



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:56 PM GMT

PDB ID : 1HWZ  
Title : BOVINE GLUTAMATE DEHYDROGENASE COMPLEXED WITH  
NADPH, GLUTAMATE, AND GTP  
Authors : Smith, T.J.; Peterson, P.E.; Schmidt, T.; Fang, J.; Stanley, C.A.  
Deposited on : 2001-01-10  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

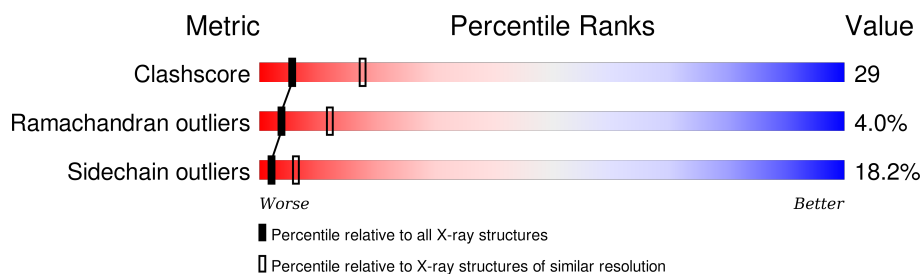
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	501	
1	B	501	
1	C	501	
1	D	501	
1	E	501	
1	F	501	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	A	550	-	-	X	-
2	GLU	B	554	-	-	X	-
2	GLU	C	555	-	-	X	-
2	GLU	D	556	-	-	X	-
2	GLU	E	557	-	-	X	-
2	GLU	F	558	-	-	X	-
3	NDP	A	551	-	-	X	-
3	NDP	B	559	-	-	X	-
3	NDP	C	560	-	-	X	-
3	NDP	D	561	-	-	X	-
3	NDP	E	562	-	-	X	-
3	NDP	F	563	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24000 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	B	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	C	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	D	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	E	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			
1	F	501	Total	C	N	O	S	0	0	0
			3910	2468	690	733	19			

There are 30 discrepancies between the modelled and reference sequences:

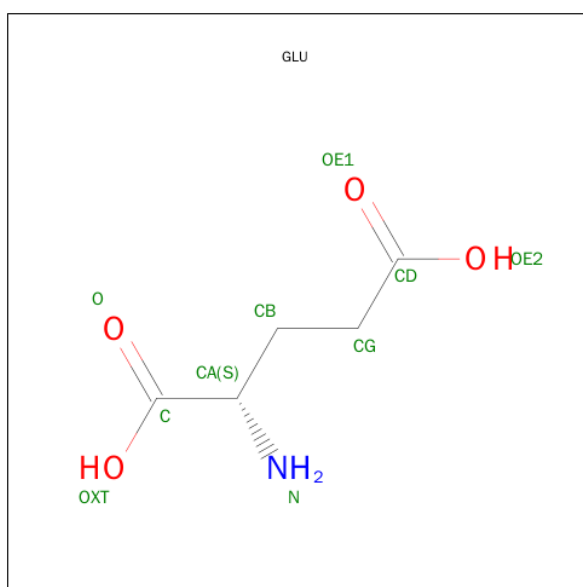
Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	LYS	SEE REMARK 999	UNP P00366
A	201	LYS	PRO	SEE REMARK 999	UNP P00366
A	202	PRO	GLY	SEE REMARK 999	UNP P00366
A	221	HIS	GLY	SEE REMARK 999	UNP P00366
A	222	GLY	HIS	SEE REMARK 999	UNP P00366
B	200	GLY	LYS	SEE REMARK 999	UNP P00366
B	201	LYS	PRO	SEE REMARK 999	UNP P00366
B	202	PRO	GLY	SEE REMARK 999	UNP P00366
B	221	HIS	GLY	SEE REMARK 999	UNP P00366
B	222	GLY	HIS	SEE REMARK 999	UNP P00366
C	200	GLY	LYS	SEE REMARK 999	UNP P00366
C	201	LYS	PRO	SEE REMARK 999	UNP P00366
C	202	PRO	GLY	SEE REMARK 999	UNP P00366
C	221	HIS	GLY	SEE REMARK 999	UNP P00366
C	222	GLY	HIS	SEE REMARK 999	UNP P00366
D	200	GLY	LYS	SEE REMARK 999	UNP P00366
D	201	LYS	PRO	SEE REMARK 999	UNP P00366

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Chain	Residue	Modelled	Actual	Comment	Reference
D	202	PRO	GLY	SEE REMARK 999	UNP P00366
D	221	HIS	GLY	SEE REMARK 999	UNP P00366
D	222	GLY	HIS	SEE REMARK 999	UNP P00366
E	200	GLY	LYS	SEE REMARK 999	UNP P00366
E	201	LYS	PRO	SEE REMARK 999	UNP P00366
E	202	PRO	GLY	SEE REMARK 999	UNP P00366
E	221	HIS	GLY	SEE REMARK 999	UNP P00366
E	222	GLY	HIS	SEE REMARK 999	UNP P00366
F	200	GLY	LYS	SEE REMARK 999	UNP P00366
F	201	LYS	PRO	SEE REMARK 999	UNP P00366
F	202	PRO	GLY	SEE REMARK 999	UNP P00366
F	221	HIS	GLY	SEE REMARK 999	UNP P00366
F	222	GLY	HIS	SEE REMARK 999	UNP P00366

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).



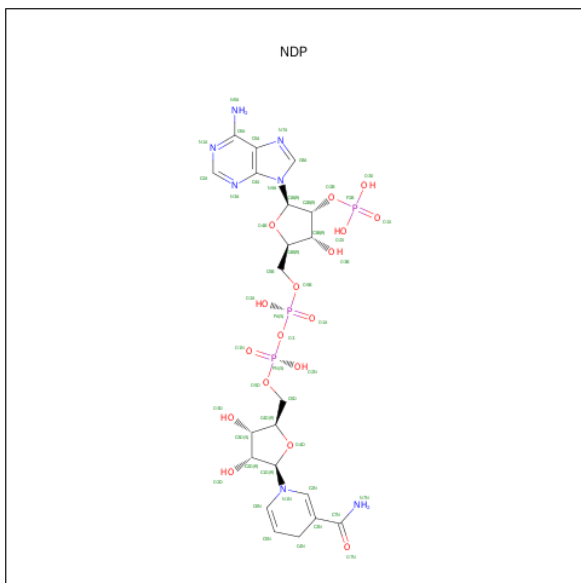
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		

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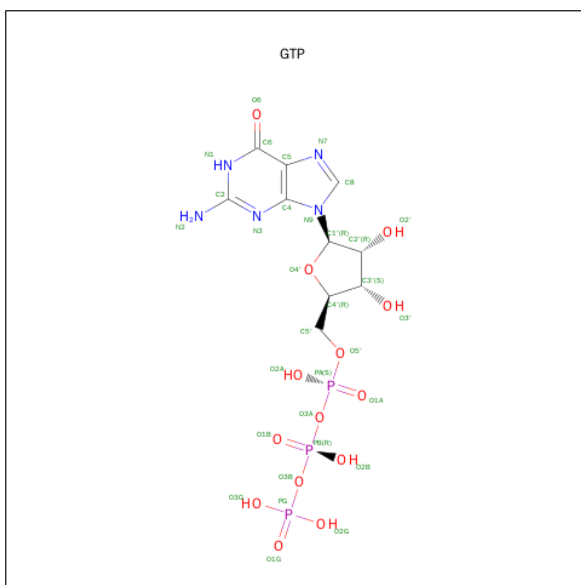
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



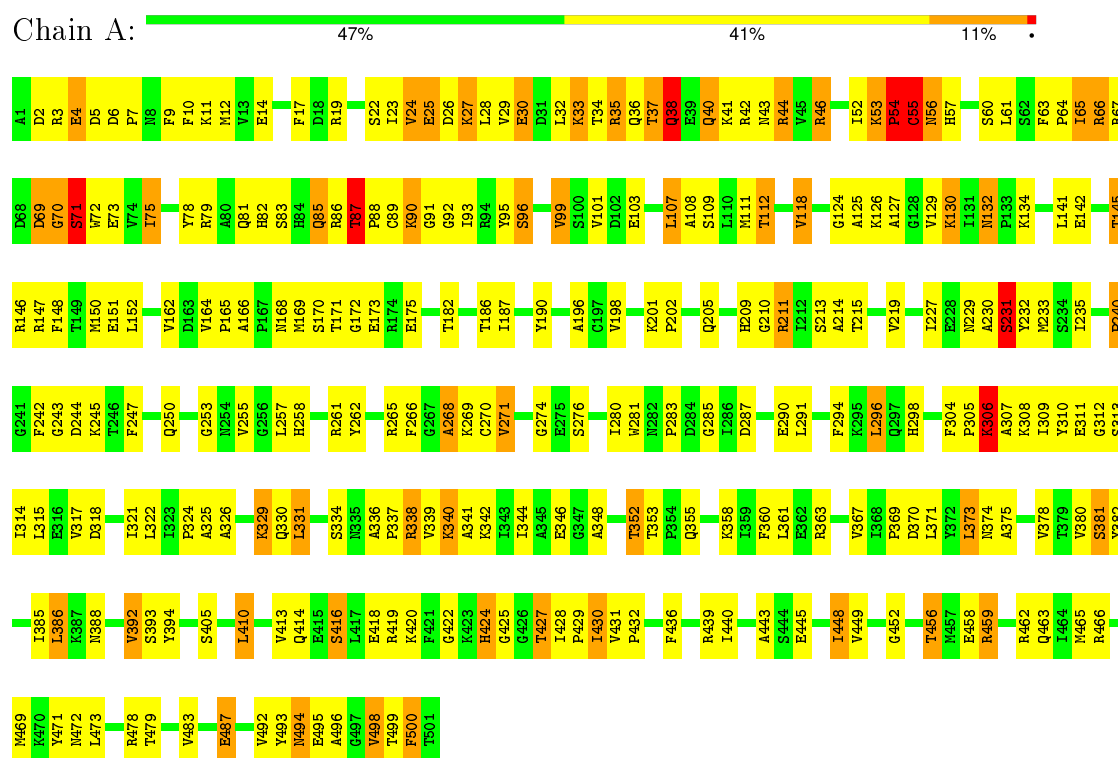
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	B	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	C	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	D	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	E	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	F	1	Total 32	C 10	N 5	O 14	P 3	0	0

### 3 Residue-property plots

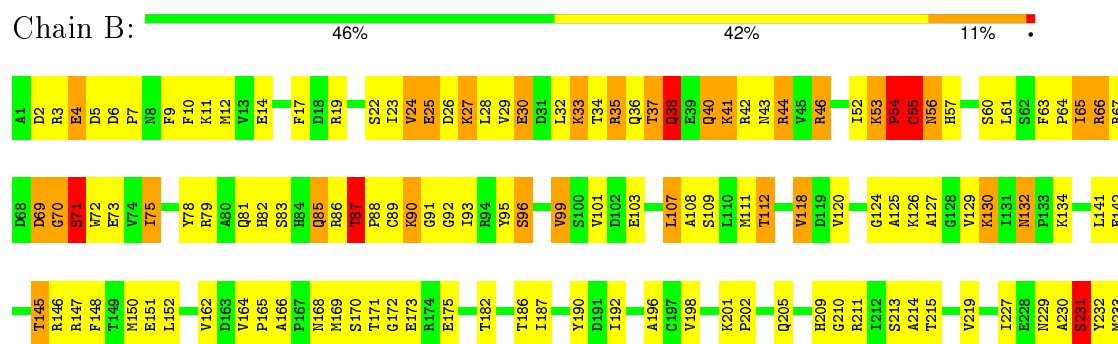
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

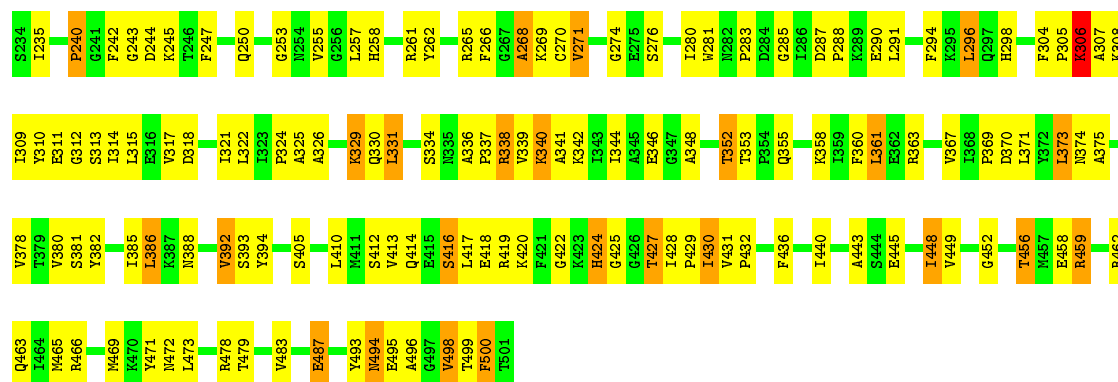
#### • Molecule 1: GLUTAMATE DEHYDROGENASE



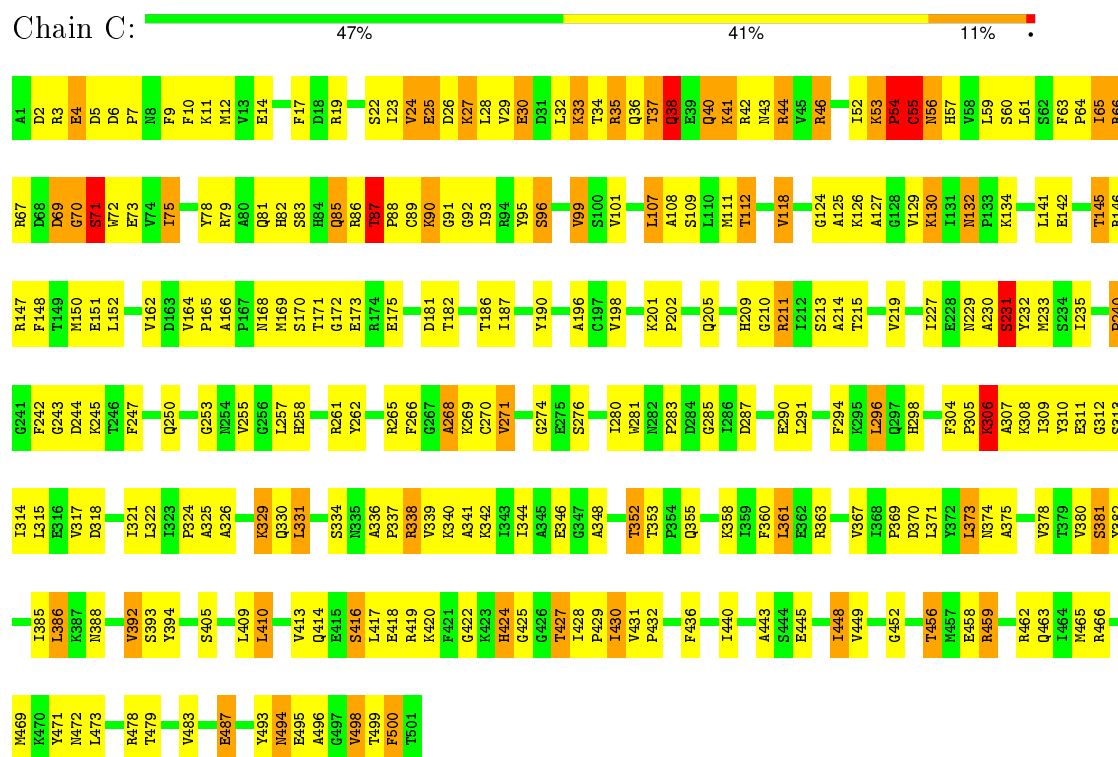
#### • Molecule 1: GLUTAMATE DEHYDROGENASE



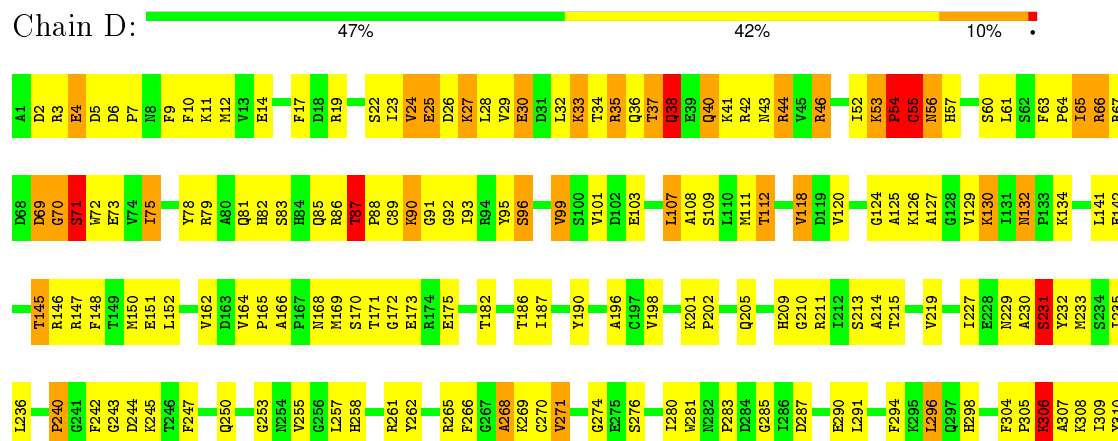


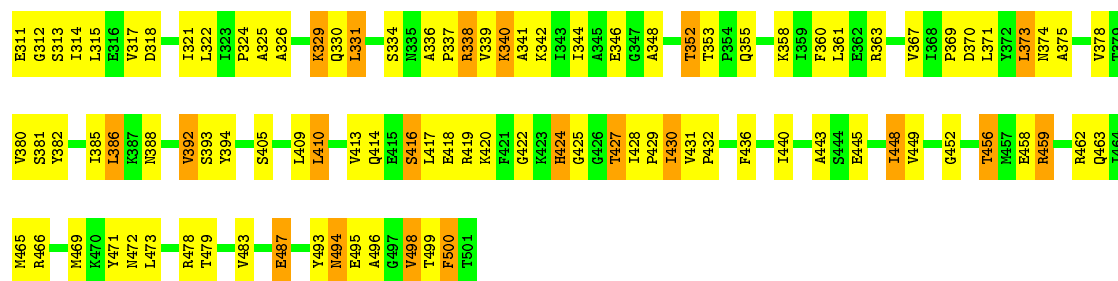


### • Molecule 1: GLUTAMATE DEHYDROGENASE



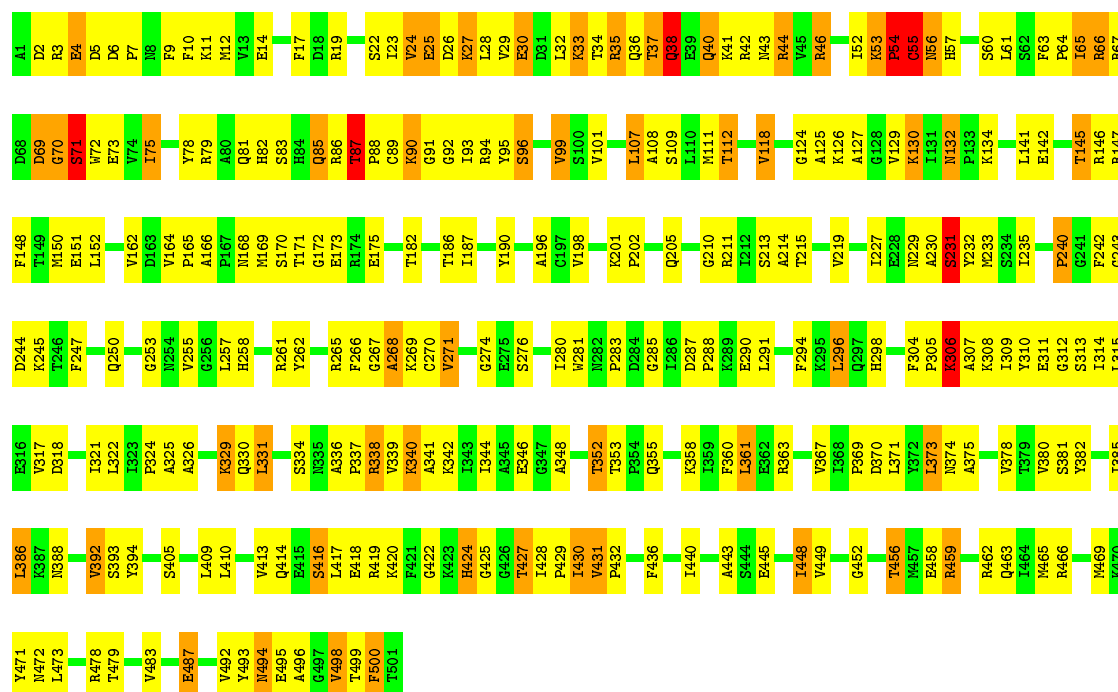
### • Molecule 1: GLUTAMATE DEHYDROGENASE





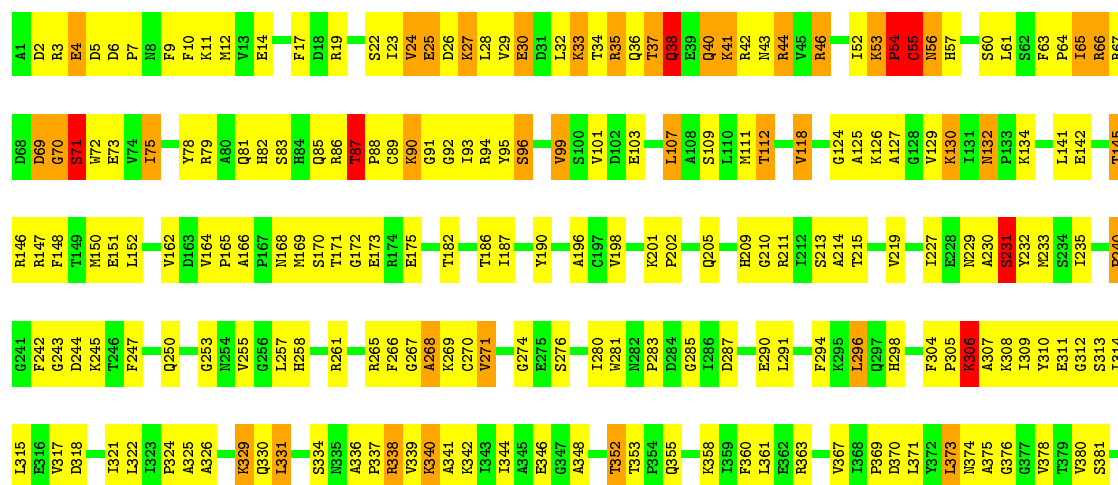
• Molecule 1: GLUTAMATE DEHYDROGENASE

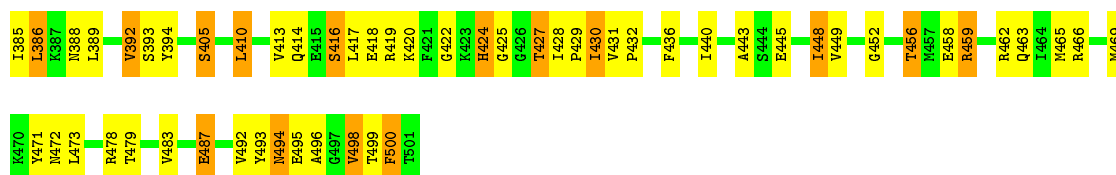
Chain E: 47% 42% 11%



• Molecule 1: GLUTAMATE DEHYDROGENASE

Chain F: 47% 41% 11%





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.30Å 102.50Å 169.20Å 90.00° 102.20° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.250 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, NDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.58	0/3991	0.84	8/5384 (0.1%)
1	B	0.58	0/3991	0.84	8/5384 (0.1%)
1	C	0.58	0/3991	0.84	8/5384 (0.1%)
1	D	0.58	0/3991	0.84	8/5384 (0.1%)
1	E	0.58	0/3991	0.84	8/5384 (0.1%)
1	F	0.58	0/3991	0.84	8/5384 (0.1%)
All	All	0.58	0/23946	0.84	48/32304 (0.1%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	LYS	N-CA-C	8.29	133.39	111.00
1	F	33	LYS	N-CA-C	8.29	133.38	111.00
1	E	33	LYS	N-CA-C	8.28	133.37	111.00
1	D	33	LYS	N-CA-C	8.28	133.36	111.00
1	C	33	LYS	N-CA-C	8.28	133.35	111.00
1	A	33	LYS	N-CA-C	8.28	133.34	111.00
1	B	87	THR	N-CA-C	7.38	130.93	111.00
1	C	87	THR	N-CA-C	7.38	130.91	111.00
1	D	87	THR	N-CA-C	7.37	130.89	111.00
1	E	87	THR	N-CA-C	7.36	130.87	111.00
1	F	87	THR	N-CA-C	7.36	130.86	111.00
1	A	87	THR	N-CA-C	7.36	130.86	111.00
1	B	231	SER	N-CA-C	-7.04	91.98	111.00
1	D	231	SER	N-CA-C	-7.04	92.00	111.00
1	C	231	SER	N-CA-C	-7.04	92.00	111.00
1	A	231	SER	N-CA-C	-7.03	92.01	111.00
1	F	231	SER	N-CA-C	-7.03	92.01	111.00
1	E	231	SER	N-CA-C	-7.03	92.02	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	54	PRO	N-CA-C	6.76	129.67	112.10
1	D	54	PRO	N-CA-C	6.75	129.65	112.10
1	B	54	PRO	N-CA-C	6.75	129.65	112.10
1	A	54	PRO	N-CA-C	6.75	129.64	112.10
1	C	54	PRO	N-CA-C	6.74	129.63	112.10
1	E	54	PRO	N-CA-C	6.74	129.62	112.10
1	B	34	THR	N-CA-C	5.92	127.00	111.00
1	F	34	THR	N-CA-C	5.92	126.99	111.00
1	A	34	THR	N-CA-C	5.92	126.98	111.00
1	C	34	THR	N-CA-C	5.91	126.96	111.00
1	D	34	THR	N-CA-C	5.91	126.96	111.00
1	E	34	THR	N-CA-C	5.91	126.96	111.00
1	D	40	GLN	N-CA-C	-5.60	95.88	111.00
1	B	40	GLN	N-CA-C	-5.60	95.89	111.00
1	C	40	GLN	N-CA-C	-5.60	95.89	111.00
1	E	40	GLN	N-CA-C	-5.60	95.89	111.00
1	F	40	GLN	N-CA-C	-5.60	95.89	111.00
1	A	40	GLN	N-CA-C	-5.59	95.91	111.00
1	D	86	ARG	N-CA-C	-5.37	96.51	111.00
1	F	86	ARG	N-CA-C	-5.36	96.52	111.00
1	A	86	ARG	N-CA-C	-5.36	96.53	111.00
1	E	86	ARG	N-CA-C	-5.35	96.55	111.00
1	C	86	ARG	N-CA-C	-5.35	96.56	111.00
1	B	86	ARG	N-CA-C	-5.34	96.57	111.00
1	D	392	VAL	CB-CA-C	-5.13	101.65	111.40
1	B	392	VAL	CB-CA-C	-5.13	101.66	111.40
1	F	392	VAL	CB-CA-C	-5.13	101.66	111.40
1	C	392	VAL	CB-CA-C	-5.13	101.66	111.40
1	E	392	VAL	CB-CA-C	-5.12	101.67	111.40
1	A	392	VAL	CB-CA-C	-5.12	101.68	111.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3910	0	3889	233	0
1	B	3910	0	3889	239	0
1	C	3910	0	3889	239	0
1	D	3910	0	3889	240	0
1	E	3910	0	3889	245	0
1	F	3910	0	3889	241	0
2	A	10	0	5	7	0
2	B	10	0	5	7	0
2	C	10	0	5	7	0
2	D	10	0	5	7	0
2	E	10	0	5	7	0
2	F	10	0	5	7	0
3	A	48	0	26	24	0
3	B	48	0	26	22	0
3	C	48	0	26	24	0
3	D	48	0	26	23	0
3	E	48	0	26	25	0
3	F	48	0	26	23	0
4	A	32	0	12	2	0
4	B	32	0	12	2	0
4	C	32	0	12	2	0
4	D	32	0	12	2	0
4	E	32	0	12	2	0
4	F	32	0	12	1	0
All	All	24000	0	23592	1401	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (1401) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:THR:HG21	3:A:551:NDP:H42N	1.15	1.15
1:B:374:ASN:HB2	3:B:559:NDP:H41N	1.16	1.14
1:A:374:ASN:HB2	3:A:551:NDP:H41N	1.16	1.13
1:F:215:THR:HG21	3:F:563:NDP:H42N	1.15	1.12
1:C:374:ASN:HB2	3:C:560:NDP:H41N	1.16	1.12
1:E:374:ASN:HB2	3:E:562:NDP:H41N	1.16	1.11
1:D:374:ASN:HB2	3:D:561:NDP:H41N	1.16	1.10
1:D:215:THR:HG21	3:D:561:NDP:H42N	1.15	1.10
1:E:215:THR:HG21	3:E:562:NDP:H42N	1.15	1.09
1:B:215:THR:HG21	3:B:559:NDP:H42N	1.15	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:THR:HG21	3:C:560:NDP:H42N	1.15	1.07
1:F:374:ASN:HB2	3:F:563:NDP:H41N	1.16	1.07
1:D:215:THR:CG2	3:D:561:NDP:H42N	1.85	1.06
1:C:215:THR:CG2	3:C:560:NDP:H42N	1.85	1.06
1:E:215:THR:CG2	3:E:562:NDP:H42N	1.85	1.06
1:B:215:THR:CG2	3:B:559:NDP:H42N	1.85	1.06
1:F:215:THR:CG2	3:F:563:NDP:H42N	1.85	1.05
1:A:215:THR:CG2	3:A:551:NDP:H42N	1.85	1.05
2:E:557:GLU:HA	3:E:562:NDP:H71N	1.25	1.01
2:D:556:GLU:HA	3:D:561:NDP:H71N	1.25	1.00
2:F:558:GLU:HA	3:F:563:NDP:H71N	1.25	0.99
1:F:82:HIS:CD2	1:F:112:THR:HG21	1.98	0.99
2:A:550:GLU:HA	3:A:551:NDP:N7N	1.78	0.99
2:A:550:GLU:HA	3:A:551:NDP:H71N	1.25	0.99
1:C:82:HIS:CD2	1:C:112:THR:HG21	1.98	0.99
2:C:555:GLU:HA	3:C:560:NDP:N7N	1.78	0.99
1:A:82:HIS:CD2	1:A:112:THR:HG21	1.98	0.99
2:F:558:GLU:HA	3:F:563:NDP:N7N	1.78	0.98
1:B:82:HIS:CD2	1:B:112:THR:HG21	1.98	0.98
2:B:554:GLU:HA	3:B:559:NDP:N7N	1.78	0.98
2:E:557:GLU:HA	3:E:562:NDP:N7N	1.78	0.98
1:E:82:HIS:CD2	1:E:112:THR:HG21	1.98	0.98
2:D:556:GLU:HA	3:D:561:NDP:N7N	1.78	0.97
1:A:374:ASN:HB2	3:A:551:NDP:C4N	1.94	0.97
2:C:555:GLU:HA	3:C:560:NDP:H71N	1.25	0.97
2:B:554:GLU:HA	3:B:559:NDP:H71N	1.25	0.97
1:D:374:ASN:HB2	3:D:561:NDP:C4N	1.94	0.97
1:D:82:HIS:CD2	1:D:112:THR:HG21	1.98	0.97
1:B:374:ASN:HB2	3:B:559:NDP:C4N	1.94	0.96
1:F:374:ASN:HB2	3:F:563:NDP:C4N	1.94	0.96
1:C:374:ASN:HB2	3:C:560:NDP:C4N	1.94	0.96
1:E:374:ASN:HB2	3:E:562:NDP:C4N	1.94	0.96
1:E:79:ARG:HD2	1:E:127:ALA:HB2	1.51	0.93
1:D:24:VAL:HG22	1:D:483:VAL:HG13	1.52	0.92
1:A:79:ARG:HD2	1:A:127:ALA:HB2	1.51	0.92
1:D:79:ARG:HD2	1:D:127:ALA:HB2	1.51	0.92
1:F:79:ARG:HD2	1:F:127:ALA:HB2	1.51	0.92
1:C:79:ARG:HD2	1:C:127:ALA:HB2	1.51	0.92
1:A:24:VAL:HG22	1:A:483:VAL:HG13	1.52	0.92
1:C:24:VAL:HG22	1:C:483:VAL:HG13	1.52	0.91
1:D:215:THR:HG21	3:D:561:NDP:C4N	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ARG:HD2	1:B:127:ALA:HB2	1.51	0.90
1:E:24:VAL:HG22	1:E:483:VAL:HG13	1.51	0.90
1:B:215:THR:HG21	3:B:559:NDP:C4N	2.02	0.90
1:C:215:THR:HG21	3:C:560:NDP:C4N	2.02	0.90
1:E:374:ASN:CB	3:E:562:NDP:H41N	2.03	0.89
1:A:374:ASN:CB	3:A:551:NDP:H41N	2.03	0.89
1:D:374:ASN:CB	3:D:561:NDP:H41N	2.03	0.89
1:B:24:VAL:HG22	1:B:483:VAL:HG13	1.51	0.89
1:E:215:THR:HG21	3:E:562:NDP:C4N	2.02	0.89
1:F:24:VAL:HG22	1:F:483:VAL:HG13	1.52	0.89
1:E:168:ASN:ND2	1:E:169:MET:H	1.72	0.88
1:C:374:ASN:CB	3:C:560:NDP:H41N	2.03	0.87
1:A:168:ASN:ND2	1:A:169:MET:H	1.72	0.87
1:A:215:THR:HG21	3:A:551:NDP:C4N	2.02	0.87
1:E:168:ASN:HD22	1:E:169:MET:H	1.22	0.87
1:D:168:ASN:ND2	1:D:169:MET:H	1.72	0.87
1:F:168:ASN:ND2	1:F:169:MET:H	1.72	0.87
1:F:215:THR:HG21	3:F:563:NDP:C4N	2.02	0.87
1:B:168:ASN:HD22	1:B:169:MET:H	1.22	0.87
1:C:168:ASN:ND2	1:C:169:MET:H	1.72	0.87
1:C:168:ASN:HD22	1:C:169:MET:H	1.22	0.86
1:B:374:ASN:CB	3:B:559:NDP:H41N	2.03	0.86
1:B:168:ASN:ND2	1:B:169:MET:H	1.72	0.86
1:F:374:ASN:CB	3:F:563:NDP:H41N	2.03	0.86
1:E:173:GLU:HG2	1:E:202:PRO:HG3	1.58	0.86
1:F:168:ASN:HD22	1:F:169:MET:H	1.22	0.85
1:F:173:GLU:HG2	1:F:202:PRO:HG3	1.58	0.85
1:C:173:GLU:HG2	1:C:202:PRO:HG3	1.58	0.85
1:D:168:ASN:HD22	1:D:169:MET:H	1.22	0.85
1:A:173:GLU:HG2	1:A:202:PRO:HG3	1.58	0.84
1:B:173:GLU:HG2	1:B:202:PRO:HG3	1.58	0.84
1:D:173:GLU:HG2	1:D:202:PRO:HG3	1.58	0.83
1:A:168:ASN:HD22	1:A:169:MET:H	1.22	0.83
1:B:392:VAL:CG1	1:F:386:LEU:HD21	2.10	0.82
2:F:558:GLU:CA	3:F:563:NDP:H71N	1.94	0.81
2:E:557:GLU:CA	3:E:562:NDP:H71N	1.94	0.81
2:D:556:GLU:CA	3:D:561:NDP:H71N	1.94	0.80
1:C:287:ASP:HB3	1:C:290:GLU:HG2	1.64	0.80
1:C:72:TRP:CH2	1:F:498:VAL:HB	2.16	0.79
1:B:287:ASP:HB3	1:B:290:GLU:HG2	1.64	0.79
2:C:555:GLU:CA	3:C:560:NDP:H71N	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:550:GLU:CA	3:A:551:NDP:H71N	1.94	0.79
1:A:386:LEU:HD21	1:F:392:VAL:CG1	2.13	0.79
1:D:287:ASP:HB3	1:D:290:GLU:HG2	1.64	0.79
2:B:554:GLU:CA	3:B:559:NDP:H71N	1.94	0.78
1:E:287:ASP:HB3	1:E:290:GLU:HG2	1.64	0.78
1:A:287:ASP:HB3	1:A:290:GLU:HG2	1.64	0.78
1:B:498:VAL:HB	1:E:72:TRP:CH2	2.19	0.78
1:F:287:ASP:HB3	1:F:290:GLU:HG2	1.64	0.77
1:E:150:MET:HE1	1:E:187:ILE:HD11	1.67	0.77
1:B:150:MET:HE1	1:B:187:ILE:HD11	1.67	0.76
1:D:150:MET:HE1	1:D:187:ILE:HD11	1.67	0.76
1:F:150:MET:HE1	1:F:187:ILE:HD11	1.67	0.76
1:A:150:MET:HE1	1:A:187:ILE:HD11	1.67	0.76
1:C:150:MET:HE1	1:C:187:ILE:HD11	1.67	0.75
1:C:91:GLY:HA3	1:C:125:ALA:O	1.87	0.75
1:D:91:GLY:HA3	1:D:125:ALA:O	1.86	0.75
1:A:91:GLY:HA3	1:A:125:ALA:O	1.86	0.75
1:E:112:THR:HB	1:E:124:GLY:H	1.52	0.75
1:A:386:LEU:HD21	1:F:392:VAL:HG11	1.68	0.75
1:A:498:VAL:HB	1:D:72:TRP:CH2	2.22	0.74
1:B:250:GLN:OE1	1:B:330:GLN:HG2	1.87	0.74
1:E:250:GLN:OE1	1:E:330:GLN:HG2	1.87	0.74
1:A:250:GLN:OE1	1:A:330:GLN:HG2	1.87	0.74
1:F:67:ARG:HG2	1:F:71:SER:O	1.88	0.74
1:C:112:THR:HB	1:C:124:GLY:H	1.52	0.74
1:E:91:GLY:HA3	1:E:125:ALA:O	1.86	0.74
1:C:496:ALA:N	1:D:205:GLN:HE22	1.85	0.74
1:D:67:ARG:HG2	1:D:71:SER:O	1.88	0.74
1:F:91:GLY:HA3	1:F:125:ALA:O	1.86	0.74
1:B:67:ARG:HG2	1:B:71:SER:O	1.88	0.74
1:F:112:THR:HB	1:F:124:GLY:H	1.52	0.74
1:F:250:GLN:OE1	1:F:330:GLN:HG2	1.87	0.74
1:B:91:GLY:HA3	1:B:125:ALA:O	1.86	0.73
1:B:112:THR:HB	1:B:124:GLY:H	1.52	0.73
1:A:67:ARG:HG2	1:A:71:SER:O	1.88	0.73
1:D:112:THR:HB	1:D:124:GLY:H	1.52	0.73
1:C:67:ARG:HG2	1:C:71:SER:O	1.88	0.73
1:C:250:GLN:OE1	1:C:330:GLN:HG2	1.88	0.73
1:A:112:THR:HB	1:A:124:GLY:H	1.52	0.73
1:E:67:ARG:HG2	1:E:71:SER:O	1.88	0.73
1:D:479:THR:O	1:D:483:VAL:HG23	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:TRP:CH2	1:E:498:VAL:HB	2.24	0.72
1:C:479:THR:O	1:C:483:VAL:HG23	1.89	0.72
1:C:498:VAL:HB	1:F:72:TRP:CH2	2.25	0.72
1:D:250:GLN:OE1	1:D:330:GLN:HG2	1.87	0.72
1:A:479:THR:O	1:A:483:VAL:HG23	1.89	0.72
1:F:479:THR:O	1:F:483:VAL:HG23	1.89	0.72
1:E:479:THR:O	1:E:483:VAL:HG23	1.89	0.71
1:D:496:ALA:N	1:E:205:GLN:HE22	1.87	0.71
1:B:479:THR:O	1:B:483:VAL:HG23	1.89	0.71
2:B:554:GLU:CA	3:B:559:NDP:N7N	2.53	0.71
1:A:392:VAL:CG1	1:B:386:LEU:HD21	2.21	0.71
1:B:392:VAL:HG11	1:F:386:LEU:HD21	1.71	0.71
1:A:392:VAL:HG11	1:B:386:LEU:HD21	1.73	0.70
1:A:33:LYS:HE3	1:A:33:LYS:O	1.92	0.70
1:D:75:ILE:HD13	1:D:129:VAL:HG13	1.74	0.70
1:E:33:LYS:O	1:E:33:LYS:HE3	1.92	0.70
1:C:205:GLN:HE22	1:E:496:ALA:N	1.88	0.70
1:D:258:HIS:HD2	1:D:261:ARG:HH11	1.40	0.70
1:A:75:ILE:HD13	1:A:129:VAL:HG13	1.74	0.70
1:C:33:LYS:HE3	1:C:33:LYS:O	1.92	0.70
1:F:75:ILE:HD13	1:F:129:VAL:HG13	1.74	0.69
1:B:33:LYS:HE3	1:B:33:LYS:O	1.92	0.69
1:A:258:HIS:HD2	1:A:261:ARG:HH11	1.40	0.69
1:C:258:HIS:HD2	1:C:261:ARG:HH11	1.40	0.69
2:F:558:GLU:CA	3:F:563:NDP:N7N	2.53	0.69
1:C:75:ILE:HD13	1:C:129:VAL:HG13	1.74	0.69
1:E:75:ILE:HD13	1:E:129:VAL:HG13	1.74	0.69
1:F:169:MET:HG3	3:F:563:NDP:H3D	1.75	0.69
1:C:169:MET:HG3	3:C:560:NDP:H3D	1.75	0.69
1:B:75:ILE:HD13	1:B:129:VAL:HG13	1.74	0.69
1:E:258:HIS:CD2	1:E:261:ARG:HH11	2.11	0.69
1:A:169:MET:HG3	3:A:551:NDP:H3D	1.75	0.69
1:F:33:LYS:HE3	1:F:33:LYS:O	1.92	0.69
1:B:374:ASN:HB2	3:B:559:NDP:C5N	2.23	0.68
1:D:33:LYS:O	1:D:33:LYS:HE3	1.92	0.68
1:F:374:ASN:HB2	3:F:563:NDP:C5N	2.23	0.68
1:D:169:MET:HG3	3:D:561:NDP:H3D	1.75	0.68
1:D:169:MET:CG	3:D:561:NDP:H3D	2.24	0.68
1:C:258:HIS:CD2	1:C:261:ARG:HH11	2.11	0.68
1:B:169:MET:HG3	3:B:559:NDP:H3D	1.75	0.68
1:F:258:HIS:CD2	1:F:261:ARG:HH11	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MET:CG	3:B:559:NDP:H3D	2.24	0.68
1:D:374:ASN:HB2	3:D:561:NDP:C5N	2.23	0.68
1:E:169:MET:HG3	3:E:562:NDP:H3D	1.75	0.68
1:A:374:ASN:HB2	3:A:551:NDP:C5N	2.23	0.68
1:E:374:ASN:HB2	3:E:562:NDP:C5N	2.23	0.68
1:A:169:MET:CG	3:A:551:NDP:H3D	2.24	0.68
1:A:258:HIS:CD2	1:A:261:ARG:HH11	2.11	0.68
1:B:258:HIS:CD2	1:B:261:ARG:HH11	2.11	0.68
1:D:258:HIS:CD2	1:D:261:ARG:HH11	2.11	0.68
1:A:281:TRP:HB3	1:A:310:TYR:HB2	1.76	0.68
1:C:169:MET:CG	3:C:560:NDP:H3D	2.24	0.67
2:E:557:GLU:CA	3:E:562:NDP:N7N	2.53	0.67
1:E:169:MET:CG	3:E:562:NDP:H3D	2.24	0.67
1:B:280:ILE:HD11	1:B:304:PHE:HB3	1.76	0.67
1:B:281:TRP:HB3	1:B:310:TYR:HB2	1.76	0.67
1:B:258:HIS:HD2	1:B:261:ARG:HH11	1.40	0.67
1:C:374:ASN:HB2	3:C:560:NDP:C5N	2.23	0.67
1:F:280:ILE:HD11	1:F:304:PHE:HB3	1.76	0.67
1:E:280:ILE:HD11	1:E:304:PHE:HB3	1.76	0.67
1:A:3:ARG:O	1:A:4:GLU:HG3	1.94	0.67
1:C:280:ILE:HD11	1:C:304:PHE:HB3	1.76	0.67
1:F:258:HIS:HD2	1:F:261:ARG:HH11	1.40	0.67
1:E:3:ARG:O	1:E:4:GLU:HG3	1.94	0.67
1:C:3:ARG:O	1:C:4:GLU:HG3	1.94	0.67
1:F:169:MET:CG	3:F:563:NDP:H3D	2.24	0.67
1:F:326:ALA:O	3:F:563:NDP:H4D	1.95	0.66
1:C:326:ALA:O	3:C:560:NDP:H4D	1.95	0.66
1:A:326:ALA:O	3:A:551:NDP:H4D	1.95	0.66
1:A:280:ILE:HD11	1:A:304:PHE:HB3	1.76	0.66
1:F:281:TRP:HB3	1:F:310:TYR:HB2	1.76	0.66
1:F:3:ARG:O	1:F:4:GLU:HG3	1.94	0.66
1:E:326:ALA:O	3:E:562:NDP:H4D	1.95	0.66
1:E:281:TRP:HB3	1:E:310:TYR:HB2	1.76	0.66
1:B:3:ARG:O	1:B:4:GLU:HG3	1.94	0.66
1:E:172:GLY:H	1:E:175:GLU:HG2	1.60	0.66
2:C:555:GLU:CA	3:C:560:NDP:N7N	2.53	0.66
1:D:3:ARG:O	1:D:4:GLU:HG3	1.94	0.66
1:F:172:GLY:H	1:F:175:GLU:HG2	1.60	0.66
1:D:280:ILE:HD11	1:D:304:PHE:HB3	1.76	0.66
1:B:315:LEU:HD11	1:B:330:GLN:HG3	1.78	0.66
1:D:172:GLY:H	1:D:175:GLU:HG2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LYS:HZ1	1:B:388:ASN:HD21	1.42	0.66
1:C:392:VAL:CG1	1:E:386:LEU:HD21	2.25	0.66
1:D:326:ALA:O	3:D:561:NDP:H4D	1.95	0.66
2:D:556:GLU:CA	3:D:561:NDP:N7N	2.53	0.66
1:E:258:HIS:HD2	1:E:261:ARG:HH11	1.40	0.66
2:A:550:GLU:CA	3:A:551:NDP:N7N	2.53	0.66
1:C:281:TRP:HB3	1:C:310:TYR:HB2	1.76	0.66
1:D:281:TRP:HB3	1:D:310:TYR:HB2	1.76	0.66
1:B:326:ALA:O	3:B:559:NDP:H4D	1.95	0.65
1:C:23:ILE:CD1	1:C:473:LEU:HD21	2.27	0.65
1:C:315:LEU:HD11	1:C:330:GLN:HG3	1.78	0.65
1:F:23:ILE:CD1	1:F:473:LEU:HD21	2.27	0.65
1:E:315:LEU:HD11	1:E:330:GLN:HG3	1.78	0.65
1:A:172:GLY:H	1:A:175:GLU:HG2	1.60	0.65
1:D:23:ILE:CD1	1:D:473:LEU:HD21	2.27	0.65
1:A:315:LEU:HD11	1:A:330:GLN:HG3	1.78	0.65
1:E:201:LYS:HZ1	1:E:388:ASN:HD21	1.43	0.65
1:D:168:ASN:HD22	1:D:169:MET:N	1.94	0.65
1:E:23:ILE:CD1	1:E:473:LEU:HD21	2.27	0.65
1:F:315:LEU:HD11	1:F:330:GLN:HG3	1.78	0.65
1:A:168:ASN:HD22	1:A:169:MET:N	1.94	0.65
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.80	0.64
1:C:172:GLY:H	1:C:175:GLU:HG2	1.60	0.64
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.80	0.64
1:A:190:TYR:CD2	1:B:162:VAL:HG11	2.33	0.64
1:D:132:ASN:ND2	1:D:134:LYS:HB2	2.13	0.64
1:E:132:ASN:ND2	1:E:134:LYS:HB2	2.13	0.64
1:E:168:ASN:HD22	1:E:169:MET:N	1.94	0.64
1:A:23:ILE:CD1	1:A:473:LEU:HD21	2.27	0.64
1:C:392:VAL:HG11	1:E:386:LEU:HD21	1.79	0.64
1:B:172:GLY:H	1:B:175:GLU:HG2	1.60	0.64
1:B:23:ILE:CD1	1:B:473:LEU:HD21	2.27	0.64
1:F:336:ALA:HB3	1:F:337:PRO:HD3	1.79	0.64
1:A:132:ASN:ND2	1:A:134:LYS:HB2	2.13	0.64
1:D:336:ALA:HB3	1:D:337:PRO:HD3	1.80	0.64
1:F:281:TRP:CB	1:F:310:TYR:HB2	2.28	0.64
1:D:23:ILE:HD13	1:D:473:LEU:HD21	1.80	0.64
1:E:23:ILE:HD13	1:E:473:LEU:HD21	1.80	0.63
1:E:258:HIS:HD2	1:E:261:ARG:NH1	1.96	0.63
1:B:281:TRP:CB	1:B:310:TYR:HB2	2.28	0.63
1:F:132:ASN:ND2	1:F:134:LYS:HB2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:HIS:HD2	1:B:261:ARG:NH1	1.96	0.63
1:C:452:GLY:O	1:C:456:THR:HG23	1.99	0.63
1:D:315:LEU:HD11	1:D:330:GLN:HG3	1.78	0.63
1:E:281:TRP:CB	1:E:310:TYR:HB2	2.28	0.63
1:C:132:ASN:ND2	1:C:134:LYS:HB2	2.13	0.63
1:E:336:ALA:HB3	1:E:337:PRO:HD3	1.80	0.63
1:F:168:ASN:HD22	1:F:169:MET:N	1.94	0.63
1:B:132:ASN:ND2	1:B:134:LYS:HB2	2.13	0.63
1:F:7:PRO:O	1:F:329:LYS:HE2	1.99	0.63
1:A:258:HIS:HD2	1:A:261:ARG:NH1	1.96	0.63
1:D:452:GLY:O	1:D:456:THR:HG23	1.99	0.63
1:C:168:ASN:HD22	1:C:169:MET:N	1.94	0.63
1:B:7:PRO:O	1:B:329:LYS:HE2	1.99	0.63
1:B:168:ASN:HD22	1:B:169:MET:N	1.94	0.63
1:F:258:HIS:HD2	1:F:261:ARG:NH1	1.97	0.63
1:F:452:GLY:O	1:F:456:THR:HG23	1.99	0.63
1:A:23:ILE:HD13	1:A:473:LEU:HD21	1.80	0.63
1:D:281:TRP:CB	1:D:310:TYR:HB2	2.28	0.63
1:A:205:GLN:HE22	1:B:496:ALA:N	1.97	0.63
1:A:7:PRO:O	1:A:329:LYS:HE2	1.99	0.62
1:A:281:TRP:CB	1:A:310:TYR:HB2	2.28	0.62
1:C:281:TRP:CB	1:C:310:TYR:HB2	2.28	0.62
1:B:23:ILE:HD13	1:B:473:LEU:HD21	1.80	0.62
1:D:258:HIS:HD2	1:D:261:ARG:NH1	1.96	0.62
1:F:17:PHE:CD2	1:F:53:LYS:HD2	2.35	0.62
1:E:7:PRO:O	1:E:329:LYS:HE2	1.99	0.62
1:A:17:PHE:CD2	1:A:53:LYS:HD2	2.35	0.62
1:A:452:GLY:O	1:A:456:THR:HG23	1.99	0.62
1:D:269:LYS:HE3	1:D:283:PRO:O	2.00	0.62
1:B:452:GLY:O	1:B:456:THR:HG23	1.99	0.62
1:E:452:GLY:O	1:E:456:THR:HG23	1.99	0.62
1:B:17:PHE:CD2	1:B:53:LYS:HD2	2.35	0.62
1:C:17:PHE:CD2	1:C:53:LYS:HD2	2.35	0.62
1:E:269:LYS:HE3	1:E:283:PRO:O	2.00	0.62
1:D:7:PRO:O	1:D:329:LYS:HE2	1.99	0.62
1:B:190:TYR:CD2	1:F:162:VAL:HG11	2.35	0.61
1:C:336:ALA:HB3	1:C:337:PRO:HD3	1.80	0.61
1:C:258:HIS:HD2	1:C:261:ARG:NH1	1.96	0.61
1:D:201:LYS:HZ1	1:D:388:ASN:HD21	1.46	0.61
1:D:150:MET:HE3	1:D:182:THR:HG22	1.83	0.61
1:C:7:PRO:O	1:C:329:LYS:HE2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:LYS:HZ1	1:F:388:ASN:HD21	1.48	0.61
1:B:265:ARG:HG3	1:B:266:PHE:CD1	2.36	0.61
1:F:23:ILE:HD13	1:F:473:LEU:HD21	1.80	0.61
1:F:269:LYS:HE3	1:F:283:PRO:O	2.00	0.61
1:C:269:LYS:HE3	1:C:283:PRO:O	2.00	0.61
1:C:201:LYS:HZ1	1:C:388:ASN:HD21	1.46	0.61
1:A:269:LYS:HE3	1:A:283:PRO:O	2.00	0.61
1:B:269:LYS:HE3	1:B:283:PRO:O	2.00	0.61
1:B:416:SER:OG	1:F:430:ILE:HA	2.01	0.61
1:D:141:LEU:O	1:D:145:THR:HG23	2.01	0.61
1:E:17:PHE:CD2	1:E:53:LYS:HD2	2.35	0.61
1:F:265:ARG:HG3	1:F:266:PHE:CD1	2.36	0.61
1:D:265:ARG:HG3	1:D:266:PHE:CD1	2.36	0.61
1:B:304:PHE:CE2	1:B:306:LYS:HB3	2.36	0.61
1:F:304:PHE:CE2	1:F:306:LYS:HB3	2.36	0.61
1:C:141:LEU:O	1:C:145:THR:HG23	2.01	0.61
1:C:417:LEU:HD13	1:D:417:LEU:HD21	1.81	0.61
1:C:265:ARG:HG3	1:C:266:PHE:CD1	2.36	0.61
1:D:17:PHE:CD2	1:D:53:LYS:HD2	2.35	0.61
1:F:348:ALA:HA	3:F:563:NDP:O4D	2.01	0.61
1:C:348:ALA:HA	3:C:560:NDP:O4D	2.01	0.61
1:B:141:LEU:O	1:B:145:THR:HG23	2.01	0.61
1:C:230:ALA:HA	1:C:233:MET:HB2	1.83	0.61
1:B:348:ALA:HA	3:B:559:NDP:O4D	2.01	0.60
1:C:23:ILE:HD13	1:C:473:LEU:HD21	1.80	0.60
1:D:348:ALA:HA	3:D:561:NDP:O4D	2.01	0.60
1:F:271:VAL:HG22	1:F:283:PRO:HA	1.83	0.60
1:A:265:ARG:HG3	1:A:266:PHE:CD1	2.36	0.60
1:A:141:LEU:O	1:A:145:THR:HG23	2.01	0.60
1:A:348:ALA:HA	3:A:551:NDP:O4D	2.01	0.60
1:C:112:THR:HB	1:C:124:GLY:N	2.17	0.60
1:B:271:VAL:HG22	1:B:283:PRO:HA	1.83	0.60
1:B:230:ALA:HA	1:B:233:MET:HB2	1.83	0.60
1:D:430:ILE:HA	1:E:416:SER:OG	2.01	0.60
1:E:348:ALA:HA	3:E:562:NDP:O4D	2.01	0.60
1:C:304:PHE:CE2	1:C:306:LYS:HB3	2.36	0.60
1:D:271:VAL:HG22	1:D:283:PRO:HA	1.83	0.60
1:F:230:ALA:HA	1:F:233:MET:HB2	1.83	0.60
1:E:141:LEU:O	1:E:145:THR:HG23	2.01	0.60
1:A:271:VAL:HG22	1:A:283:PRO:HA	1.83	0.60
1:E:271:VAL:HG22	1:E:283:PRO:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:PHE:CE2	1:E:306:LYS:HB3	2.36	0.60
1:D:112:THR:HB	1:D:124:GLY:N	2.17	0.60
1:D:304:PHE:CE2	1:D:306:LYS:HB3	2.36	0.60
1:F:201:LYS:NZ	1:F:388:ASN:HD21	2.00	0.60
1:B:432:PRO:HB3	1:B:436:PHE:HD2	1.67	0.60
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.67	0.60
1:E:265:ARG:HG3	1:E:266:PHE:CD1	2.36	0.60
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.67	0.59
1:E:171:THR:HB	1:E:175:GLU:HG3	1.85	0.59
1:B:201:LYS:NZ	1:B:388:ASN:HD21	2.00	0.59
1:C:271:VAL:HG22	1:C:283:PRO:HA	1.83	0.59
1:A:171:THR:HB	1:A:175:GLU:HG3	1.84	0.59
1:A:432:PRO:HB3	1:A:436:PHE:HD2	1.67	0.59
1:B:112:THR:HB	1:B:124:GLY:N	2.17	0.59
1:A:112:THR:HB	1:A:124:GLY:N	2.17	0.59
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.85	0.59
1:A:304:PHE:CE2	1:A:306:LYS:HB3	2.36	0.59
1:D:201:LYS:NZ	1:D:388:ASN:HD21	2.00	0.59
1:A:201:LYS:NZ	1:A:388:ASN:HD21	2.00	0.59
1:E:201:LYS:NZ	1:E:388:ASN:HD21	2.00	0.59
1:A:230:ALA:HA	1:A:233:MET:HB2	1.83	0.59
1:D:417:LEU:HD13	1:E:417:LEU:HD21	1.84	0.59
1:D:230:ALA:HA	1:D:233:MET:HB2	1.83	0.59
1:E:230:ALA:HA	1:E:233:MET:HB2	1.83	0.59
1:F:339:VAL:HG23	1:F:341:ALA:H	1.68	0.59
1:F:141:LEU:O	1:F:145:THR:HG23	2.01	0.59
1:A:339:VAL:HG23	1:A:341:ALA:H	1.68	0.59
1:E:112:THR:HB	1:E:124:GLY:N	2.17	0.59
1:C:89:CYS:HB3	1:C:125:ALA:HB2	1.85	0.59
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.67	0.59
1:C:339:VAL:HG23	1:C:341:ALA:H	1.68	0.59
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.85	0.59
1:D:89:CYS:HB3	1:D:125:ALA:HB2	1.85	0.58
1:F:89:CYS:HB3	1:F:125:ALA:HB2	1.85	0.58
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.67	0.58
1:B:171:THR:HB	1:B:175:GLU:HG3	1.85	0.58
1:C:417:LEU:CD1	1:D:417:LEU:HD21	2.33	0.58
1:C:430:ILE:HA	1:D:416:SER:OG	2.03	0.58
1:D:171:THR:HB	1:D:175:GLU:HG3	1.85	0.58
1:C:171:THR:HB	1:C:175:GLU:HG3	1.84	0.58
1:C:201:LYS:NZ	1:C:388:ASN:HD21	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:VAL:HG23	1:E:341:ALA:H	1.68	0.58
1:B:276:SER:HB2	3:B:559:NDP:O2X	2.04	0.58
1:A:499:THR:O	1:A:500:PHE:CG	2.57	0.58
1:D:417:LEU:CD1	1:E:417:LEU:HD21	2.33	0.58
1:A:496:ALA:N	1:F:205:GLN:HE22	2.01	0.58
1:F:276:SER:HB2	3:F:563:NDP:O2X	2.04	0.58
1:B:55:CYS:HA	1:B:82:HIS:HA	1.86	0.58
1:E:499:THR:O	1:E:500:PHE:CG	2.57	0.58
1:D:499:THR:O	1:D:500:PHE:CG	2.57	0.58
1:C:276:SER:HB2	3:C:560:NDP:O2X	2.04	0.58
1:A:55:CYS:HA	1:A:82:HIS:HA	1.86	0.58
1:B:499:THR:O	1:B:500:PHE:CG	2.57	0.58
1:F:171:THR:HB	1:F:175:GLU:HG3	1.85	0.58
1:C:499:THR:O	1:C:500:PHE:CG	2.57	0.58
1:A:201:LYS:HZ1	1:A:388:ASN:HD21	1.52	0.58
1:A:276:SER:HB2	3:A:551:NDP:O2X	2.04	0.58
1:C:287:ASP:HB3	1:C:290:GLU:CG	2.33	0.58
1:F:499:THR:O	1:F:500:PHE:CG	2.57	0.58
1:E:150:MET:HE3	1:E:182:THR:HG22	1.85	0.58
1:E:89:CYS:HB3	1:E:125:ALA:HB2	1.85	0.58
1:D:142:GLU:O	1:D:146:ARG:HG2	2.04	0.58
1:C:55:CYS:HA	1:C:82:HIS:HA	1.86	0.58
1:B:142:GLU:O	1:B:146:ARG:HG2	2.04	0.58
1:D:150:MET:HE1	1:D:187:ILE:CD1	2.34	0.58
1:B:339:VAL:HG23	1:B:341:ALA:H	1.68	0.58
1:A:82:HIS:CG	1:A:112:THR:HG21	2.38	0.57
1:A:142:GLU:O	1:A:146:ARG:HG2	2.04	0.57
1:E:55:CYS:HA	1:E:82:HIS:HA	1.86	0.57
1:D:339:VAL:HG23	1:D:341:ALA:H	1.68	0.57
1:E:276:SER:HB2	3:E:562:NDP:O2X	2.04	0.57
1:C:82:HIS:CG	1:C:112:THR:HG21	2.38	0.57
1:F:112:THR:HB	1:F:124:GLY:N	2.17	0.57
1:F:142:GLU:O	1:F:146:ARG:HG2	2.04	0.57
1:D:55:CYS:HA	1:D:82:HIS:HA	1.86	0.57
1:E:287:ASP:HB3	1:E:290:GLU:CG	2.34	0.57
1:F:55:CYS:HA	1:F:82:HIS:HA	1.86	0.57
1:B:82:HIS:CG	1:B:112:THR:HG21	2.38	0.57
1:E:82:HIS:CG	1:E:112:THR:HG21	2.38	0.57
1:A:150:MET:HE1	1:A:187:ILE:CD1	2.35	0.57
1:D:276:SER:HB2	3:D:561:NDP:O2X	2.04	0.56
1:C:142:GLU:O	1:C:146:ARG:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASP:HB3	1:B:290:GLU:CG	2.33	0.56
1:B:186:THR:OG1	1:B:187:ILE:HD12	2.05	0.56
1:A:150:MET:HE3	1:A:182:THR:HG22	1.87	0.56
1:A:186:THR:OG1	1:A:187:ILE:HD12	2.05	0.56
1:C:186:THR:OG1	1:C:187:ILE:HD12	2.05	0.56
1:C:416:SER:OG	1:E:430:ILE:HA	2.05	0.56
1:E:142:GLU:O	1:E:146:ARG:HG2	2.04	0.56
1:D:386:LEU:HD21	1:E:392:VAL:HG11	1.88	0.56
2:A:550:GLU:C	3:A:551:NDP:H71N	2.09	0.56
1:F:258:HIS:CD2	1:F:261:ARG:NH1	2.73	0.56
1:D:386:LEU:HD21	1:E:392:VAL:CG1	2.35	0.56
1:F:186:THR:OG1	1:F:187:ILE:HD12	2.05	0.56
1:D:82:HIS:CG	1:D:112:THR:HG21	2.38	0.56
1:F:150:MET:HE3	1:F:182:THR:HG22	1.87	0.56
1:A:72:TRP:CH2	1:D:498:VAL:HB	2.41	0.56
2:F:558:GLU:C	3:F:563:NDP:H71N	2.09	0.56
1:E:150:MET:HE1	1:E:187:ILE:CD1	2.35	0.56
1:D:186:THR:OG1	1:D:187:ILE:HD12	2.05	0.56
1:D:258:HIS:CD2	1:D:261:ARG:NH1	2.73	0.56
1:E:258:HIS:CD2	1:E:261:ARG:NH1	2.73	0.56
2:E:557:GLU:C	3:E:562:NDP:H71N	2.09	0.56
1:E:186:THR:OG1	1:E:187:ILE:HD12	2.05	0.56
2:B:554:GLU:C	3:B:559:NDP:H71N	2.09	0.55
1:C:109:SER:O	1:C:112:THR:HG23	2.07	0.55
1:B:187:ILE:HD12	1:B:187:ILE:H	1.72	0.55
1:F:150:MET:HE1	1:F:187:ILE:CD1	2.35	0.55
1:F:187:ILE:H	1:F:187:ILE:HD12	1.71	0.55
1:A:428:ILE:N	1:A:428:ILE:HD12	2.22	0.55
1:F:82:HIS:CG	1:F:112:THR:HG21	2.38	0.55
1:E:150:MET:CE	1:E:182:THR:HG22	2.37	0.55
1:D:150:MET:CE	1:D:182:THR:HG22	2.37	0.55
1:D:187:ILE:H	1:D:187:ILE:HD12	1.72	0.55
1:B:265:ARG:HG3	1:B:266:PHE:HD1	1.72	0.55
1:B:205:GLN:NE2	1:F:492:VAL:O	2.39	0.55
1:B:109:SER:O	1:B:112:THR:HG23	2.07	0.55
1:D:428:ILE:N	1:D:428:ILE:HD12	2.22	0.55
1:C:428:ILE:N	1:C:428:ILE:HD12	2.22	0.55
1:E:242:PHE:O	1:E:244:ASP:N	2.40	0.55
1:A:150:MET:CE	1:A:182:THR:HG22	2.37	0.55
1:C:265:ARG:HG3	1:C:266:PHE:HD1	1.72	0.55
1:C:242:PHE:O	1:C:244:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ILE:HD12	1:C:187:ILE:H	1.71	0.55
1:A:242:PHE:O	1:A:244:ASP:N	2.40	0.55
1:D:37:THR:O	1:D:38:GLN:HB3	2.07	0.55
1:A:287:ASP:HB3	1:A:290:GLU:CG	2.34	0.55
1:E:187:ILE:H	1:E:187:ILE:HD12	1.71	0.55
1:F:150:MET:CE	1:F:182:THR:HG22	2.37	0.55
1:B:72:TRP:CZ2	1:E:498:VAL:HB	2.41	0.55
1:E:428:ILE:N	1:E:428:ILE:HD12	2.22	0.55
1:E:37:THR:O	1:E:38:GLN:HB3	2.07	0.55
1:B:150:MET:CE	1:B:182:THR:HG22	2.37	0.55
1:B:150:MET:HE1	1:B:187:ILE:CD1	2.37	0.55
1:D:265:ARG:HG3	1:D:266:PHE:HD1	1.72	0.55
1:E:265:ARG:HG3	1:E:266:PHE:HD1	1.72	0.55
1:A:187:ILE:H	1:A:187:ILE:HD12	1.71	0.55
1:E:109:SER:O	1:E:112:THR:HG23	2.07	0.55
1:A:250:GLN:HE22	1:A:330:GLN:HE21	1.55	0.55
1:C:95:TYR:OH	1:C:145:THR:HB	2.07	0.55
1:A:265:ARG:HG3	1:A:266:PHE:HD1	1.72	0.55
1:F:242:PHE:O	1:F:244:ASP:N	2.40	0.55
1:D:242:PHE:O	1:D:244:ASP:N	2.40	0.55
2:D:556:GLU:C	3:D:561:NDP:H71N	2.09	0.54
1:D:287:ASP:HB3	1:D:290:GLU:CG	2.34	0.54
1:C:258:HIS:CD2	1:C:261:ARG:NH1	2.73	0.54
1:F:428:ILE:N	1:F:428:ILE:HD12	2.22	0.54
1:C:339:VAL:H	1:C:363:ARG:HH21	1.55	0.54
1:C:150:MET:HE1	1:C:187:ILE:CD1	2.37	0.54
1:D:95:TYR:OH	1:D:145:THR:HB	2.07	0.54
1:E:428:ILE:O	1:E:430:ILE:HD12	2.08	0.54
1:A:428:ILE:O	1:A:430:ILE:HD12	2.08	0.54
1:B:428:ILE:O	1:B:430:ILE:HD12	2.07	0.54
1:C:150:MET:CE	1:C:182:THR:HG22	2.37	0.54
1:D:250:GLN:HE22	1:D:330:GLN:HE21	1.55	0.54
1:A:95:TYR:OH	1:A:145:THR:HB	2.07	0.54
1:F:339:VAL:H	1:F:363:ARG:HH21	1.55	0.54
1:C:37:THR:O	1:C:38:GLN:HB3	2.07	0.54
2:C:555:GLU:C	3:C:560:NDP:H71N	2.09	0.54
1:F:428:ILE:O	1:F:430:ILE:HD12	2.08	0.54
1:D:428:ILE:O	1:D:430:ILE:HD12	2.08	0.54
1:B:242:PHE:O	1:B:244:ASP:N	2.40	0.54
1:F:109:SER:O	1:F:112:THR:HG23	2.07	0.54
1:B:498:VAL:HB	1:E:72:TRP:CZ2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:ASP:HB3	1:F:290:GLU:CG	2.33	0.54
1:E:339:VAL:H	1:E:363:ARG:HH21	1.55	0.54
1:B:428:ILE:N	1:B:428:ILE:HD12	2.22	0.54
1:F:37:THR:O	1:F:38:GLN:HB3	2.07	0.54
1:D:109:SER:O	1:D:112:THR:HG23	2.07	0.54
1:C:261:ARG:NH2	4:C:565:GTP:C8	2.76	0.54
1:E:261:ARG:NH2	4:E:567:GTP:C8	2.76	0.54
1:B:258:HIS:CD2	1:B:261:ARG:NH1	2.73	0.54
1:B:95:TYR:OH	1:B:145:THR:HB	2.07	0.54
1:F:95:TYR:OH	1:F:145:THR:HB	2.07	0.54
1:B:37:THR:O	1:B:38:GLN:HB3	2.07	0.54
1:A:109:SER:O	1:A:112:THR:HG23	2.07	0.54
1:D:261:ARG:NH2	4:D:566:GTP:C8	2.76	0.54
1:E:250:GLN:HE22	1:E:330:GLN:HE21	1.55	0.54
1:B:67:ARG:HD3	1:B:73:GLU:HB2	1.90	0.54
1:C:250:GLN:HE22	1:C:330:GLN:HE21	1.55	0.54
1:A:261:ARG:NH2	4:A:553:GTP:C8	2.76	0.54
1:A:37:THR:O	1:A:38:GLN:HB3	2.07	0.54
1:A:492:VAL:O	1:F:205:GLN:NE2	2.41	0.53
1:A:67:ARG:HD3	1:A:73:GLU:HB2	1.90	0.53
1:E:95:TYR:OH	1:E:145:THR:HB	2.07	0.53
1:D:230:ALA:HB2	1:D:240:PRO:CG	2.39	0.53
1:C:56:ASN:O	1:C:57:HIS:CG	2.62	0.53
1:B:250:GLN:HE22	1:B:330:GLN:HE21	1.55	0.53
1:F:250:GLN:HE22	1:F:330:GLN:HE21	1.55	0.53
1:C:67:ARG:HD3	1:C:73:GLU:HB2	1.90	0.53
1:B:261:ARG:NH2	4:B:564:GTP:C8	2.76	0.53
1:F:56:ASN:O	1:F:57:HIS:CG	2.62	0.53
1:A:56:ASN:O	1:A:57:HIS:CG	2.62	0.53
1:C:150:MET:HE3	1:C:182:THR:HG22	1.89	0.53
1:E:67:ARG:HD3	1:E:73:GLU:HB2	1.90	0.53
1:F:261:ARG:NH2	4:F:568:GTP:C8	2.76	0.53
1:E:230:ALA:HB2	1:E:240:PRO:CG	2.39	0.53
1:A:339:VAL:H	1:A:363:ARG:HH21	1.55	0.53
1:F:22:SER:O	1:F:25:GLU:HB2	2.09	0.53
1:B:150:MET:HE3	1:B:182:THR:HG22	1.91	0.53
1:F:67:ARG:HD3	1:F:73:GLU:HB2	1.90	0.53
1:D:67:ARG:HD3	1:D:73:GLU:HB2	1.90	0.53
1:C:147:ARG:O	1:C:151:GLU:HG2	2.09	0.53
1:D:231:SER:O	1:D:235:ILE:HG13	2.09	0.53
1:E:315:LEU:HD13	1:E:331:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:ILE:O	1:C:430:ILE:HD12	2.08	0.53
1:B:231:SER:O	1:B:235:ILE:HG13	2.09	0.53
1:D:56:ASN:O	1:D:57:HIS:CG	2.62	0.53
1:B:22:SER:O	1:B:25:GLU:HB2	2.09	0.53
1:C:230:ALA:HB2	1:C:240:PRO:CG	2.39	0.53
1:F:230:ALA:HB2	1:F:240:PRO:CG	2.39	0.53
1:E:22:SER:O	1:E:25:GLU:HB2	2.09	0.53
1:F:24:VAL:CG2	1:F:483:VAL:HG13	2.33	0.53
1:B:339:VAL:H	1:B:363:ARG:HH21	1.55	0.53
1:F:27:LYS:C	1:F:27:LYS:HD3	2.30	0.53
1:A:22:SER:O	1:A:25:GLU:HB2	2.09	0.53
1:E:231:SER:O	1:E:235:ILE:HG13	2.09	0.53
1:C:24:VAL:CG2	1:C:483:VAL:HG13	2.33	0.53
1:F:315:LEU:HD13	1:F:331:LEU:HD13	1.91	0.53
1:E:147:ARG:O	1:E:151:GLU:HG2	2.09	0.53
1:D:22:SER:O	1:D:25:GLU:HB2	2.09	0.53
1:A:315:LEU:HD13	1:A:331:LEU:HD13	1.91	0.52
1:D:147:ARG:O	1:D:151:GLU:HG2	2.09	0.52
1:A:258:HIS:CD2	1:A:261:ARG:NH1	2.73	0.52
1:F:265:ARG:HG3	1:F:266:PHE:HD1	1.72	0.52
1:E:56:ASN:O	1:E:57:HIS:CG	2.62	0.52
1:A:162:VAL:HG11	1:F:190:TYR:CD2	2.44	0.52
1:C:22:SER:O	1:C:25:GLU:HB2	2.09	0.52
1:B:56:ASN:O	1:B:57:HIS:CG	2.62	0.52
1:A:147:ARG:O	1:A:151:GLU:HG2	2.09	0.52
1:A:255:VAL:HG22	1:A:325:ALA:HB1	1.91	0.52
1:D:27:LYS:C	1:D:27:LYS:HD3	2.30	0.52
1:F:231:SER:O	1:F:235:ILE:HG13	2.09	0.52
1:C:27:LYS:C	1:C:27:LYS:HD3	2.29	0.52
1:D:458:GLU:OE2	1:D:462:ARG:HD3	2.10	0.52
1:E:27:LYS:HD3	1:E:27:LYS:C	2.30	0.52
1:C:315:LEU:HD13	1:C:331:LEU:HD13	1.91	0.52
1:B:147:ARG:O	1:B:151:GLU:HG2	2.09	0.52
1:D:339:VAL:H	1:D:363:ARG:HH21	1.55	0.52
1:A:227:ILE:HD11	1:A:245:LYS:CD	2.40	0.52
1:C:146:ARG:NH2	1:E:500:PHE:CE1	2.77	0.52
1:B:255:VAL:HG22	1:B:325:ALA:HB1	1.91	0.52
1:A:458:GLU:OE2	1:A:462:ARG:HD3	2.10	0.52
1:D:344:ILE:HB	1:D:367:VAL:HG22	1.92	0.52
1:C:386:LEU:HD21	1:D:392:VAL:CG1	2.40	0.52
1:B:215:THR:CG2	3:B:559:NDP:C4N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ILE:HD11	1:B:245:LYS:CD	2.40	0.52
1:C:231:SER:O	1:C:235:ILE:HG13	2.09	0.52
1:E:227:ILE:HD11	1:E:245:LYS:CD	2.40	0.52
1:B:458:GLU:OE2	1:B:462:ARG:HD3	2.10	0.52
1:A:24:VAL:CG2	1:A:483:VAL:HG13	2.33	0.52
1:E:458:GLU:OE2	1:E:462:ARG:HD3	2.10	0.52
1:D:227:ILE:HD11	1:D:245:LYS:CD	2.40	0.52
1:F:227:ILE:HD11	1:F:245:LYS:CD	2.40	0.52
1:B:63:PHE:CZ	1:B:75:ILE:HD11	2.45	0.52
1:A:231:SER:O	1:A:235:ILE:HG13	2.09	0.52
1:C:458:GLU:OE2	1:C:462:ARG:HD3	2.10	0.52
1:C:255:VAL:HG22	1:C:325:ALA:HB1	1.91	0.52
1:F:255:VAL:HG22	1:F:325:ALA:HB1	1.91	0.52
1:C:205:GLN:NE2	1:E:492:VAL:O	2.43	0.52
1:F:63:PHE:CZ	1:F:75:ILE:HD11	2.45	0.52
1:C:63:PHE:CZ	1:C:75:ILE:HD11	2.45	0.52
1:D:63:PHE:CZ	1:D:75:ILE:HD11	2.45	0.52
1:E:63:PHE:CZ	1:E:75:ILE:HD11	2.45	0.52
1:B:230:ALA:HB2	1:B:240:PRO:CG	2.39	0.52
1:F:344:ILE:HB	1:F:367:VAL:HG22	1.92	0.52
1:C:344:ILE:HB	1:C:367:VAL:HG22	1.92	0.52
1:A:230:ALA:HB2	1:A:240:PRO:CG	2.39	0.52
1:F:35:ARG:HG3	1:F:36:GLN:OE1	2.11	0.52
1:A:27:LYS:C	1:A:27:LYS:HD3	2.30	0.52
1:B:27:LYS:C	1:B:27:LYS:HD3	2.30	0.52
1:F:147:ARG:O	1:F:151:GLU:HG2	2.09	0.51
1:D:499:THR:O	1:D:500:PHE:CD1	2.63	0.51
1:F:458:GLU:OE2	1:F:462:ARG:HD3	2.10	0.51
1:C:90:LYS:HE2	1:C:164:VAL:HB	1.93	0.51
1:E:255:VAL:HG22	1:E:325:ALA:HB1	1.91	0.51
1:A:63:PHE:CZ	1:A:75:ILE:HD11	2.45	0.51
1:E:35:ARG:HG3	1:E:36:GLN:OE1	2.10	0.51
1:A:90:LYS:HE2	1:A:164:VAL:HB	1.93	0.51
1:B:24:VAL:CG2	1:B:483:VAL:HG13	2.33	0.51
1:C:417:LEU:HD21	1:E:417:LEU:HD13	1.92	0.51
1:B:344:ILE:HB	1:B:367:VAL:HG22	1.92	0.51
1:C:499:THR:O	1:C:500:PHE:CD1	2.63	0.51
1:D:315:LEU:HD13	1:D:331:LEU:HD13	1.91	0.51
1:C:227:ILE:HD11	1:C:245:LYS:CD	2.40	0.51
1:D:255:VAL:HG22	1:D:325:ALA:HB1	1.91	0.51
1:C:215:THR:HG21	3:C:560:NDP:C5N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:VAL:HB	1:F:72:TRP:CZ2	2.44	0.51
1:A:35:ARG:HG3	1:A:36:GLN:OE1	2.10	0.51
1:B:35:ARG:HG3	1:B:36:GLN:OE1	2.10	0.51
1:D:90:LYS:HE2	1:D:164:VAL:HB	1.93	0.51
1:E:215:THR:HG21	3:E:562:NDP:C5N	2.41	0.51
1:A:346:GLU:OE1	1:A:352:THR:HG23	2.11	0.51
1:C:96:SER:O	1:C:130:LYS:HA	2.11	0.51
1:D:443:ALA:HB1	1:D:448:ILE:HD12	1.93	0.51
1:A:344:ILE:HB	1:A:367:VAL:HG22	1.92	0.51
1:F:96:SER:O	1:F:130:LYS:HA	2.11	0.51
1:A:96:SER:O	1:A:130:LYS:HA	2.11	0.51
1:F:499:THR:O	1:F:500:PHE:CD1	2.63	0.51
1:B:499:THR:O	1:B:500:PHE:CD1	2.63	0.51
1:F:346:GLU:OE1	1:F:352:THR:HG23	2.11	0.51
1:A:392:VAL:HG12	1:B:382:TYR:OH	2.11	0.51
1:A:443:ALA:HB1	1:A:448:ILE:HD12	1.93	0.51
1:C:72:TRP:CZ2	1:F:498:VAL:HB	2.46	0.51
1:E:499:THR:O	1:E:500:PHE:CD1	2.63	0.51
1:B:190:TYR:CE2	1:F:162:VAL:HG11	2.46	0.51
1:A:499:THR:O	1:A:500:PHE:CD1	2.63	0.51
1:B:96:SER:O	1:B:130:LYS:HA	2.11	0.51
1:B:315:LEU:HD13	1:B:331:LEU:HD13	1.91	0.51
1:B:346:GLU:OE1	1:B:352:THR:HG23	2.11	0.51
1:B:90:LYS:HE2	1:B:164:VAL:HB	1.93	0.51
1:E:344:ILE:HB	1:E:367:VAL:HG22	1.92	0.50
1:D:35:ARG:HG3	1:D:36:GLN:OE1	2.10	0.50
1:A:23:ILE:HD12	1:A:479:THR:HG21	1.93	0.50
1:D:28:LEU:HD21	1:D:487:GLU:HG2	1.94	0.50
1:B:28:LEU:HD21	1:B:487:GLU:HG2	1.94	0.50
1:C:28:LEU:HD21	1:C:487:GLU:HG2	1.94	0.50
2:B:554:GLU:C	3:B:559:NDP:N7N	2.65	0.50
1:C:23:ILE:HD12	1:C:479:THR:HG21	1.94	0.50
1:E:24:VAL:CG2	1:E:483:VAL:HG13	2.33	0.50
2:A:550:GLU:C	3:A:551:NDP:N7N	2.65	0.50
2:C:555:GLU:C	3:C:560:NDP:N7N	2.65	0.50
1:E:28:LEU:HD21	1:E:487:GLU:HG2	1.94	0.50
1:C:417:LEU:HD21	1:E:417:LEU:CD1	2.42	0.50
1:F:23:ILE:HD12	1:F:479:THR:HG21	1.94	0.50
1:D:346:GLU:OE1	1:D:352:THR:HG23	2.11	0.50
1:A:230:ALA:HB2	1:A:240:PRO:HG2	1.94	0.50
1:C:443:ALA:HB1	1:C:448:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:557:GLU:C	3:E:562:NDP:N7N	2.65	0.50
1:D:215:THR:HG21	3:D:561:NDP:C5N	2.41	0.50
1:A:427:THR:O	1:A:429:PRO:HD3	2.12	0.50
1:F:90:LYS:HE2	1:F:164:VAL:HB	1.92	0.50
1:F:427:THR:O	1:F:429:PRO:HD3	2.12	0.50
1:D:23:ILE:HD12	1:D:479:THR:HG21	1.93	0.50
1:C:346:GLU:OE2	1:C:478:ARG:NH2	2.45	0.50
1:C:386:LEU:HD21	1:D:392:VAL:HG11	1.93	0.50
1:C:35:ARG:HG3	1:C:36:GLN:OE1	2.11	0.50
1:E:331:LEU:HD23	1:E:352:THR:HG22	1.94	0.50
1:E:346:GLU:OE1	1:E:352:THR:HG23	2.11	0.50
1:F:215:THR:CG2	3:F:563:NDP:C4N	2.73	0.49
2:F:558:GLU:C	3:F:563:NDP:N7N	2.65	0.49
1:C:7:PRO:HD2	1:C:329:LYS:HD2	1.94	0.49
1:E:96:SER:O	1:E:130:LYS:HA	2.11	0.49
1:E:427:THR:O	1:E:429:PRO:HD3	2.12	0.49
1:C:346:GLU:OE1	1:C:352:THR:HG23	2.11	0.49
1:D:331:LEU:HD23	1:D:352:THR:HG22	1.94	0.49
1:A:280:ILE:HD11	1:A:304:PHE:CB	2.42	0.49
1:F:280:ILE:HD11	1:F:304:PHE:CB	2.42	0.49
1:B:427:THR:O	1:B:429:PRO:HD3	2.12	0.49
1:E:346:GLU:OE2	1:E:478:ARG:NH2	2.45	0.49
1:F:346:GLU:OE2	1:F:478:ARG:NH2	2.45	0.49
1:F:443:ALA:HB1	1:F:448:ILE:HD12	1.93	0.49
1:F:215:THR:HG21	3:F:563:NDP:C5N	2.41	0.49
1:F:7:PRO:HD2	1:F:329:LYS:HD2	1.94	0.49
1:B:40:GLN:O	1:B:43:ASN:HB2	2.13	0.49
1:D:96:SER:O	1:D:130:LYS:HA	2.11	0.49
1:E:90:LYS:HE2	1:E:164:VAL:HB	1.93	0.49
1:A:215:THR:HG21	3:A:551:NDP:C5N	2.41	0.49
1:E:132:ASN:C	1:E:132:ASN:HD22	2.16	0.49
1:B:132:ASN:C	1:B:132:ASN:HD22	2.16	0.49
1:C:230:ALA:HB2	1:C:240:PRO:HG2	1.94	0.49
1:D:230:ALA:HB2	1:D:240:PRO:HG2	1.94	0.49
1:F:92:GLY:HA2	1:F:166:ALA:O	2.13	0.49
1:B:232:TYR:CE2	1:B:465:MET:HG2	2.48	0.49
1:D:24:VAL:CG2	1:D:483:VAL:HG13	2.33	0.49
1:D:346:GLU:OE2	1:D:478:ARG:NH2	2.45	0.49
1:D:280:ILE:HD11	1:D:304:PHE:CB	2.42	0.49
1:A:7:PRO:HD2	1:A:329:LYS:HD2	1.94	0.49
1:C:219:VAL:HA	1:C:373:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:VAL:HA	1:F:373:LEU:HD22	1.95	0.49
1:C:92:GLY:HA2	1:C:166:ALA:O	2.13	0.49
1:B:7:PRO:HD2	1:B:329:LYS:HD2	1.94	0.49
1:B:230:ALA:HB2	1:B:240:PRO:HG2	1.94	0.49
1:F:230:ALA:HB2	1:F:240:PRO:HG2	1.94	0.49
1:E:230:ALA:HB2	1:E:240:PRO:HG2	1.94	0.49
1:E:443:ALA:HB1	1:E:448:ILE:HD12	1.93	0.49
1:D:232:TYR:CE2	1:D:465:MET:HG2	2.48	0.49
1:D:92:GLY:HA2	1:D:166:ALA:O	2.13	0.49
1:C:215:THR:CG2	3:C:560:NDP:C4N	2.73	0.49
1:C:132:ASN:HD22	1:C:134:LYS:H	1.61	0.49
1:D:40:GLN:O	1:D:43:ASN:HB2	2.13	0.49
1:C:40:GLN:O	1:C:43:ASN:HB2	2.13	0.49
1:C:232:TYR:CE2	1:C:465:MET:HG2	2.48	0.49
1:C:427:THR:O	1:C:429:PRO:HD3	2.12	0.49
1:B:215:THR:HG21	3:B:559:NDP:C5N	2.41	0.49
2:D:556:GLU:C	3:D:561:NDP:N7N	2.65	0.49
1:B:54:PRO:O	1:B:55:CYS:HB2	2.13	0.49
1:A:430:ILE:HA	1:F:416:SER:OG	2.12	0.49
1:A:92:GLY:HA2	1:A:166:ALA:O	2.13	0.49
1:B:443:ALA:HB1	1:B:448:ILE:HD12	1.93	0.49
1:C:54:PRO:O	1:C:55:CYS:HB2	2.13	0.49
1:E:82:HIS:CE1	1:E:109:SER:HB3	2.48	0.49
1:C:147:ARG:HG2	1:C:147:ARG:HH11	1.78	0.49
1:A:40:GLN:O	1:A:43:ASN:HB2	2.13	0.49
1:B:92:GLY:HA2	1:B:166:ALA:O	2.13	0.49
1:D:23:ILE:HG23	1:D:471:TYR:CD2	2.48	0.48
1:A:23:ILE:HG23	1:A:471:TYR:CD2	2.48	0.48
1:C:23:ILE:HG23	1:C:471:TYR:CD2	2.48	0.48
1:E:23:ILE:HG23	1:E:471:TYR:CD2	2.48	0.48
1:B:23:ILE:HD12	1:B:479:THR:HG21	1.93	0.48
1:F:23:ILE:HG23	1:F:471:TYR:CD2	2.48	0.48
1:A:331:LEU:HD23	1:A:352:THR:HG22	1.94	0.48
1:A:346:GLU:OE2	1:A:478:ARG:NH2	2.45	0.48
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.78	0.48
1:B:132:ASN:HD22	1:B:134:LYS:H	1.61	0.48
1:E:7:PRO:HD2	1:E:329:LYS:HD2	1.94	0.48
1:D:7:PRO:HD2	1:D:329:LYS:HD2	1.94	0.48
1:C:339:VAL:HG11	1:C:360:PHE:CZ	2.48	0.48
1:F:40:GLN:O	1:F:43:ASN:HB2	2.13	0.48
1:E:219:VAL:HA	1:E:373:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:TYR:CE2	1:F:465:MET:HG2	2.48	0.48
1:A:87:THR:HG22	1:A:88:PRO:HD3	1.95	0.48
1:F:82:HIS:CE1	1:F:109:SER:HB3	2.48	0.48
1:B:82:HIS:CE1	1:B:109:SER:HB3	2.48	0.48
1:D:82:HIS:CE1	1:D:109:SER:HB3	2.48	0.48
1:B:346:GLU:OE2	1:B:478:ARG:NH2	2.45	0.48
1:F:69:ASP:O	1:F:71:SER:N	2.46	0.48
1:F:132:ASN:HD21	1:F:134:LYS:HB2	1.78	0.48
1:E:339:VAL:HG11	1:E:360:PHE:CZ	2.48	0.48
1:E:40:GLN:O	1:E:43:ASN:HB2	2.13	0.48
1:C:87:THR:HG22	1:C:88:PRO:HD3	1.95	0.48
1:D:87:THR:HG22	1:D:88:PRO:HD3	1.95	0.48
1:D:427:THR:O	1:D:429:PRO:HD3	2.12	0.48
1:B:331:LEU:HD23	1:B:352:THR:HG22	1.94	0.48
1:D:69:ASP:O	1:D:71:SER:N	2.47	0.48
1:B:69:ASP:O	1:B:71:SER:N	2.46	0.48
1:E:280:ILE:HD11	1:E:304:PHE:CB	2.42	0.48
1:F:339:VAL:HG11	1:F:360:PHE:CZ	2.48	0.48
1:D:99:VAL:O	1:D:130:LYS:HE2	2.14	0.48
1:F:28:LEU:HD21	1:F:487:GLU:HG2	1.94	0.48
1:A:219:VAL:HA	1:A:373:LEU:HD22	1.95	0.48
1:C:82:HIS:CE1	1:C:109:SER:HB3	2.48	0.48
1:E:69:ASP:O	1:E:71:SER:N	2.47	0.48
1:A:132:ASN:C	1:A:132:ASN:HD22	2.16	0.48
1:A:99:VAL:O	1:A:130:LYS:HE2	2.14	0.48
1:C:465:MET:O	1:C:469:MET:HG2	2.13	0.48
1:F:465:MET:O	1:F:469:MET:HG2	2.14	0.48
1:D:87:THR:O	1:D:88:PRO:C	2.51	0.48
1:B:87:THR:HG22	1:B:88:PRO:HD3	1.95	0.48
1:E:232:TYR:CE2	1:E:465:MET:HG2	2.48	0.48
1:A:232:TYR:CE2	1:A:465:MET:HG2	2.48	0.48
1:B:219:VAL:HA	1:B:373:LEU:HD22	1.95	0.48
1:D:54:PRO:O	1:D:55:CYS:HB2	2.13	0.48
1:F:331:LEU:HD23	1:F:352:THR:HG22	1.94	0.48
1:C:69:ASP:O	1:C:71:SER:N	2.47	0.48
1:B:147:ARG:HG2	1:B:147:ARG:HH11	1.78	0.48
1:C:132:ASN:C	1:C:132:ASN:HD22	2.16	0.48
1:C:443:ALA:CB	1:C:448:ILE:HD12	2.44	0.48
1:B:465:MET:O	1:B:469:MET:HG2	2.14	0.48
1:D:10:PHE:O	1:D:14:GLU:HG3	2.14	0.48
1:D:54:PRO:O	1:D:55:CYS:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ARG:HD3	1:B:70:GLY:O	2.14	0.48
1:A:69:ASP:O	1:A:71:SER:N	2.47	0.48
1:A:281:TRP:CZ3	1:A:308:LYS:HE2	2.49	0.48
1:F:132:ASN:C	1:F:132:ASN:HD22	2.16	0.48
1:C:132:ASN:HD21	1:C:134:LYS:HB2	1.79	0.48
1:B:339:VAL:HG11	1:B:360:PHE:CZ	2.48	0.48
1:D:339:VAL:HG11	1:D:360:PHE:CZ	2.48	0.48
1:E:92:GLY:HA2	1:E:166:ALA:O	2.13	0.48
1:B:23:ILE:HG23	1:B:471:TYR:CD2	2.48	0.48
1:F:66:ARG:HD3	1:F:70:GLY:O	2.14	0.48
1:E:147:ARG:HH11	1:E:147:ARG:HG2	1.78	0.48
1:C:281:TRP:CZ3	1:C:308:LYS:HE2	2.49	0.48
1:F:132:ASN:HD22	1:F:134:LYS:H	1.61	0.48
1:F:443:ALA:CB	1:F:448:ILE:HD12	2.44	0.48
1:D:465:MET:O	1:D:469:MET:HG2	2.13	0.48
1:B:443:ALA:CB	1:B:448:ILE:HD12	2.44	0.48
1:E:459:ARG:HG2	1:E:463:GLN:HE21	1.79	0.48
1:B:107:LEU:HB3	1:B:126:LYS:HG2	1.96	0.48
1:F:459:ARG:HG2	1:F:463:GLN:HE21	1.79	0.48
1:D:219:VAL:HA	1:D:373:LEU:HD22	1.95	0.48
1:A:28:LEU:HD21	1:A:487:GLU:HG2	1.94	0.48
1:E:10:PHE:O	1:E:14:GLU:HG3	2.14	0.48
1:A:168:ASN:ND2	1:A:169:MET:N	2.53	0.48
1:A:54:PRO:O	1:A:55:CYS:CB	2.62	0.48
1:F:281:TRP:CZ3	1:F:308:LYS:HE2	2.49	0.48
1:D:132:ASN:C	1:D:132:ASN:HD22	2.16	0.48
1:A:339:VAL:HG11	1:A:360:PHE:CZ	2.48	0.48
1:A:458:GLU:O	1:A:462:ARG:HG3	2.14	0.48
1:D:443:ALA:CB	1:D:448:ILE:HD12	2.44	0.48
1:A:196:ALA:HA	1:A:388:ASN:HD22	1.79	0.48
1:A:465:MET:O	1:A:469:MET:HG2	2.14	0.48
1:F:10:PHE:O	1:F:14:GLU:HG3	2.14	0.48
1:E:274:GLY:N	1:E:314:ILE:HD13	2.29	0.48
1:C:107:LEU:HB3	1:C:126:LYS:HG2	1.96	0.48
1:C:274:GLY:N	1:C:314:ILE:HD13	2.29	0.48
1:F:54:PRO:O	1:F:55:CYS:CB	2.62	0.48
1:A:82:HIS:CE1	1:A:109:SER:HB3	2.48	0.48
1:E:54:PRO:O	1:E:55:CYS:CB	2.62	0.48
1:E:23:ILE:HD12	1:E:479:THR:HG21	1.94	0.48
1:C:66:ARG:HD3	1:C:70:GLY:O	2.14	0.48
1:C:392:VAL:HG12	1:E:382:TYR:OH	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:VAL:HG11	1:B:360:PHE:CE2	2.49	0.48
1:E:458:GLU:O	1:E:462:ARG:HG3	2.14	0.48
1:E:465:MET:O	1:E:469:MET:HG2	2.14	0.48
1:C:10:PHE:O	1:C:14:GLU:HG3	2.14	0.48
1:B:274:GLY:N	1:B:314:ILE:HD13	2.29	0.48
1:A:107:LEU:HB3	1:A:126:LYS:HG2	1.96	0.48
1:F:87:THR:O	1:F:88:PRO:C	2.52	0.48
1:A:215:THR:CG2	3:A:551:NDP:C4N	2.73	0.47
1:B:374:ASN:O	3:B:559:NDP:O7N	2.32	0.47
1:E:54:PRO:O	1:E:55:CYS:HB2	2.13	0.47
1:D:147:ARG:HG2	1:D:147:ARG:HH11	1.78	0.47
1:C:280:ILE:HD11	1:C:304:PHE:CB	2.42	0.47
1:F:339:VAL:HG11	1:F:360:PHE:CE2	2.49	0.47
1:C:339:VAL:HG11	1:C:360:PHE:CE2	2.49	0.47
1:D:339:VAL:HG11	1:D:360:PHE:CE2	2.49	0.47
1:D:27:LYS:O	1:D:30:GLU:HB2	2.14	0.47
1:B:458:GLU:O	1:B:462:ARG:HG3	2.14	0.47
1:A:27:LYS:O	1:A:30:GLU:HB2	2.14	0.47
1:C:99:VAL:O	1:C:130:LYS:HE2	2.14	0.47
1:F:87:THR:HG22	1:F:88:PRO:HD3	1.95	0.47
1:A:459:ARG:HG2	1:A:463:GLN:HE21	1.79	0.47
1:F:274:GLY:N	1:F:314:ILE:HD13	2.29	0.47
1:D:274:GLY:N	1:D:314:ILE:HD13	2.29	0.47
1:A:274:GLY:N	1:A:314:ILE:HD13	2.29	0.47
1:C:374:ASN:O	3:C:560:NDP:O7N	2.33	0.47
1:B:54:PRO:O	1:B:55:CYS:CB	2.62	0.47
1:A:66:ARG:HD3	1:A:70:GLY:O	2.14	0.47
1:B:196:ALA:HA	1:B:388:ASN:HD22	1.79	0.47
1:E:196:ALA:HA	1:E:388:ASN:HD22	1.79	0.47
1:B:337:PRO:O	1:B:338:ARG:HB3	2.14	0.47
1:D:132:ASN:HD21	1:D:134:LYS:HB2	1.79	0.47
1:E:339:VAL:HG11	1:E:360:PHE:CE2	2.49	0.47
1:B:27:LYS:O	1:B:30:GLU:HB2	2.14	0.47
1:F:99:VAL:O	1:F:130:LYS:HE2	2.14	0.47
1:E:443:ALA:CB	1:E:448:ILE:HD12	2.44	0.47
1:D:107:LEU:HB3	1:D:126:LYS:HG2	1.96	0.47
1:C:331:LEU:HD23	1:C:352:THR:HG22	1.94	0.47
1:A:242:PHE:HB3	1:A:268:ALA:HB2	1.97	0.47
1:C:38:GLN:N	1:C:38:GLN:OE1	2.47	0.47
1:E:87:THR:HG22	1:E:88:PRO:HD3	1.95	0.47
1:D:459:ARG:HG2	1:D:463:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:ARG:HD3	1:E:70:GLY:O	2.14	0.47
1:E:337:PRO:O	1:E:338:ARG:HB3	2.14	0.47
1:C:87:THR:O	1:C:88:PRO:C	2.51	0.47
1:A:32:LEU:HD21	1:A:44:ARG:HG2	1.97	0.47
1:C:32:LEU:HD21	1:C:44:ARG:HG2	1.96	0.47
1:B:281:TRP:CZ3	1:B:308:LYS:HE2	2.49	0.47
1:A:132:ASN:HD22	1:A:134:LYS:H	1.61	0.47
1:C:337:PRO:O	1:C:338:ARG:HB3	2.14	0.47
1:C:196:ALA:HA	1:C:388:ASN:HD22	1.79	0.47
1:E:414:GLN:HA	1:E:430:ILE:HD13	1.97	0.47
1:B:99:VAL:O	1:B:130:LYS:HE2	2.14	0.47
1:C:162:VAL:HG11	1:D:190:TYR:CD2	2.49	0.47
1:D:374:ASN:O	3:D:561:NDP:O7N	2.33	0.47
1:C:54:PRO:O	1:C:55:CYS:CB	2.62	0.47
1:B:280:ILE:HD11	1:B:304:PHE:CB	2.42	0.47
1:E:132:ASN:HD21	1:E:134:LYS:HB2	1.78	0.47
1:E:38:GLN:N	1:E:38:GLN:OE1	2.48	0.47
1:A:416:SER:OG	1:B:430:ILE:HA	2.14	0.47
1:C:27:LYS:O	1:C:30:GLU:HB2	2.14	0.47
1:D:46:ARG:HG3	1:D:46:ARG:HH11	1.80	0.47
1:F:374:ASN:O	3:F:563:NDP:O7N	2.33	0.47
1:E:281:TRP:CZ3	1:E:308:LYS:HE2	2.49	0.47
1:D:281:TRP:CZ3	1:D:308:LYS:HE2	2.49	0.47
1:A:190:TYR:CE2	1:B:162:VAL:HG11	2.49	0.47
1:A:337:PRO:O	1:A:338:ARG:HB3	2.14	0.47
1:E:132:ASN:HD22	1:E:134:LYS:H	1.61	0.47
1:F:337:PRO:O	1:F:338:ARG:HB3	2.14	0.47
1:A:339:VAL:HG11	1:A:360:PHE:CE2	2.49	0.47
1:C:414:GLN:HA	1:C:430:ILE:HD13	1.97	0.47
1:B:205:GLN:HE22	1:F:496:ALA:N	2.12	0.47
1:B:38:GLN:N	1:B:38:GLN:OE1	2.48	0.47
1:F:27:LYS:O	1:F:30:GLU:HB2	2.14	0.47
1:D:458:GLU:O	1:D:462:ARG:HG3	2.14	0.47
1:E:394:TYR:CE2	1:E:448:ILE:HD13	2.50	0.47
1:A:87:THR:O	1:A:88:PRO:C	2.51	0.47
1:B:87:THR:O	1:B:88:PRO:C	2.51	0.47
1:C:459:ARG:HG2	1:C:463:GLN:HE21	1.79	0.47
1:D:32:LEU:HD21	1:D:44:ARG:HG2	1.97	0.47
1:B:32:LEU:HD21	1:B:44:ARG:HG2	1.96	0.47
1:C:294:PHE:CE2	1:C:298:HIS:CD2	3.03	0.47
1:A:374:ASN:O	3:A:551:NDP:O7N	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:ILE:HA	1:E:127:ALA:O	2.15	0.47
1:A:382:TYR:OH	1:F:392:VAL:HG12	2.14	0.47
1:F:147:ARG:HH11	1:F:147:ARG:HG2	1.78	0.47
1:C:242:PHE:HB3	1:C:268:ALA:HB2	1.97	0.47
1:F:242:PHE:HB3	1:F:268:ALA:HB2	1.96	0.47
1:E:99:VAL:O	1:E:130:LYS:HE2	2.14	0.47
1:B:10:PHE:O	1:B:14:GLU:HG3	2.14	0.47
1:C:424:HIS:CG	1:C:425:GLY:N	2.83	0.47
1:F:107:LEU:HB3	1:F:126:LYS:HG2	1.96	0.47
1:B:253:GLY:HA3	3:B:559:NDP:O5B	2.15	0.47
1:C:253:GLY:HA3	3:C:560:NDP:O5B	2.15	0.47
1:F:54:PRO:O	1:F:55:CYS:HB2	2.13	0.47
1:A:54:PRO:O	1:A:55:CYS:HB2	2.13	0.47
1:B:70:GLY:O	1:B:71:SER:C	2.54	0.47
1:D:196:ALA:HA	1:D:388:ASN:HD22	1.79	0.47
1:F:414:GLN:HA	1:F:430:ILE:HD13	1.97	0.47
1:D:242:PHE:HB3	1:D:268:ALA:HB2	1.97	0.47
1:C:394:TYR:CE2	1:C:448:ILE:HD13	2.50	0.47
1:F:294:PHE:CE2	1:F:298:HIS:CD2	3.03	0.47
1:C:46:ARG:HH11	1:C:46:ARG:HG3	1.80	0.47
1:F:253:GLY:HA3	3:F:563:NDP:O5B	2.15	0.47
1:D:253:GLY:HA3	3:D:561:NDP:O5B	2.15	0.47
1:C:93:ILE:HA	1:C:127:ALA:O	2.15	0.47
1:D:66:ARG:HD3	1:D:70:GLY:O	2.14	0.47
1:F:458:GLU:O	1:F:462:ARG:HG3	2.14	0.47
1:A:443:ALA:CB	1:A:448:ILE:HD12	2.44	0.47
1:B:322:LEU:O	1:B:324:PRO:HD3	2.15	0.47
1:A:10:PHE:O	1:A:14:GLU:HG3	2.14	0.47
1:E:294:PHE:CE2	1:E:298:HIS:CD2	3.03	0.47
1:B:417:LEU:HD21	1:F:417:LEU:HD13	1.97	0.47
1:B:294:PHE:CE2	1:B:298:HIS:CD2	3.03	0.47
1:A:70:GLY:O	1:A:71:SER:C	2.54	0.46
1:D:337:PRO:O	1:D:338:ARG:HB3	2.14	0.46
1:B:414:GLN:HA	1:B:430:ILE:HD13	1.96	0.46
1:B:459:ARG:HG2	1:B:463:GLN:HE21	1.79	0.46
1:E:46:ARG:HH11	1:E:46:ARG:HG3	1.80	0.46
1:D:132:ASN:HD22	1:D:134:LYS:H	1.61	0.46
1:A:132:ASN:HD21	1:A:134:LYS:HB2	1.78	0.46
1:F:339:VAL:H	1:F:363:ARG:NH2	2.13	0.46
1:A:414:GLN:HA	1:A:430:ILE:HD13	1.97	0.46
1:E:242:PHE:HB3	1:E:268:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:GLU:O	1:C:462:ARG:HG3	2.14	0.46
1:B:394:TYR:CE2	1:B:448:ILE:HD13	2.50	0.46
1:A:322:LEU:O	1:A:324:PRO:HD3	2.15	0.46
1:A:46:ARG:HG3	1:A:46:ARG:HH11	1.80	0.46
1:E:253:GLY:HA3	3:E:562:NDP:O5B	2.15	0.46
1:D:215:THR:CG2	3:D:561:NDP:C4N	2.73	0.46
1:C:496:ALA:N	1:D:205:GLN:NE2	2.61	0.46
1:F:75:ILE:HD13	1:F:129:VAL:CG1	2.45	0.46
1:E:75:ILE:CD1	1:E:129:VAL:HG13	2.45	0.46
1:E:75:ILE:HD13	1:E:129:VAL:CG1	2.45	0.46
1:A:281:TRP:O	1:A:307:ALA:HB1	2.16	0.46
1:A:337:PRO:O	1:A:338:ARG:CB	2.63	0.46
1:F:196:ALA:HA	1:F:388:ASN:HD22	1.79	0.46
1:C:339:VAL:H	1:C:363:ARG:NH2	2.13	0.46
1:A:38:GLN:OE1	1:A:38:GLN:N	2.47	0.46
1:A:394:TYR:CE2	1:A:448:ILE:HD13	2.50	0.46
1:B:11:LYS:O	1:B:14:GLU:HB2	2.16	0.46
1:D:409:LEU:HD13	1:E:409:LEU:HD11	1.98	0.46
1:A:294:PHE:CE2	1:A:298:HIS:CD2	3.03	0.46
1:A:253:GLY:HA3	3:A:551:NDP:O5B	2.15	0.46
1:D:93:ILE:HA	1:D:127:ALA:O	2.15	0.46
1:E:281:TRP:O	1:E:307:ALA:HB1	2.16	0.46
1:D:57:HIS:HB2	1:D:81:GLN:HB2	1.98	0.46
1:B:57:HIS:HB2	1:B:81:GLN:HB2	1.98	0.46
1:E:11:LYS:O	1:E:14:GLU:HB2	2.16	0.46
1:B:46:ARG:HG3	1:B:46:ARG:HH11	1.80	0.46
1:E:374:ASN:O	3:E:562:NDP:O7N	2.32	0.46
1:B:337:PRO:O	1:B:338:ARG:CB	2.63	0.46
1:E:337:PRO:O	1:E:338:ARG:CB	2.63	0.46
1:D:414:GLN:HA	1:D:430:ILE:HD13	1.97	0.46
1:C:339:VAL:N	1:C:363:ARG:NH2	2.64	0.46
1:E:339:VAL:N	1:E:363:ARG:NH2	2.64	0.46
1:F:38:GLN:OE1	1:F:38:GLN:N	2.47	0.46
1:F:394:TYR:CE2	1:F:448:ILE:HD13	2.50	0.46
1:D:294:PHE:CE2	1:D:298:HIS:CD2	3.03	0.46
1:C:270:CYS:O	1:C:285:GLY:HA2	2.16	0.46
1:C:322:LEU:O	1:C:324:PRO:HD3	2.15	0.46
1:E:107:LEU:HB3	1:E:126:LYS:HG2	1.96	0.46
1:B:85:GLN:HB3	1:B:85:GLN:HE21	1.56	0.46
1:B:339:VAL:N	1:B:363:ARG:NH2	2.64	0.46
1:C:46:ARG:HG3	1:C:46:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:322:LEU:O	1:F:324:PRO:HD3	2.15	0.46
1:B:270:CYS:O	1:B:285:GLY:HA2	2.16	0.46
1:A:93:ILE:HA	1:A:127:ALA:O	2.15	0.46
1:F:93:ILE:HA	1:F:127:ALA:O	2.15	0.46
1:D:337:PRO:O	1:D:338:ARG:CB	2.63	0.46
1:C:337:PRO:O	1:C:338:ARG:CB	2.63	0.46
1:A:11:LYS:O	1:A:14:GLU:HB2	2.16	0.46
1:E:46:ARG:HG3	1:E:46:ARG:NH1	2.31	0.46
1:E:270:CYS:O	1:E:285:GLY:HA2	2.16	0.46
1:F:270:CYS:O	1:F:285:GLY:HA2	2.16	0.46
1:F:46:ARG:HG3	1:F:46:ARG:NH1	2.31	0.46
1:F:424:HIS:CG	1:F:425:GLY:N	2.83	0.46
1:D:64:PRO:HB2	1:D:72:TRP:CE3	2.51	0.46
1:D:70:GLY:O	1:D:71:SER:C	2.54	0.46
1:F:64:PRO:HB2	1:F:72:TRP:CE3	2.51	0.46
1:C:281:TRP:O	1:C:307:ALA:HB1	2.16	0.46
1:D:339:VAL:N	1:D:363:ARG:NH2	2.64	0.46
1:F:57:HIS:HB2	1:F:81:GLN:HB2	1.98	0.46
1:E:27:LYS:O	1:E:30:GLU:HB2	2.14	0.46
1:F:247:PHE:HA	1:F:321:ILE:O	2.16	0.46
1:F:32:LEU:HD21	1:F:44:ARG:HG2	1.97	0.46
1:C:247:PHE:HA	1:C:321:ILE:O	2.16	0.46
1:D:281:TRP:O	1:D:307:ALA:HB1	2.16	0.46
1:D:339:VAL:H	1:D:363:ARG:NH2	2.13	0.46
1:D:38:GLN:N	1:D:38:GLN:OE1	2.48	0.46
1:E:57:HIS:HB2	1:E:81:GLN:HB2	1.98	0.46
1:E:32:LEU:HD21	1:E:44:ARG:HG2	1.96	0.46
1:A:270:CYS:O	1:A:285:GLY:HA2	2.16	0.46
1:E:322:LEU:O	1:E:324:PRO:HD3	2.15	0.46
1:B:93:ILE:HA	1:B:127:ALA:O	2.15	0.46
1:C:70:GLY:O	1:C:71:SER:C	2.54	0.46
1:F:339:VAL:N	1:F:363:ARG:NH2	2.64	0.46
1:A:46:ARG:HG3	1:A:46:ARG:NH1	2.31	0.46
1:B:247:PHE:HA	1:B:321:ILE:O	2.16	0.46
1:E:210:GLY:O	1:E:214:ALA:HB2	2.16	0.46
1:D:322:LEU:O	1:D:324:PRO:HD3	2.15	0.46
1:C:190:TYR:CD2	1:E:162:VAL:HG11	2.50	0.46
1:F:210:GLY:O	1:F:214:ALA:HB2	2.16	0.46
1:E:424:HIS:CG	1:E:425:GLY:N	2.83	0.46
1:C:64:PRO:HB2	1:C:72:TRP:CE3	2.51	0.45
1:E:64:PRO:HB2	1:E:72:TRP:CE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:VAL:HB	1:D:72:TRP:CZ2	2.50	0.45
1:B:64:PRO:HB2	1:B:72:TRP:CE3	2.51	0.45
1:E:339:VAL:H	1:E:363:ARG:NH2	2.13	0.45
1:B:242:PHE:HB3	1:B:268:ALA:HB2	1.97	0.45
1:F:11:LYS:O	1:F:14:GLU:HB2	2.16	0.45
1:C:61:LEU:HD12	1:C:61:LEU:N	2.32	0.45
1:A:424:HIS:CG	1:A:425:GLY:N	2.83	0.45
1:D:247:PHE:HA	1:D:321:ILE:O	2.16	0.45
1:F:70:GLY:O	1:F:71:SER:C	2.53	0.45
1:E:70:GLY:O	1:E:71:SER:C	2.54	0.45
1:F:337:PRO:O	1:F:338:ARG:CB	2.63	0.45
1:D:394:TYR:CE2	1:D:448:ILE:HD13	2.50	0.45
1:C:11:LYS:O	1:C:14:GLU:HB2	2.16	0.45
1:E:247:PHE:HA	1:E:321:ILE:O	2.16	0.45
1:E:215:THR:CG2	3:E:562:NDP:C4N	2.73	0.45
1:A:339:VAL:N	1:A:363:ARG:NH2	2.64	0.45
1:A:64:PRO:HB2	1:A:72:TRP:CE3	2.51	0.45
1:E:37:THR:OG1	1:E:38:GLN:N	2.49	0.45
1:A:57:HIS:HB2	1:A:81:GLN:HB2	1.98	0.45
1:B:46:ARG:NH1	1:B:46:ARG:HG3	2.31	0.45
1:D:61:LEU:HD12	1:D:61:LEU:N	2.32	0.45
1:A:262:TYR:OH	4:A:553:GTP:O2G	2.33	0.45
1:B:37:THR:OG1	1:B:38:GLN:N	2.49	0.45
1:C:57:HIS:HB2	1:C:81:GLN:HB2	1.98	0.45
1:C:210:GLY:O	1:C:214:ALA:HB2	2.16	0.45
1:A:61:LEU:HD12	1:A:61:LEU:N	2.31	0.45
1:D:168:ASN:ND2	1:D:169:MET:N	2.53	0.45
1:F:281:TRP:O	1:F:307:ALA:HB1	2.16	0.45
1:E:87:THR:O	1:E:88:PRO:C	2.51	0.45
1:A:247:PHE:HA	1:A:321:ILE:O	2.16	0.45
1:E:61:LEU:HD12	1:E:61:LEU:N	2.31	0.45
1:B:210:GLY:O	1:B:214:ALA:HB2	2.16	0.45
1:C:37:THR:OG1	1:C:38:GLN:N	2.49	0.45
1:D:46:ARG:HG3	1:D:46:ARG:NH1	2.31	0.45
1:B:146:ARG:NH2	1:F:500:PHE:CE1	2.83	0.45
1:A:37:THR:OG1	1:A:38:GLN:N	2.49	0.45
1:D:11:LYS:O	1:D:14:GLU:HB2	2.16	0.45
1:F:355:GLN:NE2	1:F:358:LYS:HD2	2.32	0.45
1:B:355:GLN:NE2	1:B:358:LYS:HD2	2.32	0.45
1:F:75:ILE:CD1	1:F:129:VAL:HG13	2.45	0.45
1:F:37:THR:OG1	1:F:38:GLN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ARG:HH11	1:F:46:ARG:HG3	1.80	0.45
1:E:355:GLN:NE2	1:E:358:LYS:HD2	2.32	0.45
1:C:78:TYR:CE2	1:C:101:VAL:HG22	2.52	0.45
1:B:339:VAL:H	1:B:363:ARG:NH2	2.13	0.45
1:C:38:GLN:O	1:C:38:GLN:HG2	2.17	0.45
1:A:210:GLY:O	1:A:214:ALA:HB2	2.16	0.45
1:D:37:THR:OG1	1:D:38:GLN:N	2.49	0.45
1:B:424:HIS:CG	1:B:425:GLY:N	2.83	0.45
1:F:148:PHE:O	1:F:152:LEU:HG	2.17	0.45
1:B:75:ILE:HD13	1:B:129:VAL:CG1	2.45	0.44
1:B:281:TRP:O	1:B:307:ALA:HB1	2.16	0.44
1:F:38:GLN:HG2	1:F:38:GLN:O	2.17	0.44
1:D:78:TYR:CE2	1:D:101:VAL:HG22	2.52	0.44
1:D:210:GLY:O	1:D:214:ALA:HB2	2.16	0.44
1:A:35:ARG:HD2	1:A:35:ARG:HA	1.90	0.44
1:F:78:TYR:CE2	1:F:101:VAL:HG22	2.52	0.44
1:A:75:ILE:HD13	1:A:129:VAL:CG1	2.45	0.44
1:A:370:ASP:OD1	1:A:371:LEU:N	2.51	0.44
1:D:424:HIS:CG	1:D:425:GLY:N	2.83	0.44
1:B:61:LEU:HD12	1:B:61:LEU:N	2.31	0.44
1:C:296:LEU:HD13	1:C:296:LEU:O	2.18	0.44
1:D:75:ILE:HD13	1:D:129:VAL:CG1	2.45	0.44
1:E:3:ARG:HA	1:E:3:ARG:HD3	1.83	0.44
1:D:25:GLU:O	1:D:29:VAL:HG23	2.18	0.44
1:A:148:PHE:O	1:A:152:LEU:HG	2.17	0.44
1:B:148:PHE:O	1:B:152:LEU:HG	2.17	0.44
1:A:355:GLN:NE2	1:A:358:LYS:HD2	2.32	0.44
1:E:148:PHE:O	1:E:152:LEU:HG	2.17	0.44
1:E:296:LEU:HD13	1:E:296:LEU:O	2.18	0.44
1:C:361:LEU:HA	1:C:361:LEU:HD23	1.88	0.44
1:C:262:TYR:OH	4:C:565:GTP:O2G	2.33	0.44
1:D:355:GLN:NE2	1:D:358:LYS:HD2	2.32	0.44
1:D:370:ASP:OD1	1:D:371:LEU:N	2.51	0.44
1:D:270:CYS:O	1:D:285:GLY:HA2	2.16	0.44
1:B:38:GLN:HG2	1:B:38:GLN:O	2.17	0.44
1:B:25:GLU:O	1:B:29:VAL:HG23	2.18	0.44
1:D:214:ALA:HB1	1:D:380:VAL:HG21	2.00	0.44
1:F:61:LEU:N	1:F:61:LEU:HD12	2.31	0.44
1:B:370:ASP:OD1	1:B:371:LEU:N	2.50	0.44
1:E:65:ILE:HG22	1:E:73:GLU:O	2.18	0.44
1:B:132:ASN:HD21	1:B:134:LYS:HB2	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:HB1	1:B:380:VAL:HG21	2.00	0.44
1:F:370:ASP:OD1	1:F:371:LEU:N	2.51	0.44
1:F:296:LEU:HD13	1:F:296:LEU:O	2.18	0.44
1:B:75:ILE:CD1	1:B:129:VAL:HG13	2.45	0.44
1:A:38:GLN:O	1:A:38:GLN:HG2	2.17	0.44
1:F:25:GLU:O	1:F:29:VAL:HG23	2.18	0.44
1:C:370:ASP:OD1	1:C:371:LEU:N	2.51	0.44
1:D:109:SER:HA	1:D:112:THR:CG2	2.48	0.44
1:D:65:ILE:HG22	1:D:73:GLU:O	2.18	0.44
1:D:262:TYR:OH	4:D:566:GTP:O2G	2.33	0.44
1:A:63:PHE:CE2	1:A:75:ILE:HD11	2.53	0.44
1:C:63:PHE:CE2	1:C:75:ILE:HD11	2.53	0.44
1:C:280:ILE:HG12	1:C:307:ALA:HB3	2.00	0.44
1:C:25:GLU:O	1:C:29:VAL:HG23	2.18	0.44
1:C:409:LEU:HD13	1:D:409:LEU:HD11	1.99	0.44
1:A:78:TYR:CE2	1:A:101:VAL:HG22	2.52	0.44
1:C:26:ASP:HB2	1:C:42:ARG:HH22	1.83	0.44
1:D:296:LEU:HD13	1:D:296:LEU:O	2.18	0.44
1:A:296:LEU:O	1:A:296:LEU:HD13	2.18	0.44
1:B:296:LEU:O	1:B:296:LEU:HD13	2.18	0.44
1:F:109:SER:HA	1:F:112:THR:CG2	2.48	0.43
1:F:65:ILE:HG22	1:F:73:GLU:O	2.18	0.43
1:B:280:ILE:HG12	1:B:307:ALA:HB3	2.00	0.43
1:B:230:ALA:HB2	1:B:240:PRO:HG3	2.00	0.43
1:C:162:VAL:HG11	1:D:190:TYR:CE2	2.53	0.43
1:A:445:GLU:O	1:A:449:VAL:HG23	2.18	0.43
1:D:148:PHE:O	1:D:152:LEU:HG	2.17	0.43
1:D:26:ASP:HB2	1:D:42:ARG:HH22	1.83	0.43
1:A:500:PHE:CE1	1:F:146:ARG:NH2	2.86	0.43
1:D:346:GLU:OE2	1:D:369:PRO:HA	2.18	0.43
1:E:63:PHE:CE2	1:E:75:ILE:HD11	2.53	0.43
1:A:280:ILE:HG12	1:A:307:ALA:HB3	2.00	0.43
1:A:339:VAL:H	1:A:363:ARG:NH2	2.13	0.43
1:B:38:GLN:OE1	1:B:40:GLN:HB3	2.18	0.43
1:A:38:GLN:OE1	1:A:40:GLN:HB3	2.19	0.43
1:E:78:TYR:CE2	1:E:101:VAL:HG22	2.52	0.43
1:C:355:GLN:NE2	1:C:358:LYS:HD2	2.32	0.43
1:B:287:ASP:HA	1:B:288:PRO:HD3	1.86	0.43
1:A:305:PRO:O	1:A:306:LYS:HD3	2.18	0.43
1:D:38:GLN:HG2	1:D:38:GLN:O	2.17	0.43
1:F:38:GLN:OE1	1:F:40:GLN:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:445:GLU:O	1:F:449:VAL:HG23	2.18	0.43
1:E:52:ILE:HG12	1:E:493:TYR:CE1	2.53	0.43
1:B:445:GLU:O	1:B:449:VAL:HG23	2.18	0.43
1:A:118:VAL:HG11	1:A:375:ALA:HB1	2.00	0.43
1:C:52:ILE:HG12	1:C:493:TYR:CE1	2.54	0.43
1:B:78:TYR:CE2	1:B:101:VAL:HG22	2.52	0.43
1:B:109:SER:HA	1:B:112:THR:CG2	2.48	0.43
1:C:65:ILE:HG22	1:C:73:GLU:O	2.18	0.43
1:B:412:SER:OG	1:F:432:PRO:HA	2.18	0.43
1:D:445:GLU:O	1:D:449:VAL:HG23	2.18	0.43
1:E:370:ASP:OD1	1:E:371:LEU:N	2.51	0.43
1:F:118:VAL:HG11	1:F:375:ALA:HB1	2.00	0.43
1:E:111:MET:HB3	1:E:111:MET:HE2	1.89	0.43
1:E:109:SER:HA	1:E:112:THR:CG2	2.48	0.43
1:E:346:GLU:OE2	1:E:369:PRO:HA	2.19	0.43
1:C:346:GLU:OE2	1:C:369:PRO:HA	2.19	0.43
1:D:305:PRO:O	1:D:306:LYS:HD3	2.18	0.43
1:E:25:GLU:O	1:E:29:VAL:HG23	2.18	0.43
1:C:445:GLU:O	1:C:449:VAL:HG23	2.18	0.43
1:F:257:LEU:HD12	1:F:257:LEU:O	2.19	0.43
1:E:445:GLU:O	1:E:449:VAL:HG23	2.18	0.43
1:A:109:SER:HA	1:A:112:THR:CG2	2.48	0.43
1:A:346:GLU:OE2	1:A:369:PRO:HA	2.19	0.43
1:C:498:VAL:HG12	1:C:499:THR:N	2.34	0.43
1:C:281:TRP:CZ2	1:C:283:PRO:HG3	2.54	0.43
1:C:305:PRO:O	1:C:306:LYS:HD3	2.18	0.43
1:E:38:GLN:OE1	1:E:40:GLN:HB3	2.19	0.43
1:A:25:GLU:O	1:A:29:VAL:HG23	2.18	0.43
1:C:165:PRO:HB2	1:C:198:VAL:HG23	2.01	0.43
1:B:52:ILE:HG12	1:B:493:TYR:CE1	2.53	0.43
1:E:498:VAL:HG12	1:E:499:THR:N	2.34	0.43
1:D:63:PHE:CE2	1:D:75:ILE:HD11	2.53	0.43
1:F:63:PHE:CE2	1:F:75:ILE:HD11	2.53	0.43
1:A:281:TRP:CZ2	1:A:283:PRO:HG3	2.54	0.43
1:D:280:ILE:HG12	1:D:307:ALA:HB3	2.00	0.43
1:D:38:GLN:OE1	1:D:40:GLN:HB3	2.18	0.43
1:C:118:VAL:HG11	1:C:375:ALA:HB1	2.00	0.43
1:A:52:ILE:HG12	1:A:493:TYR:CE1	2.53	0.43
1:D:162:VAL:HG11	1:E:190:TYR:CD2	2.53	0.43
1:E:215:THR:HG23	3:E:562:NDP:H42N	1.91	0.43
1:B:65:ILE:HG22	1:B:73:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ILE:HG12	1:E:307:ALA:HB3	2.00	0.43
1:F:214:ALA:HB1	1:F:380:VAL:HG21	2.00	0.43
1:C:214:ALA:HB1	1:C:380:VAL:HG21	2.00	0.43
1:D:52:ILE:HG12	1:D:493:TYR:CE1	2.54	0.43
1:D:215:THR:HG23	3:D:561:NDP:H42N	1.91	0.43
1:B:63:PHE:CE2	1:B:75:ILE:HD11	2.53	0.43
1:B:281:TRP:CZ2	1:B:283:PRO:HG3	2.54	0.43
1:F:305:PRO:O	1:F:306:LYS:HD3	2.18	0.43
1:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.54	0.43
1:D:118:VAL:HG11	1:D:375:ALA:HB1	2.00	0.43
1:C:148:PHE:O	1:C:152:LEU:HG	2.17	0.43
1:B:165:PRO:HB2	1:B:198:VAL:HG23	2.01	0.43
1:C:85:GLN:HB3	1:C:85:GLN:HE21	1.56	0.43
1:B:118:VAL:HG11	1:B:375:ALA:HB1	2.00	0.43
1:B:498:VAL:HG12	1:B:499:THR:N	2.34	0.43
1:F:346:GLU:OE2	1:F:369:PRO:HA	2.19	0.43
1:A:65:ILE:HG22	1:A:73:GLU:O	2.18	0.43
1:F:280:ILE:HG12	1:F:307:ALA:HB3	2.00	0.43
1:F:281:TRP:CZ2	1:F:283:PRO:HG3	2.54	0.43
1:E:305:PRO:O	1:E:306:LYS:HD3	2.18	0.43
1:D:498:VAL:HG12	1:D:499:THR:N	2.34	0.43
1:E:38:GLN:HG2	1:E:38:GLN:O	2.17	0.43
1:E:214:ALA:HB1	1:E:380:VAL:HG21	2.00	0.43
1:A:214:ALA:HB1	1:A:380:VAL:HG21	2.00	0.43
1:F:52:ILE:HG12	1:F:493:TYR:CE1	2.53	0.43
1:F:498:VAL:HG12	1:F:499:THR:N	2.34	0.42
1:D:382:TYR:OH	1:E:392:VAL:HG12	2.19	0.42
1:B:361:LEU:HD23	1:B:361:LEU:HA	1.88	0.42
1:D:165:PRO:HB2	1:D:198:VAL:HG23	2.01	0.42
1:C:109:SER:HA	1:C:112:THR:CG2	2.48	0.42
1:B:346:GLU:OE2	1:B:369:PRO:HA	2.19	0.42
1:A:230:ALA:HB2	1:A:240:PRO:HG3	2.00	0.42
1:E:26:ASP:HB2	1:E:42:ARG:HH22	1.83	0.42
1:A:26:ASP:HB2	1:A:42:ARG:HH22	1.83	0.42
1:D:230:ALA:HB2	1:D:240:PRO:HG3	2.00	0.42
1:B:340:LYS:H	1:B:363:ARG:HH22	1.68	0.42
1:E:118:VAL:HG11	1:E:375:ALA:HB1	2.00	0.42
1:E:257:LEU:O	1:E:257:LEU:HD12	2.19	0.42
1:E:281:TRP:CZ2	1:E:283:PRO:HG3	2.54	0.42
1:F:230:ALA:HB2	1:F:240:PRO:HG3	2.00	0.42
1:A:211:ARG:HH11	1:A:381:SER:HG	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HD12	1:A:257:LEU:O	2.19	0.42
1:A:75:ILE:CD1	1:A:129:VAL:HG13	2.45	0.42
1:A:63:PHE:CD1	1:A:147:ARG:HG3	2.55	0.42
1:B:305:PRO:O	1:B:306:LYS:HD3	2.18	0.42
1:F:281:TRP:HB2	1:F:310:TYR:HB2	2.02	0.42
1:C:230:ALA:HB2	1:C:240:PRO:HG3	2.00	0.42
1:D:340:LYS:H	1:D:363:ARG:HH22	1.68	0.42
1:D:494:ASN:HB3	1:D:495:GLU:OE1	2.19	0.42
1:A:85:GLN:HB3	1:A:85:GLN:HE21	1.56	0.42
1:E:361:LEU:HD23	1:E:361:LEU:HA	1.88	0.42
1:B:257:LEU:HD12	1:B:257:LEU:O	2.19	0.42
1:D:257:LEU:O	1:D:257:LEU:HD12	2.19	0.42
1:C:38:GLN:OE1	1:C:40:GLN:HB3	2.19	0.42
1:F:26:ASP:HB2	1:F:42:ARG:HH22	1.83	0.42
1:A:165:PRO:HB2	1:A:198:VAL:HG23	2.01	0.42
1:E:494:ASN:HB3	1:E:495:GLU:OE1	2.19	0.42
1:A:498:VAL:HG12	1:A:499:THR:N	2.34	0.42
1:C:75:ILE:HD13	1:C:129:VAL:CG1	2.45	0.42
1:E:262:TYR:OH	4:E:567:GTP:O2G	2.33	0.42
1:B:213:SER:HB3	1:B:258:HIS:CD2	2.55	0.42
1:B:417:LEU:HD21	1:F:417:LEU:CD1	2.50	0.42
1:B:26:ASP:HB2	1:B:42:ARG:HH22	1.83	0.42
1:A:111:MET:SD	2:A:550:GLU:O	2.78	0.42
1:F:111:MET:SD	2:F:558:GLU:O	2.78	0.42
1:C:213:SER:HB3	1:C:258:HIS:CD2	2.55	0.42
1:B:494:ASN:HB3	1:B:495:GLU:OE1	2.19	0.42
1:C:382:TYR:OH	1:D:392:VAL:HG12	2.20	0.42
1:C:111:MET:SD	2:C:555:GLU:O	2.78	0.42
1:E:111:MET:SD	2:E:557:GLU:O	2.78	0.42
1:A:213:SER:HB3	1:A:258:HIS:CD2	2.55	0.42
1:F:418:GLU:OE2	1:F:427:THR:HG22	2.20	0.42
1:D:96:SER:O	1:D:99:VAL:CG1	2.68	0.42
1:E:165:PRO:HB2	1:E:198:VAL:HG23	2.01	0.42
1:C:257:LEU:O	1:C:257:LEU:HD12	2.19	0.42
1:B:111:MET:SD	2:B:554:GLU:O	2.78	0.42
1:F:63:PHE:CD1	1:F:147:ARG:HG3	2.55	0.42
1:C:3:ARG:HA	1:C:3:ARG:HD3	1.83	0.42
1:B:96:SER:O	1:B:99:VAL:CG1	2.68	0.42
1:F:494:ASN:HB3	1:F:495:GLU:OE1	2.19	0.42
1:D:63:PHE:CD1	1:D:147:ARG:HG3	2.55	0.41
1:E:213:SER:HB3	1:E:258:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:TYR:OH	4:B:564:GTP:O2G	2.33	0.41
1:E:280:ILE:HD13	1:E:280:ILE:HG21	1.84	0.41
1:F:340:LYS:H	1:F:363:ARG:HH22	1.68	0.41
1:F:96:SER:O	1:F:99:VAL:CG1	2.68	0.41
1:A:418:GLU:OE2	1:A:427:THR:HG22	2.20	0.41
1:F:165:PRO:HB2	1:F:198:VAL:HG23	2.01	0.41
1:D:111:MET:HE2	1:D:111:MET:HB3	1.95	0.41
1:C:494:ASN:HB3	1:C:495:GLU:OE1	2.19	0.41
1:C:75:ILE:CD1	1:C:129:VAL:HG13	2.45	0.41
1:A:340:LYS:H	1:A:363:ARG:HH22	1.68	0.41
1:B:35:ARG:HD2	1:B:35:ARG:HA	1.90	0.41
1:E:60:SER:C	1:E:61:LEU:HD12	2.41	0.41
1:B:192:ILE:HD11	1:F:389:LEU:HD11	2.02	0.41
1:E:12:MET:SD	1:E:353:THR:HG22	2.61	0.41
1:D:66:ARG:NH1	1:D:70:GLY:O	2.53	0.41
1:C:66:ARG:NH1	1:C:70:GLY:O	2.53	0.41
1:B:63:PHE:CD1	1:B:147:ARG:HG3	2.55	0.41
1:D:196:ALA:HB2	1:D:388:ASN:HB3	2.02	0.41
1:A:60:SER:C	1:A:61:LEU:HD12	2.41	0.41
1:E:494:ASN:HD22	1:E:494:ASN:HA	1.70	0.41
1:D:12:MET:SD	1:D:353:THR:HG22	2.61	0.41
1:A:494:ASN:HB3	1:A:495:GLU:OE1	2.19	0.41
1:C:495:GLU:C	1:D:205:GLN:HE22	2.24	0.41
1:A:162:VAL:HG11	1:F:190:TYR:CE2	2.55	0.41
1:D:60:SER:C	1:D:61:LEU:HD12	2.41	0.41
1:C:108:ALA:O	1:C:112:THR:HG22	2.21	0.41
1:E:108:ALA:O	1:E:112:THR:HG22	2.21	0.41
1:E:66:ARG:NH1	1:E:70:GLY:O	2.53	0.41
1:C:63:PHE:CD1	1:C:147:ARG:HG3	2.55	0.41
1:E:431:VAL:HA	1:E:432:PRO:HD3	1.96	0.41
1:E:230:ALA:HB2	1:E:240:PRO:HG3	2.00	0.41
1:C:96:SER:O	1:C:99:VAL:CG1	2.68	0.41
1:C:60:SER:C	1:C:61:LEU:HD12	2.41	0.41
1:C:181:ASP:OD2	1:E:499:THR:O	2.38	0.41
1:F:213:SER:HB3	1:F:258:HIS:CD2	2.55	0.41
1:B:196:ALA:HB2	1:B:388:ASN:HB3	2.02	0.41
1:A:196:ALA:HB2	1:A:388:ASN:HB3	2.03	0.41
1:E:267:GLY:O	1:E:268:ALA:C	2.59	0.41
1:B:427:THR:C	1:B:429:PRO:HD3	2.41	0.41
1:D:427:THR:C	1:D:429:PRO:HD3	2.41	0.41
1:F:12:MET:SD	1:F:353:THR:HG22	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:MET:SD	1:A:353:THR:HG22	2.61	0.41
1:F:168:ASN:OD1	3:F:563:NDP:O2D	2.39	0.41
1:D:111:MET:SD	2:D:556:GLU:O	2.78	0.41
1:D:213:SER:HB3	1:D:258:HIS:CD2	2.55	0.41
1:B:75:ILE:C	1:B:75:ILE:HD12	2.41	0.41
1:E:85:GLN:HB3	1:E:85:GLN:HE21	1.56	0.41
1:F:168:ASN:ND2	1:F:169:MET:N	2.53	0.41
1:F:75:ILE:C	1:F:75:ILE:HD12	2.41	0.41
1:B:3:ARG:HD3	1:B:3:ARG:HA	1.83	0.41
1:C:196:ALA:HB2	1:C:388:ASN:HB3	2.02	0.41
1:C:410:LEU:HG	1:C:430:ILE:HG22	2.03	0.41
1:A:410:LEU:HG	1:A:430:ILE:HG22	2.03	0.41
1:E:130:LYS:HE3	1:E:130:LYS:HB2	1.82	0.41
1:B:418:GLU:OE2	1:B:427:THR:HG22	2.20	0.41
1:D:418:GLU:OE2	1:D:427:THR:HG22	2.20	0.41
1:F:60:SER:C	1:F:61:LEU:HD12	2.41	0.41
1:A:209:HIS:C	1:A:209:HIS:CD2	2.94	0.41
1:D:108:ALA:O	1:D:112:THR:HG22	2.21	0.41
1:D:496:ALA:N	1:E:205:GLN:NE2	2.63	0.41
1:E:63:PHE:CD1	1:E:147:ARG:HG3	2.55	0.41
1:D:233:MET:HE1	1:D:236:LEU:HD12	2.03	0.41
1:A:96:SER:O	1:A:99:VAL:CG1	2.68	0.41
1:E:96:SER:O	1:E:99:VAL:CG1	2.68	0.41
1:E:418:GLU:OE2	1:E:427:THR:HG22	2.20	0.41
1:E:427:THR:C	1:E:429:PRO:HD3	2.41	0.41
1:D:103:GLU:HG2	1:D:107:LEU:HD22	2.03	0.41
1:F:494:ASN:HD22	1:F:494:ASN:HA	1.70	0.41
1:B:12:MET:SD	1:B:353:THR:HG22	2.61	0.41
1:C:12:MET:SD	1:C:353:THR:HG22	2.61	0.41
1:D:209:HIS:CD2	1:D:209:HIS:C	2.94	0.41
1:C:211:ARG:HH11	1:C:381:SER:HG	1.69	0.41
1:F:66:ARG:NH1	1:F:70:GLY:O	2.53	0.41
1:D:75:ILE:C	1:D:75:ILE:HD12	2.41	0.41
1:C:418:GLU:OE2	1:C:427:THR:HG22	2.20	0.41
1:C:59:LEU:O	1:C:78:TYR:HA	2.21	0.41
1:B:60:SER:C	1:B:61:LEU:HD12	2.41	0.41
1:B:118:VAL:HG13	1:B:120:VAL:HG23	2.03	0.41
1:F:209:HIS:C	1:F:209:HIS:CD2	2.94	0.41
1:E:94:ARG:HE	1:E:168:ASN:ND2	2.20	0.40
1:E:168:ASN:OD1	3:E:562:NDP:O2D	2.39	0.40
1:B:108:ALA:O	1:B:112:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:VAL:HG13	1:F:386:LEU:HD21	1.96	0.40
1:D:75:ILE:CD1	1:D:129:VAL:HG13	2.45	0.40
1:A:108:ALA:O	1:A:112:THR:HG22	2.21	0.40
1:E:75:ILE:C	1:E:75:ILE:HD12	2.41	0.40
1:C:281:TRP:HB2	1:C:310:TYR:HB2	2.02	0.40
1:E:196:ALA:HB2	1:E:388:ASN:HB3	2.02	0.40
1:B:132:ASN:ND2	1:B:134:LYS:H	2.20	0.40
1:D:410:LEU:HG	1:D:430:ILE:HG22	2.03	0.40
1:F:267:GLY:O	1:F:268:ALA:C	2.59	0.40
1:D:35:ARG:HA	1:D:35:ARG:HD2	1.90	0.40
1:B:103:GLU:HG2	1:B:107:LEU:HD22	2.03	0.40
1:D:373:LEU:HA	1:D:373:LEU:HD23	1.92	0.40
1:F:94:ARG:HE	1:F:168:ASN:ND2	2.20	0.40
1:A:66:ARG:NH1	1:A:70:GLY:O	2.53	0.40
1:E:340:LYS:H	1:E:363:ARG:HH22	1.68	0.40
1:A:103:GLU:HG2	1:A:107:LEU:HD22	2.03	0.40
1:B:32:LEU:HB2	1:B:41:LYS:HD3	2.04	0.40
1:D:118:VAL:HG13	1:D:120:VAL:HG23	2.03	0.40
1:A:439:ARG:HB3	1:F:405:SER:OG	2.22	0.40
1:F:410:LEU:HA	1:F:410:LEU:HD12	1.97	0.40
1:C:209:HIS:CD2	1:C:209:HIS:C	2.94	0.40
3:A:551:NDP:C2D	3:A:551:NDP:O5D	2.70	0.40
1:C:168:ASN:OD1	3:C:560:NDP:O2D	2.39	0.40
3:C:560:NDP:C2D	3:C:560:NDP:O5D	2.70	0.40
3:E:562:NDP:O5D	3:E:562:NDP:C2D	2.70	0.40
1:E:287:ASP:HA	1:E:288:PRO:HD3	1.86	0.40
1:A:132:ASN:ND2	1:A:134:LYS:H	2.20	0.40
1:A:205:GLN:NE2	1:B:495:GLU:HB2	2.36	0.40
1:E:227:ILE:HD11	1:E:245:LYS:HD2	2.04	0.40
1:C:32:LEU:HB2	1:C:41:LYS:HD3	2.04	0.40
1:F:103:GLU:HG2	1:F:107:LEU:HD22	2.03	0.40
1:B:209:HIS:C	1:B:209:HIS:CD2	2.94	0.40
1:A:215:THR:HG23	3:A:551:NDP:H42N	1.91	0.40
1:E:24:VAL:HG11	1:E:487:GLU:HG3	2.04	0.40
1:F:132:ASN:ND2	1:F:134:LYS:H	2.19	0.40
1:F:427:THR:C	1:F:429:PRO:HD3	2.41	0.40
1:F:32:LEU:HB2	1:F:41:LYS:HD3	2.04	0.40
1:F:376:GLY:O	1:F:380:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/501 (100%)	437 (88%)	42 (8%)	20 (4%)	4	12
1	B	499/501 (100%)	436 (87%)	43 (9%)	20 (4%)	4	12
1	C	499/501 (100%)	437 (88%)	42 (8%)	20 (4%)	4	12
1	D	499/501 (100%)	437 (88%)	42 (8%)	20 (4%)	4	12
1	E	499/501 (100%)	437 (88%)	42 (8%)	20 (4%)	4	12
1	F	499/501 (100%)	437 (88%)	42 (8%)	20 (4%)	4	12
All	All	2994/3006 (100%)	2621 (88%)	253 (8%)	120 (4%)	4	12

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	35	ARG
1	A	38	GLN
1	A	54	PRO
1	A	55	CYS
1	A	231	SER
1	A	243	GLY
1	A	338	ARG
1	A	422	GLY
1	B	5	ASP
1	B	35	ARG
1	B	38	GLN
1	B	54	PRO
1	B	55	CYS
1	B	231	SER
1	B	243	GLY
1	B	338	ARG
1	B	422	GLY
1	C	5	ASP
1	C	35	ARG

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Mol	Chain	Res	Type
1	C	38	GLN
1	C	54	PRO
1	C	55	CYS
1	C	231	SER
1	C	243	GLY
1	C	338	ARG
1	C	422	GLY
1	D	5	ASP
1	D	35	ARG
1	D	38	GLN
1	D	54	PRO
1	D	55	CYS
1	D	231	SER
1	D	243	GLY
1	D	338	ARG
1	D	422	GLY
1	E	5	ASP
1	E	35	ARG
1	E	38	GLN
1	E	54	PRO
1	E	55	CYS
1	E	231	SER
1	E	243	GLY
1	E	338	ARG
1	E	422	GLY
1	F	5	ASP
1	F	35	ARG
1	F	38	GLN
1	F	54	PRO
1	F	55	CYS
1	F	231	SER
1	F	243	GLY
1	F	338	ARG
1	F	422	GLY
1	A	71	SER
1	A	87	THR
1	A	130	LYS
1	A	306	LYS
1	B	71	SER
1	B	87	THR
1	B	130	LYS
1	B	306	LYS

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Mol	Chain	Res	Type
1	C	71	SER
1	C	87	THR
1	C	130	LYS
1	C	306	LYS
1	D	71	SER
1	D	87	THR
1	D	130	LYS
1	D	306	LYS
1	E	71	SER
1	E	87	THR
1	E	130	LYS
1	E	306	LYS
1	F	71	SER
1	F	87	THR
1	F	130	LYS
1	F	306	LYS
1	A	70	GLY
1	A	268	ALA
1	B	70	GLY
1	B	268	ALA
1	C	70	GLY
1	C	268	ALA
1	D	70	GLY
1	D	268	ALA
1	E	70	GLY
1	E	268	ALA
1	F	70	GLY
1	F	268	ALA
1	A	498	VAL
1	B	498	VAL
1	C	498	VAL
1	D	498	VAL
1	E	498	VAL
1	F	498	VAL
1	A	69	ASP
1	B	69	ASP
1	C	69	ASP
1	D	69	ASP
1	E	69	ASP
1	F	69	ASP
1	A	309	ILE
1	A	312	GLY

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Mol	Chain	Res	Type
1	B	309	ILE
1	B	312	GLY
1	C	309	ILE
1	C	312	GLY
1	D	309	ILE
1	D	312	GLY
1	E	309	ILE
1	E	312	GLY
1	F	309	ILE
1	F	312	GLY
1	A	240	PRO
1	B	240	PRO
1	C	240	PRO
1	D	240	PRO
1	E	240	PRO
1	F	240	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/417 (100%)	341 (82%)	76 (18%)	2	6
1	B	417/417 (100%)	341 (82%)	76 (18%)	2	6
1	C	417/417 (100%)	341 (82%)	76 (18%)	2	6
1	D	417/417 (100%)	341 (82%)	76 (18%)	2	6
1	E	417/417 (100%)	341 (82%)	76 (18%)	2	6
1	F	417/417 (100%)	341 (82%)	76 (18%)	2	6
All	All	2502/2502 (100%)	2046 (82%)	456 (18%)	2	6

All (456) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	4	GLU

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Mol	Chain	Res	Type
1	A	6	ASP
1	A	9	PHE
1	A	19	ARG
1	A	24	VAL
1	A	25	GLU
1	A	27	LYS
1	A	30	GLU
1	A	37	THR
1	A	38	GLN
1	A	41	LYS
1	A	44	ARG
1	A	46	ARG
1	A	53	LYS
1	A	54	PRO
1	A	55	CYS
1	A	56	ASN
1	A	65	ILE
1	A	66	ARG
1	A	71	SER
1	A	75	ILE
1	A	83	SER
1	A	85	GLN
1	A	90	LYS
1	A	96	SER
1	A	99	VAL
1	A	107	LEU
1	A	112	THR
1	A	118	VAL
1	A	132	ASN
1	A	145	THR
1	A	170	SER
1	A	211	ARG
1	A	229	ASN
1	A	231	SER
1	A	271	VAL
1	A	291	LEU
1	A	296	LEU
1	A	306	LYS
1	A	311	GLU
1	A	313	SER
1	A	317	VAL
1	A	318	ASP

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Mol	Chain	Res	Type
1	A	329	LYS
1	A	331	LEU
1	A	334	SER
1	A	340	LYS
1	A	342	LYS
1	A	352	THR
1	A	361	LEU
1	A	373	LEU
1	A	378	VAL
1	A	381	SER
1	A	385	ILE
1	A	386	LEU
1	A	393	SER
1	A	405	SER
1	A	410	LEU
1	A	413	VAL
1	A	416	SER
1	A	419	ARG
1	A	420	LYS
1	A	424	HIS
1	A	427	THR
1	A	430	ILE
1	A	431	VAL
1	A	440	ILE
1	A	448	ILE
1	A	456	THR
1	A	459	ARG
1	A	466	ARG
1	A	472	ASN
1	A	487	GLU
1	A	494	ASN
1	A	500	PHE
1	B	2	ASP
1	B	4	GLU
1	B	6	ASP
1	B	9	PHE
1	B	19	ARG
1	B	24	VAL
1	B	25	GLU
1	B	27	LYS
1	B	30	GLU
1	B	37	THR

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Mol	Chain	Res	Type
1	B	38	GLN
1	B	41	LYS
1	B	44	ARG
1	B	46	ARG
1	B	53	LYS
1	B	54	PRO
1	B	55	CYS
1	B	56	ASN
1	B	65	ILE
1	B	66	ARG
1	B	71	SER
1	B	75	ILE
1	B	83	SER
1	B	85	GLN
1	B	90	LYS
1	B	96	SER
1	B	99	VAL
1	B	107	LEU
1	B	112	THR
1	B	118	VAL
1	B	132	ASN
1	B	145	THR
1	B	170	SER
1	B	211	ARG
1	B	229	ASN
1	B	231	SER
1	B	271	VAL
1	B	291	LEU
1	B	296	LEU
1	B	306	LYS
1	B	311	GLU
1	B	313	SER
1	B	317	VAL
1	B	318	ASP
1	B	329	LYS
1	B	331	LEU
1	B	334	SER
1	B	340	LYS
1	B	342	LYS
1	B	352	THR
1	B	361	LEU
1	B	373	LEU

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Mol	Chain	Res	Type
1	B	378	VAL
1	B	381	SER
1	B	385	ILE
1	B	386	LEU
1	B	393	SER
1	B	405	SER
1	B	410	LEU
1	B	413	VAL
1	B	416	SER
1	B	419	ARG
1	B	420	LYS
1	B	424	HIS
1	B	427	THR
1	B	430	ILE
1	B	431	VAL
1	B	440	ILE
1	B	448	ILE
1	B	456	THR
1	B	459	ARG
1	B	466	ARG
1	B	472	ASN
1	B	487	GLU
1	B	494	ASN
1	B	500	PHE
1	C	2	ASP
1	C	4	GLU
1	C	6	ASP
1	C	9	PHE
1	C	19	ARG
1	C	24	VAL
1	C	25	GLU
1	C	27	LYS
1	C	30	GLU
1	C	37	THR
1	C	38	GLN
1	C	41	LYS
1	C	44	ARG
1	C	46	ARG
1	C	53	LYS
1	C	54	PRO
1	C	55	CYS
1	C	56	ASN

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Mol	Chain	Res	Type
1	C	65	ILE
1	C	66	ARG
1	C	71	SER
1	C	75	ILE
1	C	83	SER
1	C	85	GLN
1	C	90	LYS
1	C	96	SER
1	C	99	VAL
1	C	107	LEU
1	C	112	THR
1	C	118	VAL
1	C	132	ASN
1	C	145	THR
1	C	170	SER
1	C	211	ARG
1	C	229	ASN
1	C	231	SER
1	C	271	VAL
1	C	291	LEU
1	C	296	LEU
1	C	306	LYS
1	C	311	GLU
1	C	313	SER
1	C	317	VAL
1	C	318	ASP
1	C	329	LYS
1	C	331	LEU
1	C	334	SER
1	C	340	LYS
1	C	342	LYS
1	C	352	THR
1	C	361	LEU
1	C	373	LEU
1	C	378	VAL
1	C	381	SER
1	C	385	ILE
1	C	386	LEU
1	C	393	SER
1	C	405	SER
1	C	410	LEU
1	C	413	VAL

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Mol	Chain	Res	Type
1	C	416	SER
1	C	419	ARG
1	C	420	LYS
1	C	424	HIS
1	C	427	THR
1	C	430	ILE
1	C	431	VAL
1	C	440	ILE
1	C	448	ILE
1	C	456	THR
1	C	459	ARG
1	C	466	ARG
1	C	472	ASN
1	C	487	GLU
1	C	494	ASN
1	C	500	PHE
1	D	2	ASP
1	D	4	GLU
1	D	6	ASP
1	D	9	PHE
1	D	19	ARG
1	D	24	VAL
1	D	25	GLU
1	D	27	LYS
1	D	30	GLU
1	D	37	THR
1	D	38	GLN
1	D	41	LYS
1	D	44	ARG
1	D	46	ARG
1	D	53	LYS
1	D	54	PRO
1	D	55	CYS
1	D	56	ASN
1	D	65	ILE
1	D	66	ARG
1	D	71	SER
1	D	75	ILE
1	D	83	SER
1	D	85	GLN
1	D	90	LYS
1	D	96	SER

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Mol	Chain	Res	Type
1	D	99	VAL
1	D	107	LEU
1	D	112	THR
1	D	118	VAL
1	D	132	ASN
1	D	145	THR
1	D	170	SER
1	D	211	ARG
1	D	229	ASN
1	D	231	SER
1	D	271	VAL
1	D	291	LEU
1	D	296	LEU
1	D	306	LYS
1	D	311	GLU
1	D	313	SER
1	D	317	VAL
1	D	318	ASP
1	D	329	LYS
1	D	331	LEU
1	D	334	SER
1	D	340	LYS
1	D	342	LYS
1	D	352	THR
1	D	361	LEU
1	D	373	LEU
1	D	378	VAL
1	D	381	SER
1	D	385	ILE
1	D	386	LEU
1	D	393	SER
1	D	405	SER
1	D	410	LEU
1	D	413	VAL
1	D	416	SER
1	D	419	ARG
1	D	420	LYS
1	D	424	HIS
1	D	427	THR
1	D	430	ILE
1	D	431	VAL
1	D	440	ILE

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Mol	Chain	Res	Type
1	D	448	ILE
1	D	456	THR
1	D	459	ARG
1	D	466	ARG
1	D	472	ASN
1	D	487	GLU
1	D	494	ASN
1	D	500	PHE
1	E	2	ASP
1	E	4	GLU
1	E	6	ASP
1	E	9	PHE
1	E	19	ARG
1	E	24	VAL
1	E	25	GLU
1	E	27	LYS
1	E	30	GLU
1	E	37	THR
1	E	38	GLN
1	E	41	LYS
1	E	44	ARG
1	E	46	ARG
1	E	53	LYS
1	E	54	PRO
1	E	55	CYS
1	E	56	ASN
1	E	65	ILE
1	E	66	ARG
1	E	71	SER
1	E	75	ILE
1	E	83	SER
1	E	85	GLN
1	E	90	LYS
1	E	96	SER
1	E	99	VAL
1	E	107	LEU
1	E	112	THR
1	E	118	VAL
1	E	132	ASN
1	E	145	THR
1	E	170	SER
1	E	211	ARG

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Mol	Chain	Res	Type
1	E	229	ASN
1	E	231	SER
1	E	271	VAL
1	E	291	LEU
1	E	296	LEU
1	E	306	LYS
1	E	311	GLU
1	E	313	SER
1	E	317	VAL
1	E	318	ASP
1	E	329	LYS
1	E	331	LEU
1	E	334	SER
1	E	340	LYS
1	E	342	LYS
1	E	352	THR
1	E	361	LEU
1	E	373	LEU
1	E	378	VAL
1	E	381	SER
1	E	385	ILE
1	E	386	LEU
1	E	393	SER
1	E	405	SER
1	E	410	LEU
1	E	413	VAL
1	E	416	SER
1	E	419	ARG
1	E	420	LYS
1	E	424	HIS
1	E	427	THR
1	E	430	ILE
1	E	431	VAL
1	E	440	ILE
1	E	448	ILE
1	E	456	THR
1	E	459	ARG
1	E	466	ARG
1	E	472	ASN
1	E	487	GLU
1	E	494	ASN
1	E	500	PHE

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Mol	Chain	Res	Type
1	F	2	ASP
1	F	4	GLU
1	F	6	ASP
1	F	9	PHE
1	F	19	ARG
1	F	24	VAL
1	F	25	GLU
1	F	27	LYS
1	F	30	GLU
1	F	37	THR
1	F	38	GLN
1	F	41	LYS
1	F	44	ARG
1	F	46	ARG
1	F	53	LYS
1	F	54	PRO
1	F	55	CYS
1	F	56	ASN
1	F	65	ILE
1	F	66	ARG
1	F	71	SER
1	F	75	ILE
1	F	83	SER
1	F	85	GLN
1	F	90	LYS
1	F	96	SER
1	F	99	VAL
1	F	107	LEU
1	F	112	THR
1	F	118	VAL
1	F	132	ASN
1	F	145	THR
1	F	170	SER
1	F	211	ARG
1	F	229	ASN
1	F	231	SER
1	F	271	VAL
1	F	291	LEU
1	F	296	LEU
1	F	306	LYS
1	F	311	GLU
1	F	313	SER

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Mol	Chain	Res	Type
1	F	317	VAL
1	F	318	ASP
1	F	329	LYS
1	F	331	LEU
1	F	334	SER
1	F	340	LYS
1	F	342	LYS
1	F	352	THR
1	F	361	LEU
1	F	373	LEU
1	F	378	VAL
1	F	381	SER
1	F	385	ILE
1	F	386	LEU
1	F	393	SER
1	F	405	SER
1	F	410	LEU
1	F	413	VAL
1	F	416	SER
1	F	419	ARG
1	F	420	LYS
1	F	424	HIS
1	F	427	THR
1	F	430	ILE
1	F	431	VAL
1	F	440	ILE
1	F	448	ILE
1	F	456	THR
1	F	459	ARG
1	F	466	ARG
1	F	472	ASN
1	F	487	GLU
1	F	494	ASN
1	F	500	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	82	HIS
1	A	85	GLN
1	A	132	ASN

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Mol	Chain	Res	Type
1	A	168	ASN
1	A	209	HIS
1	A	254	ASN
1	A	258	HIS
1	A	330	GLN
1	A	388	ASN
1	A	406	ASN
1	A	437	GLN
1	A	450	HIS
1	A	463	GLN
1	A	494	ASN
1	B	43	ASN
1	B	82	HIS
1	B	85	GLN
1	B	132	ASN
1	B	168	ASN
1	B	209	HIS
1	B	254	ASN
1	B	258	HIS
1	B	330	GLN
1	B	388	ASN
1	B	406	ASN
1	B	437	GLN
1	B	450	HIS
1	B	463	GLN
1	B	494	ASN
1	C	43	ASN
1	C	82	HIS
1	C	85	GLN
1	C	132	ASN
1	C	168	ASN
1	C	189	HIS
1	C	209	HIS
1	C	254	ASN
1	C	258	HIS
1	C	330	GLN
1	C	388	ASN
1	C	406	ASN
1	C	437	GLN
1	C	450	HIS
1	C	463	GLN
1	C	494	ASN

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Mol	Chain	Res	Type
1	D	43	ASN
1	D	82	HIS
1	D	85	GLN
1	D	132	ASN
1	D	168	ASN
1	D	205	GLN
1	D	209	HIS
1	D	254	ASN
1	D	258	HIS
1	D	330	GLN
1	D	388	ASN
1	D	406	ASN
1	D	437	GLN
1	D	450	HIS
1	D	463	GLN
1	D	494	ASN
1	E	43	ASN
1	E	82	HIS
1	E	85	GLN
1	E	132	ASN
1	E	168	ASN
1	E	205	GLN
1	E	209	HIS
1	E	254	ASN
1	E	258	HIS
1	E	330	GLN
1	E	388	ASN
1	E	406	ASN
1	E	437	GLN
1	E	450	HIS
1	E	463	GLN
1	E	494	ASN
1	F	43	ASN
1	F	82	HIS
1	F	85	GLN
1	F	132	ASN
1	F	168	ASN
1	F	209	HIS
1	F	254	ASN
1	F	258	HIS
1	F	330	GLN
1	F	388	ASN

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Mol	Chain	Res	Type
1	F	406	ASN
1	F	437	GLN
1	F	450	HIS
1	F	463	GLN
1	F	494	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GLU	A	550	-	3,9,9	0.68	0	2,11,11	0.42	0
3	NDP	A	551	-	42,52,52	1.98	9 (21%)	55,80,80	2.25	19 (34%)
4	GTP	A	553	-	25,34,34	1.34	2 (8%)	34,54,54	2.34	10 (29%)
2	GLU	B	554	-	3,9,9	0.68	0	2,11,11	0.42	0
3	NDP	B	559	-	42,52,52	1.98	9 (21%)	55,80,80	2.25	19 (34%)
4	GTP	B	564	-	25,34,34	1.34	2 (8%)	34,54,54	2.34	10 (29%)
2	GLU	C	555	-	3,9,9	0.68	0	2,11,11	0.42	0
3	NDP	C	560	-	42,52,52	1.98	9 (21%)	55,80,80	2.25	19 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GTP	C	565	-	25,34,34	1.34	2 (8%)	34,54,54	2.34	10 (29%)
2	GLU	D	556	-	3,9,9	0.67	0	2,11,11	0.42	0
3	NDP	D	561	-	42,52,52	1.98	9 (21%)	55,80,80	2.25	19 (34%)
4	GTP	D	566	-	25,34,34	1.35	3 (12%)	34,54,54	2.34	10 (29%)
2	GLU	E	557	-	3,9,9	0.68	0	2,11,11	0.42	0
3	NDP	E	562	-	42,52,52	1.98	9 (21%)	55,80,80	2.25	19 (34%)
4	GTP	E	567	-	25,34,34	1.35	2 (8%)	34,54,54	2.34	10 (29%)
2	GLU	F	558	-	3,9,9	0.69	0	2,11,11	0.42	0
3	NDP	F	563	-	42,52,52	1.98	9 (21%)	55,80,80	2.25	19 (34%)
4	GTP	F	568	-	25,34,34	1.34	2 (8%)	34,54,54	2.33	10 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	A	550	-	-	0/3/9/9	0/0/0/0
3	NDP	A	551	-	-	0/30/77/77	0/5/5/5
4	GTP	A	553	-	-	0/18/38/38	0/3/3/3
2	GLU	B	554	-	-	0/3/9/9	0/0/0/0
3	NDP	B	559	-	-	0/30/77/77	0/5/5/5
4	GTP	B	564	-	-	0/18/38/38	0/3/3/3
2	GLU	C	555	-	-	0/3/9/9	0/0/0/0
3	NDP	C	560	-	-	0/30/77/77	0/5/5/5
4	GTP	C	565	-	-	0/18/38/38	0/3/3/3
2	GLU	D	556	-	-	0/3/9/9	0/0/0/0
3	NDP	D	561	-	-	0/30/77/77	0/5/5/5
4	GTP	D	566	-	-	0/18/38/38	0/3/3/3
2	GLU	E	557	-	-	0/3/9/9	0/0/0/0
3	NDP	E	562	-	-	0/30/77/77	0/5/5/5
4	GTP	E	567	-	-	0/18/38/38	0/3/3/3
2	GLU	F	558	-	-	0/3/9/9	0/0/0/0
3	NDP	F	563	-	-	0/30/77/77	0/5/5/5
4	GTP	F	568	-	-	0/18/38/38	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	551	NDP	C3B-C2B	-6.14	1.39	1.53
3	D	561	NDP	C3B-C2B	-6.14	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	560	NDP	C3B-C2B	-6.14	1.39	1.53
3	E	562	NDP	C3B-C2B	-6.13	1.39	1.53
3	B	559	NDP	C3B-C2B	-6.12	1.39	1.53
3	F	563	NDP	C3B-C2B	-6.11	1.39	1.53
3	E	562	NDP	C4N-C5N	-4.68	1.39	1.49
3	D	561	NDP	C4N-C5N	-4.67	1.39	1.49
3	A	551	NDP	C4N-C5N	-4.66	1.39	1.49
3	C	560	NDP	C4N-C5N	-4.66	1.39	1.49
3	B	559	NDP	C4N-C5N	-4.64	1.39	1.49
3	F	563	NDP	C4N-C5N	-4.63	1.39	1.49
3	E	562	NDP	P2B-O2X	-2.43	1.46	1.54
3	C	560	NDP	P2B-O2X	-2.42	1.46	1.54
3	B	559	NDP	P2B-O2X	-2.42	1.46	1.54
3	A	551	NDP	P2B-O2X	-2.41	1.46	1.54
3	D	561	NDP	P2B-O2X	-2.41	1.46	1.54
3	F	563	NDP	P2B-O2X	-2.41	1.46	1.54
4	D	566	GTP	O6-C6	-2.00	1.20	1.24
3	C	560	NDP	O4D-C1D	2.10	1.47	1.42
3	F	563	NDP	O4D-C1D	2.10	1.47	1.42
3	A	551	NDP	O4D-C1D	2.10	1.47	1.42
3	E	562	NDP	O4D-C1D	2.10	1.47	1.42
3	D	561	NDP	O4D-C1D	2.10	1.47	1.42
3	B	559	NDP	O4D-C1D	2.11	1.47	1.42
3	B	559	NDP	O2D-C2D	2.18	1.48	1.43
4	C	565	GTP	O4'-C4'	2.19	1.50	1.45
4	D	566	GTP	O4'-C4'	2.19	1.50	1.45
4	A	553	GTP	O4'-C4'	2.20	1.50	1.45
3	C	560	NDP	O2D-C2D	2.20	1.48	1.43
4	F	568	GTP	O4'-C4'	2.20	1.50	1.45
4	E	567	GTP	O4'-C4'	2.21	1.50	1.45
3	A	551	NDP	O2D-C2D	2.21	1.48	1.43
3	E	562	NDP	O2D-C2D	2.22	1.48	1.43
3	F	563	NDP	O2D-C2D	2.22	1.48	1.43
3	D	561	NDP	O2D-C2D	2.22	1.48	1.43
3	B	559	NDP	O4D-C4D	2.23	1.50	1.45
4	B	564	GTP	O4'-C4'	2.23	1.50	1.45
3	D	561	NDP	O4D-C4D	2.23	1.50	1.45
3	F	563	NDP	O4D-C4D	2.23	1.50	1.45
3	A	551	NDP	O4D-C4D	2.25	1.50	1.45
3	C	560	NDP	O4D-C4D	2.26	1.50	1.45
3	E	562	NDP	O4D-C4D	2.27	1.50	1.45
3	B	559	NDP	O4B-C1B	2.84	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	562	NDP	O4B-C1B	2.84	1.44	1.41
3	D	561	NDP	O4B-C1B	2.84	1.44	1.41
3	A	551	NDP	O4B-C1B	2.88	1.44	1.41
3	F	563	NDP	O4B-C1B	2.89	1.44	1.41
3	C	560	NDP	O4B-C1B	2.89	1.44	1.41
4	F	568	GTP	O4'-C1'	2.96	1.44	1.41
4	C	565	GTP	O4'-C1'	2.96	1.44	1.41
4	A	553	GTP	O4'-C1'	2.99	1.45	1.41
4	D	566	GTP	O4'-C1'	2.99	1.45	1.41
4	E	567	GTP	O4'-C1'	3.01	1.45	1.41
4	B	564	GTP	O4'-C1'	3.03	1.45	1.41
3	C	560	NDP	C2N-C3N	4.24	1.45	1.34
3	E	562	NDP	C2N-C3N	4.25	1.45	1.34
3	D	561	NDP	C2N-C3N	4.27	1.45	1.34
3	B	559	NDP	C2N-C3N	4.27	1.45	1.34
3	A	551	NDP	C2N-C3N	4.27	1.45	1.34
3	F	563	NDP	C2N-C3N	4.27	1.45	1.34
3	C	560	NDP	O4B-C4B	5.04	1.56	1.45
3	E	562	NDP	O4B-C4B	5.05	1.56	1.45
3	B	559	NDP	O4B-C4B	5.05	1.56	1.45
3	A	551	NDP	O4B-C4B	5.05	1.56	1.45
3	D	561	NDP	O4B-C4B	5.07	1.56	1.45
3	F	563	NDP	O4B-C4B	5.08	1.56	1.45

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	567	GTP	C5-C6-N1	-7.56	113.26	123.59
4	D	566	GTP	C5-C6-N1	-7.54	113.28	123.59
4	C	565	GTP	C5-C6-N1	-7.54	113.28	123.59
4	A	553	GTP	C5-C6-N1	-7.52	113.30	123.59
4	B	564	GTP	C5-C6-N1	-7.51	113.31	123.59
4	F	568	GTP	C5-C6-N1	-7.49	113.35	123.59
3	E	562	NDP	N3A-C2A-N1A	-5.75	124.49	128.89
3	A	551	NDP	N3A-C2A-N1A	-5.74	124.50	128.89
3	F	563	NDP	N3A-C2A-N1A	-5.73	124.50	128.89
3	C	560	NDP	N3A-C2A-N1A	-5.72	124.51	128.89
3	B	559	NDP	N3A-C2A-N1A	-5.70	124.53	128.89
3	D	561	NDP	N3A-C2A-N1A	-5.70	124.53	128.89
3	F	563	NDP	C3N-C2N-N1N	-5.37	115.45	123.14
3	C	560	NDP	C3N-C2N-N1N	-5.37	115.45	123.14
3	B	559	NDP	C3N-C2N-N1N	-5.35	115.48	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	551	NDP	C3N-C2N-N1N	-5.35	115.48	123.14
3	D	561	NDP	C3N-C2N-N1N	-5.33	115.50	123.14
3	E	562	NDP	C3N-C2N-N1N	-5.33	115.50	123.14
3	E	562	NDP	O4B-C4B-C3B	-5.07	94.93	105.15
3	D	561	NDP	O4B-C4B-C3B	-5.05	94.98	105.15
3	A	551	NDP	O4B-C4B-C3B	-5.05	94.98	105.15
3	B	559	NDP	O4B-C4B-C3B	-5.03	95.01	105.15
3	F	563	NDP	O4B-C4B-C3B	-5.03	95.01	105.15
3	C	560	NDP	O4B-C4B-C3B	-5.02	95.02	105.15
3	E	562	NDP	O4D-C4D-C3D	-4.84	95.40	105.15
3	D	561	NDP	O4D-C4D-C3D	-4.83	95.41	105.15
3	B	559	NDP	O4D-C4D-C3D	-4.83	95.42	105.15
3	C	560	NDP	O4D-C4D-C3D	-4.83	95.42	105.15
3	A	551	NDP	O4D-C4D-C3D	-4.82	95.43	105.15
3	F	563	NDP	O4D-C4D-C3D	-4.82	95.44	105.15
3	E	562	NDP	C3B-C2B-C1B	-3.92	95.14	102.73
3	F	563	NDP	C3B-C2B-C1B	-3.90	95.18	102.73
3	A	551	NDP	C3B-C2B-C1B	-3.90	95.19	102.73
3	D	561	NDP	C3B-C2B-C1B	-3.90	95.19	102.73
3	C	560	NDP	C3B-C2B-C1B	-3.89	95.20	102.73
3	B	559	NDP	C3B-C2B-C1B	-3.88	95.22	102.73
3	B	559	NDP	PN-O3-PA	-3.79	122.08	132.73
3	D	561	NDP	PN-O3-PA	-3.79	122.09	132.73
3	C	560	NDP	PN-O3-PA	-3.79	122.09	132.73
3	A	551	NDP	PN-O3-PA	-3.78	122.10	132.73
3	F	563	NDP	PN-O3-PA	-3.78	122.11	132.73
3	E	562	NDP	PN-O3-PA	-3.77	122.15	132.73
3	F	563	NDP	C4B-O4B-C1B	-3.36	106.03	109.72
3	C	560	NDP	C4B-O4B-C1B	-3.36	106.03	109.72
3	B	559	NDP	C4B-O4B-C1B	-3.34	106.04	109.72
3	D	561	NDP	C4B-O4B-C1B	-3.34	106.05	109.72
3	A	551	NDP	C4B-O4B-C1B	-3.34	106.05	109.72
4	D	566	GTP	C4'-O4'-C1'	-3.30	106.09	109.72
4	B	564	GTP	C4'-O4'-C1'	-3.30	106.10	109.72
3	E	562	NDP	C4B-O4B-C1B	-3.30	106.10	109.72
4	F	568	GTP	C4'-O4'-C1'	-3.28	106.11	109.72
4	A	553	GTP	C4'-O4'-C1'	-3.28	106.12	109.72
4	E	567	GTP	C4'-O4'-C1'	-3.27	106.13	109.72
4	C	565	GTP	C4'-O4'-C1'	-3.27	106.13	109.72
4	D	566	GTP	PB-O3B-PG	-3.15	122.10	132.67
4	C	565	GTP	PB-O3B-PG	-3.15	122.12	132.67
4	A	553	GTP	PB-O3B-PG	-3.15	122.12	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	564	GTP	PB-O3B-PG	-3.15	122.12	132.67
4	E	567	GTP	PB-O3B-PG	-3.14	122.12	132.67
4	F	568	GTP	PB-O3B-PG	-3.14	122.15	132.67
3	A	551	NDP	O4B-C1B-C2B	-3.12	100.96	106.60
3	C	560	NDP	O4B-C1B-C2B	-3.12	100.96	106.60
3	D	561	NDP	O4B-C1B-C2B	-3.12	100.97	106.60
3	E	562	NDP	O4B-C1B-C2B	-3.11	100.97	106.60
3	F	563	NDP	O4B-C1B-C2B	-3.11	100.98	106.60
3	B	559	NDP	O4B-C1B-C2B	-3.10	100.99	106.60
3	C	560	NDP	C3D-C2D-C1D	-2.93	95.51	101.40
3	B	559	NDP	C3D-C2D-C1D	-2.93	95.51	101.40
3	D	561	NDP	C3D-C2D-C1D	-2.93	95.51	101.40
3	A	551	NDP	C3D-C2D-C1D	-2.93	95.52	101.40
3	F	563	NDP	C3D-C2D-C1D	-2.91	95.56	101.40
3	E	562	NDP	C3D-C2D-C1D	-2.90	95.57	101.40
4	E	567	GTP	PA-O3A-PB	-2.88	124.63	132.73
4	B	564	GTP	PA-O3A-PB	-2.88	124.65	132.73
4	F	568	GTP	PA-O3A-PB	-2.88	124.65	132.73
4	A	553	GTP	PA-O3A-PB	-2.87	124.67	132.73
4	C	565	GTP	PA-O3A-PB	-2.87	124.67	132.73
4	D	566	GTP	PA-O3A-PB	-2.86	124.70	132.73
4	B	564	GTP	N3-C2-N1	-2.63	123.44	127.44
4	F	568	GTP	N3-C2-N1	-2.63	123.44	127.44
4	C	565	GTP	N3-C2-N1	-2.62	123.45	127.44
4	A	553	GTP	N3-C2-N1	-2.62	123.45	127.44
4	E	567	GTP	N3-C2-N1	-2.62	123.46	127.44
4	D	566	GTP	N3-C2-N1	-2.61	123.46	127.44
4	B	564	GTP	O3A-PA-O5'	-2.55	96.17	102.94
4	C	565	GTP	O3A-PA-O5'	-2.55	96.17	102.94
4	D	566	GTP	O3A-PA-O5'	-2.55	96.18	102.94
4	A	553	GTP	O3A-PA-O5'	-2.55	96.18	102.94
4	E	567	GTP	O3A-PA-O5'	-2.54	96.19	102.94
4	F	568	GTP	O3A-PA-O5'	-2.54	96.19	102.94
4	E	567	GTP	C5'-C4'-C3'	-2.47	105.40	115.21
4	C	565	GTP	C5'-C4'-C3'	-2.47	105.41	115.21
4	A	553	GTP	C5'-C4'-C3'	-2.47	105.42	115.21
4	D	566	GTP	C5'-C4'-C3'	-2.47	105.42	115.21
4	F	568	GTP	C5'-C4'-C3'	-2.46	105.43	115.21
4	B	564	GTP	C5'-C4'-C3'	-2.46	105.44	115.21
4	F	568	GTP	C6-C5-C4	-2.46	117.96	120.90
4	A	553	GTP	C6-C5-C4	-2.43	117.99	120.90
4	B	564	GTP	C6-C5-C4	-2.42	118.01	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	566	GTP	C6-C5-C4	-2.41	118.02	120.90
4	C	565	GTP	C6-C5-C4	-2.40	118.02	120.90
4	E	567	GTP	C6-C5-C4	-2.39	118.04	120.90
3	C	560	NDP	C1D-N1N-C6N	-2.33	115.59	120.81
3	D	561	NDP	C1D-N1N-C6N	-2.33	115.60	120.81
3	A	551	NDP	C1D-N1N-C6N	-2.32	115.62	120.81
3	B	559	NDP	C1D-N1N-C6N	-2.32	115.62	120.81
3	F	563	NDP	C1D-N1N-C6N	-2.31	115.64	120.81
3	E	562	NDP	C1D-N1N-C6N	-2.30	115.65	120.81
3	F	563	NDP	O3D-C3D-C4D	-2.20	104.44	111.05
3	D	561	NDP	O4B-C4B-C5B	-2.20	101.47	109.32
3	F	563	NDP	O4B-C4B-C5B	-2.19	101.47	109.32
3	C	560	NDP	O4B-C4B-C5B	-2.19	101.47	109.32
3	E	562	NDP	O3D-C3D-C4D	-2.19	104.48	111.05
3	A	551	NDP	O4B-C4B-C5B	-2.19	101.48	109.32
3	A	551	NDP	O3D-C3D-C4D	-2.19	104.48	111.05
3	E	562	NDP	O4B-C4B-C5B	-2.19	101.49	109.32
3	B	559	NDP	O3D-C3D-C4D	-2.19	104.49	111.05
3	B	559	NDP	O4B-C4B-C5B	-2.19	101.50	109.32
3	D	561	NDP	O3D-C3D-C4D	-2.18	104.50	111.05
3	C	560	NDP	O3D-C3D-C4D	-2.17	104.54	111.05
3	C	560	NDP	O2A-PA-O5B	2.10	119.04	108.46
3	F	563	NDP	O2A-PA-O5B	2.10	119.05	108.46
3	A	551	NDP	O2A-PA-O5B	2.10	119.07	108.46
3	B	559	NDP	O2A-PA-O5B	2.10	119.08	108.46
3	D	561	NDP	O2A-PA-O5B	2.11	119.08	108.46
3	E	562	NDP	O2A-PA-O5B	2.11	119.11	108.46
3	B	559	NDP	O3-PN-O5D	2.20	108.78	102.94
3	C	560	NDP	O3-PN-O5D	2.21	108.80	102.94
3	A	551	NDP	O3-PN-O5D	2.21	108.81	102.94
3	D	561	NDP	O3-PN-O5D	2.22	108.82	102.94
3	F	563	NDP	O3-PN-O5D	2.22	108.82	102.94
3	E	562	NDP	O3-PN-O5D	2.22	108.83	102.94
3	C	560	NDP	C4A-C5A-N7A	2.37	111.66	109.48
3	B	559	NDP	C4A-C5A-N7A	2.38	111.67	109.48
3	B	559	NDP	C2B-C3B-C4B	2.41	107.56	101.85
3	E	562	NDP	C4A-C5A-N7A	2.41	111.70	109.48
3	D	561	NDP	C4A-C5A-N7A	2.42	111.70	109.48
3	C	560	NDP	C2B-C3B-C4B	2.42	107.59	101.85
3	F	563	NDP	C4A-C5A-N7A	2.42	111.71	109.48
3	F	563	NDP	C2B-C3B-C4B	2.43	107.60	101.85
3	A	551	NDP	C2B-C3B-C4B	2.43	107.60	101.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	562	NDP	C2B-C3B-C4B	2.44	107.62	101.85
3	D	561	NDP	C2B-C3B-C4B	2.44	107.63	101.85
3	A	551	NDP	C4A-C5A-N7A	2.44	111.72	109.48
3	B	559	NDP	C5N-C4N-C3N	2.60	119.68	112.52
3	C	560	NDP	C5N-C4N-C3N	2.60	119.68	112.52
3	A	551	NDP	C5N-C4N-C3N	2.60	119.69	112.52
3	E	562	NDP	C5N-C4N-C3N	2.60	119.69	112.52
3	F	563	NDP	C5N-C4N-C3N	2.61	119.71	112.52
3	D	561	NDP	C5N-C4N-C3N	2.63	119.75	112.52
3	E	562	NDP	O2B-P2B-O1X	2.77	114.03	107.11
3	C	560	NDP	O2B-P2B-O1X	2.78	114.04	107.11
3	A	551	NDP	O2B-P2B-O1X	2.78	114.04	107.11
3	F	563	NDP	O2B-P2B-O1X	2.78	114.05	107.11
3	B	559	NDP	O2B-P2B-O1X	2.78	114.05	107.11
3	D	561	NDP	O2B-P2B-O1X	2.78	114.06	107.11
4	E	567	GTP	O2A-PA-O3A	3.34	120.23	105.09
4	F	568	GTP	O2A-PA-O3A	3.34	120.26	105.09
4	B	564	GTP	O2A-PA-O3A	3.34	120.27	105.09
4	A	553	GTP	O2A-PA-O3A	3.35	120.27	105.09
4	D	566	GTP	O2A-PA-O3A	3.35	120.28	105.09
4	C	565	GTP	O2A-PA-O3A	3.35	120.29	105.09
3	D	561	NDP	C2D-C1D-N1N	3.51	122.83	113.34
3	B	559	NDP	C2D-C1D-N1N	3.52	122.85	113.34
3	C	560	NDP	C2D-C1D-N1N	3.52	122.85	113.34
3	A	551	NDP	C2D-C1D-N1N	3.53	122.87	113.34
3	E	562	NDP	C2D-C1D-N1N	3.53	122.88	113.34
3	F	563	NDP	C2D-C1D-N1N	3.54	122.92	113.34
4	F	568	GTP	C6-N1-C2	6.16	124.49	115.94
4	B	564	GTP	C6-N1-C2	6.16	124.49	115.94
4	A	553	GTP	C6-N1-C2	6.17	124.50	115.94
4	C	565	GTP	C6-N1-C2	6.18	124.52	115.94
4	D	566	GTP	C6-N1-C2	6.19	124.53	115.94
4	E	567	GTP	C6-N1-C2	6.19	124.53	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 158 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	550	GLU	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	551	NDP	24	0
4	A	553	GTP	2	0
2	B	554	GLU	7	0
3	B	559	NDP	22	0
4	B	564	GTP	2	0
2	C	555	GLU	7	0
3	C	560	NDP	24	0
4	C	565	GTP	2	0
2	D	556	GLU	7	0
3	D	561	NDP	23	0
4	D	566	GTP	2	0
2	E	557	GLU	7	0
3	E	562	NDP	25	0
4	E	567	GTP	2	0
2	F	558	GLU	7	0
3	F	563	NDP	23	0
4	F	568	GTP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.