Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:44 AM GMT

PDB ID	:	3MW9
Title	:	Bovine glutamate dehydrogenase complexed with NADH, GTP, glutamate
Authors	:	Smith, T.J.; Peterson, P.
Deposited on	:	2010-05-05
Resolution	:	2.40 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

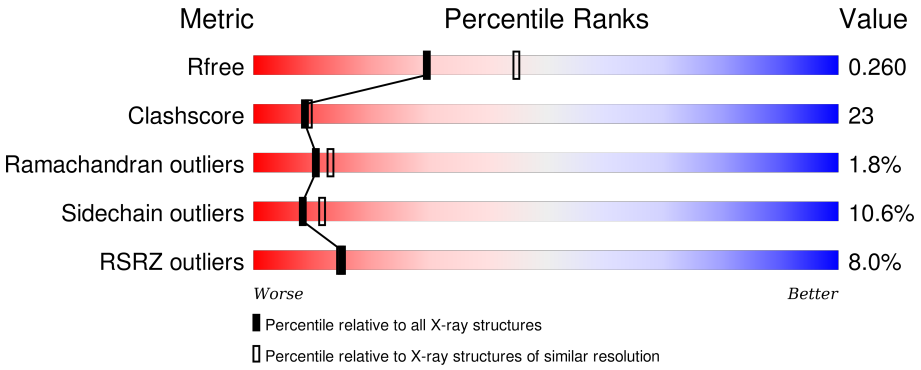
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 >=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 <=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.

Mol	Chain	Length	Quality of chain
1	A	501	7% 64% 28% 7%
1	B	501	7% 67% 27% 6%
1	C	501	9% 67% 26% 7%
1	D	501	8% 62% 32% 6%
1	E	501	9% 62% 32% 7%

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Mol	Chain	Length	Quality of chain
1	F	501	9% 64% 29% 7%

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	601	-	-	X	-
2	GLU	B	601	-	-	X	-
2	GLU	C	601	-	-	X	-
2	GLU	D	601	-	-	X	-
2	GLU	E	601	-	-	X	-
2	GLU	F	601	-	-	X	-
3	NAI	A	603	X	-	X	-
3	NAI	A	604	X	-	-	-
3	NAI	B	603	X	-	-	-
3	NAI	C	603	X	-	-	-
3	NAI	C	604	X	-	-	-
3	NAI	C	605	X	-	-	-
3	NAI	D	603	X	-	X	-
3	NAI	D	605	X	-	-	-
3	NAI	E	603	X	-	-	-
3	NAI	F	604	X	-	-	-
4	GTP	C	602	X	-	-	-
4	GTP	D	602	X	-	-	-
4	GTP	F	603	X	-	-	-

2 Entry composition

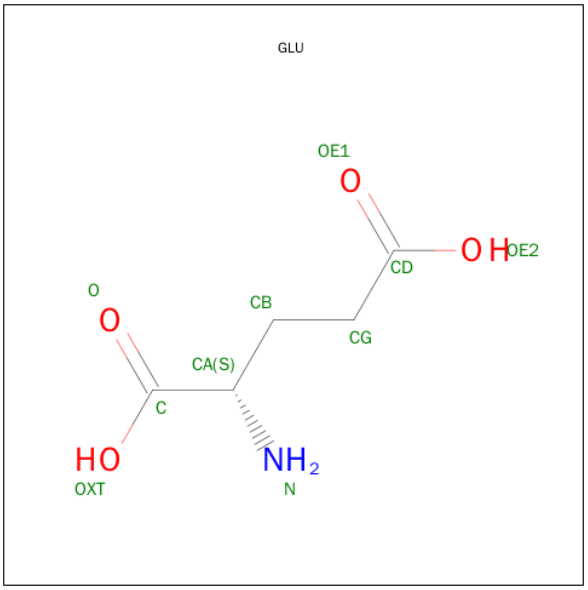
There are 5 unique types of molecules in this entry. The entry contains 24707 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1.

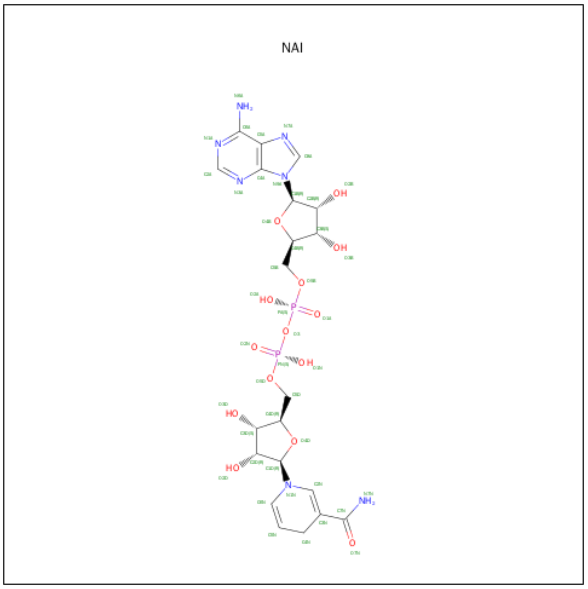
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3922	2476	687	740	19			
1	B	501	Total	C	N	O	S	0	0	0
			3922	2476	687	740	19			
1	C	501	Total	C	N	O	S	0	0	0
			3922	2476	687	740	19			
1	D	501	Total	C	N	O	S	0	0	0
			3922	2476	687	740	19			
1	E	501	Total	C	N	O	S	0	0	0
			3922	2476	687	740	19			
1	F	501	Total	C	N	O	S	0	0	0
			3922	2476	687	740	19			

- 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		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	A	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	11	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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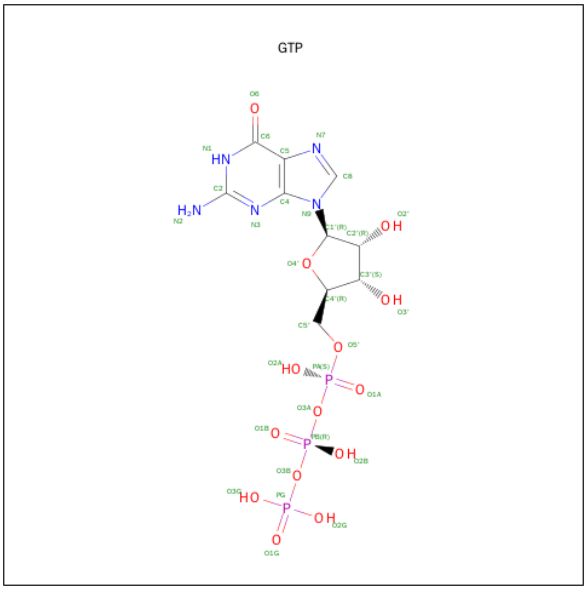
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	6	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- 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	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

- Molecule 5 is water.

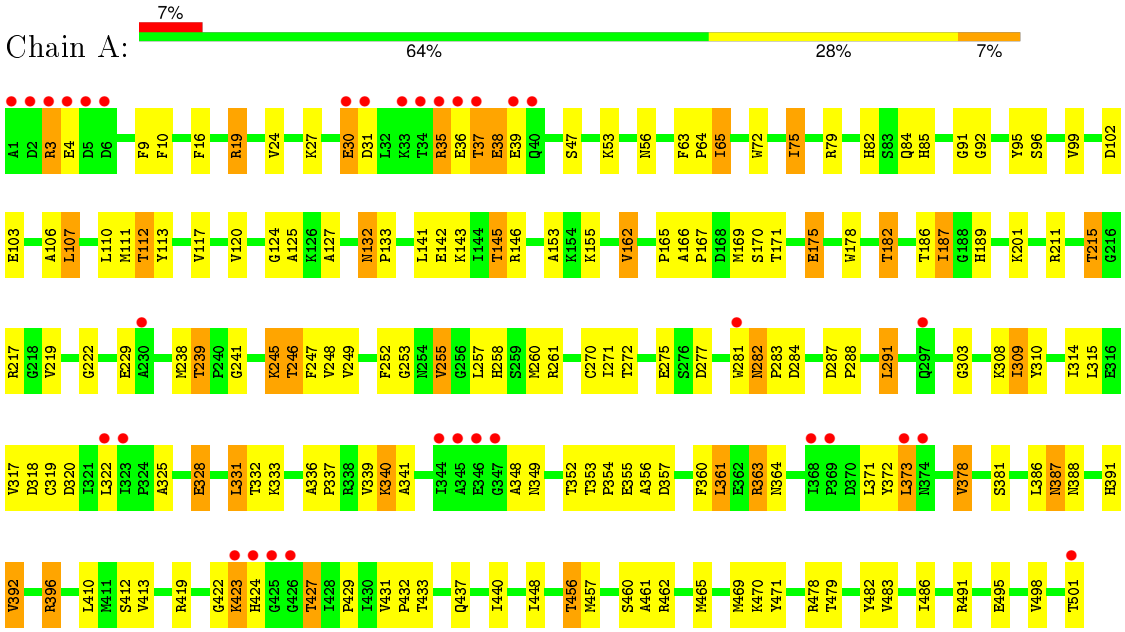
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	73	Total	O	0	0
			73	73		
5	B	69	Total	O	0	0
			69	69		
5	C	65	Total	O	0	0
			65	65		
5	D	66	Total	O	0	0
			66	66		
5	E	55	Total	O	0	0
			55	55		
5	F	67	Total	O	0	0
			67	67		

3 Residue-property plots (i)

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.

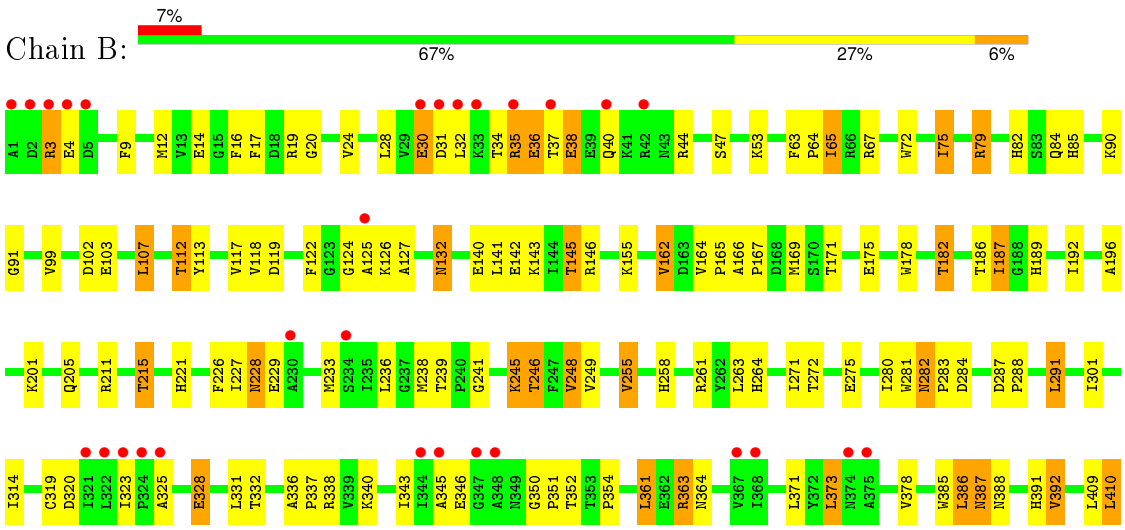
- Molecule 1: Glutamate dehydrogenase 1

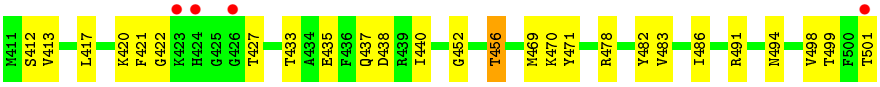
Chain A:



- Molecule 1: Glutamate dehydrogenase 1

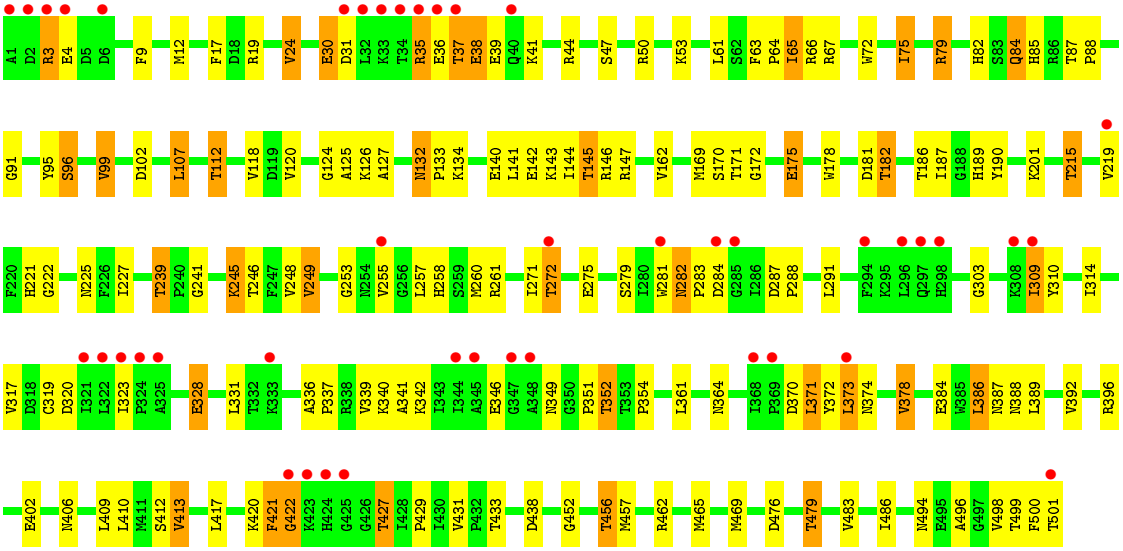
Chain B:





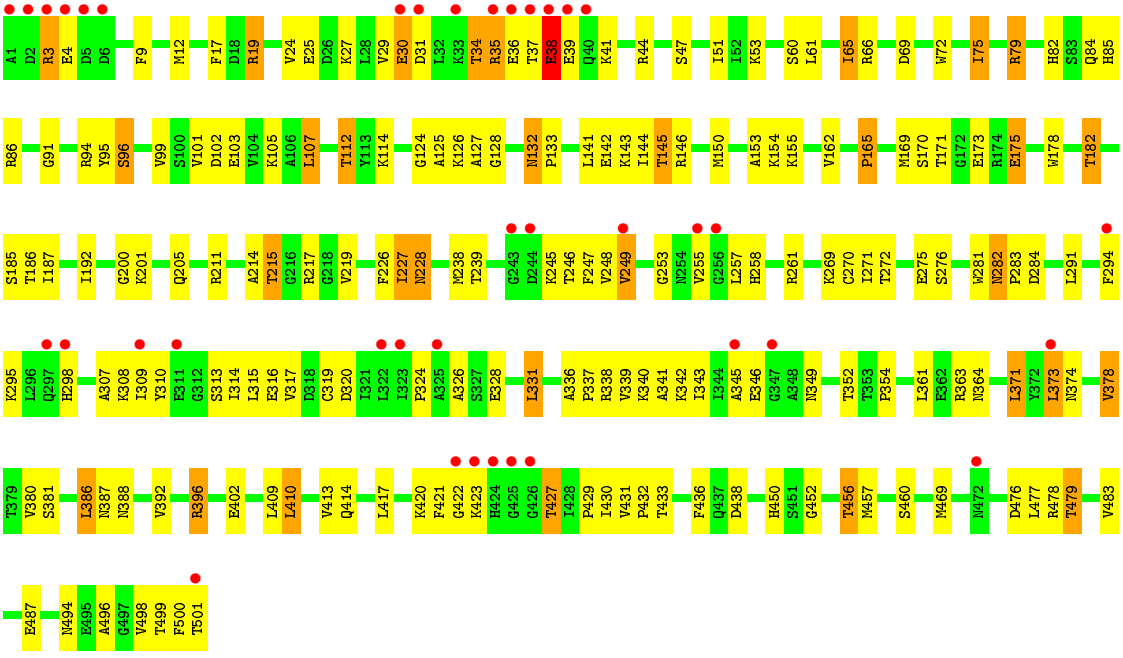
• Molecule 1: Glutamate dehydrogenase 1

Chain C:



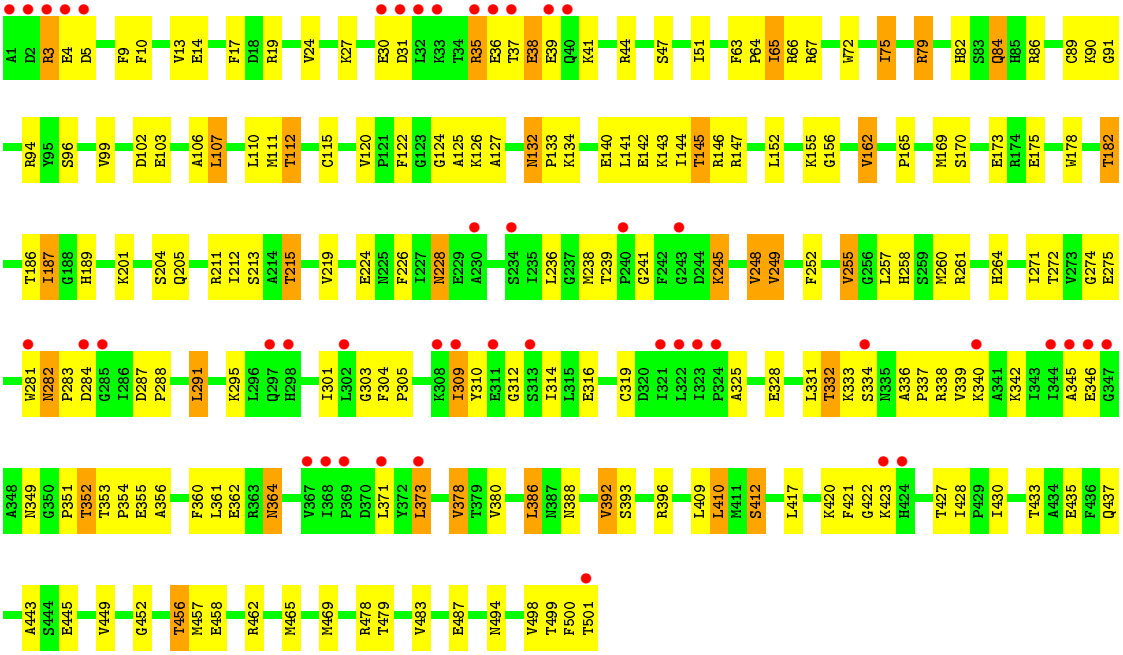
• Molecule 1: Glutamate dehydrogenase 1

Chain D:



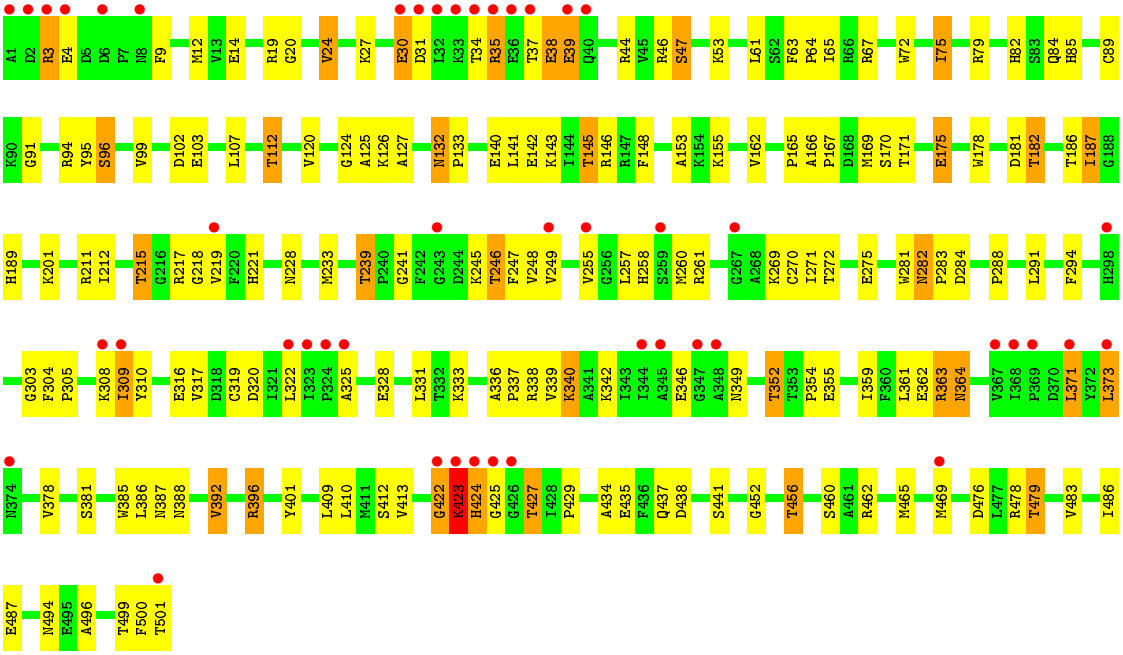
• Molecule 1: Glutamate dehydrogenase 1

Chain E:



• Molecule 1: Glutamate dehydrogenase 1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.00Å 102.50Å 167.30Å 90.00° 101.64° 90.00°	Depositor
Resolution (Å)	28.59 – 2.40 28.59 – 2.28	Depositor EDS
% Data completeness (in resolution range)	79.8 (28.59-2.40) 69.4 (28.59-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, R_{free}	0.204 , 0.261 0.206 , 0.260	Depositor DCC
R_{free} test set	1961 reflections (1.56%)	DCC
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 130469 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24707	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.45	0/4005	0.61	0/5406
1	B	0.45	0/4005	0.62	1/5406 (0.0%)
1	C	0.46	0/4005	0.59	0/5406
1	D	0.45	0/4005	0.61	0/5406
1	E	0.45	0/4005	0.61	1/5406 (0.0%)
1	F	0.44	0/4005	0.60	0/5406
All	All	0.45	0/24030	0.61	2/32436 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	162	VAL	CB-CA-C	-5.67	100.62	111.40
1	B	162	VAL	CB-CA-C	-5.06	101.78	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	3922	0	3883	189	0
1	B	3922	0	3883	167	0
1	C	3922	0	3883	176	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3922	0	3883	208	0
1	E	3922	0	3883	198	0
1	F	3922	0	3883	190	0
2	A	10	0	5	5	0
2	B	10	0	5	8	0
2	C	10	0	5	9	0
2	D	10	0	5	8	0
2	E	10	0	5	9	0
2	F	10	0	5	7	0
3	A	88	0	54	31	0
3	B	44	0	27	10	0
3	C	132	0	81	24	0
3	D	132	0	81	44	0
3	E	44	0	27	19	0
3	F	88	0	54	26	0
4	A	32	0	12	0	0
4	B	32	0	12	1	0
4	C	32	0	12	4	0
4	D	32	0	12	2	0
4	E	32	0	12	0	0
4	F	32	0	12	2	0
5	A	73	0	0	13	0
5	B	69	0	0	8	0
5	C	65	0	0	3	0
5	D	66	0	0	5	0
5	E	55	0	0	5	0
5	F	67	0	0	10	0
All	All	24707	0	23724	1124	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 23.

All (1124) 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)
2:B:601:GLU:HA	3:B:603:NAI:H4N	1.22	1.12
1:A:272:THR:HG21	1:A:317:VAL:HG21	1.30	1.12
1:E:272:THR:CG2	1:E:281:TRP:HD1	1.64	1.10
1:A:38:GLU:HG2	1:A:39:GLU:H	1.16	1.08
1:C:82:HIS:HD2	1:C:112:THR:HG21	1.13	1.08
1:C:82:HIS:CD2	1:C:112:THR:HG21	1.89	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:THR:HG21	1:E:281:TRP:HD1	1.18	1.06
1:D:272:THR:HG22	1:D:281:TRP:HD1	1.12	1.05
1:B:82:HIS:CD2	1:B:112:THR:HG21	1.90	1.05
1:D:275:GLU:C	3:D:603:NAI:H2A	1.77	1.04
1:C:258:HIS:HD2	1:C:261:ARG:HH11	1.05	1.02
1:F:272:THR:HG21	1:F:317:VAL:HG11	1.42	1.01
1:E:82:HIS:CD2	1:E:112:THR:HG21	1.95	1.01
4:C:602:GTP:H4'	4:C:602:GTP:C8	1.94	1.01
1:D:271:ILE:HG13	1:D:272:THR:HG23	1.36	1.00
1:D:272:THR:HG22	1:D:281:TRP:CD1	1.98	0.99
1:F:272:THR:HG22	1:F:281:TRP:HD1	1.28	0.97
1:A:258:HIS:HD2	1:A:261:ARG:HH11	1.08	0.97
2:C:601:GLU:HA	3:C:604:NAI:H4N	1.45	0.97
1:A:253:GLY:HA3	3:A:603:NAI:H52A	1.47	0.97
1:C:186:THR:HG22	1:C:187:ILE:H	1.30	0.95
1:B:47:SER:HB3	1:E:72:TRP:HB2	1.47	0.94
1:D:112:THR:HG22	1:D:124:GLY:HA3	1.50	0.94
1:C:271:ILE:HG13	1:C:272:THR:HG23	1.50	0.94
1:F:82:HIS:CD2	1:F:112:THR:HG21	2.03	0.94
1:E:272:THR:CG2	1:E:281:TRP:CD1	2.50	0.94
1:C:272:THR:CG2	1:C:281:TRP:HD1	1.82	0.93
1:E:126:LYS:HZ2	2:E:601:GLU:N	1.64	0.93
1:B:186:THR:HG22	1:B:187:ILE:N	1.84	0.92
1:A:363:ARG:NH2	5:A:763:HOH:O	2.02	0.92
1:A:82:HIS:HD2	1:A:112:THR:HG21	1.33	0.92
1:B:75:ILE:H	1:B:75:ILE:HD13	1.33	0.92
1:E:44:ARG:HH12	1:E:494:ASN:HD21	1.18	0.92
1:B:38:GLU:HG3	1:B:40:GLN:H	1.35	0.91
2:B:601:GLU:HA	3:B:603:NAI:C4N	1.99	0.91
1:B:82:HIS:HD2	1:B:112:THR:HG21	1.26	0.91
2:B:601:GLU:CA	3:B:603:NAI:H4N	2.00	0.90
3:D:604:NAI:O2A	1:E:393:SER:HB3	1.72	0.90
1:D:44:ARG:HH12	1:D:494:ASN:HD21	1.18	0.90
1:D:272:THR:CG2	1:D:281:TRP:HD1	1.84	0.89
1:B:143:LYS:HD3	1:E:501:THR:HG22	1.53	0.88
1:D:246:THR:HG22	1:D:320:ASP:OD2	1.73	0.88
2:A:601:GLU:HA	3:A:603:NAI:H4N	1.55	0.87
1:F:82:HIS:HD2	1:F:112:THR:HG21	1.37	0.87
1:A:82:HIS:CD2	1:A:112:THR:HG21	2.11	0.86
1:F:271:ILE:HD11	1:F:319:CYS:HB3	1.58	0.85
1:F:112:THR:HG22	1:F:124:GLY:HA3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:HIS:CD2	1:C:261:ARG:HH11	1.94	0.84
1:B:9:PHE:CE1	1:B:328:GLU:HG2	2.12	0.84
1:E:272:THR:HG21	1:E:281:TRP:CD1	2.10	0.84
1:F:248:VAL:HG12	1:F:319:CYS:SG	2.17	0.84
1:B:186:THR:HG22	1:B:187:ILE:H	1.41	0.84
1:D:82:HIS:CD2	1:D:112:THR:HG21	2.13	0.83
1:D:217:ARG:HD3	5:D:754:HOH:O	1.78	0.83
1:C:186:THR:HG22	1:C:187:ILE:N	1.89	0.83
1:D:178:TRP:O	1:D:182:THR:HG23	1.77	0.83
1:D:24:VAL:HG11	1:D:483:VAL:HG13	1.60	0.83
1:F:282:ASN:HD22	1:F:284:ASP:H	1.22	0.83
1:F:37:THR:O	1:F:38:GLU:HG3	1.78	0.83
1:A:47:SER:HB3	1:D:72:TRP:HB2	1.57	0.83
1:E:99:VAL:HA	1:E:103:GLU:OE1	1.79	0.82
1:A:272:THR:HG23	1:A:281:TRP:HD1	1.44	0.82
1:E:456:THR:HG21	1:F:396:ARG:HH21	1.44	0.81
1:D:186:THR:HG22	1:D:187:ILE:H	1.43	0.81
1:A:37:THR:O	1:A:38:GLU:HB2	1.79	0.81
1:D:82:HIS:HD2	1:D:112:THR:HG21	1.46	0.81
1:A:391:HIS:HA	3:A:604:NAI:H1D	1.62	0.81
1:D:282:ASN:HD22	1:D:284:ASP:H	1.27	0.81
1:C:38:GLU:HG2	1:C:39:GLU:H	1.42	0.81
1:D:349:ASN:ND2	3:D:603:NAI:H6N	1.95	0.80
1:C:82:HIS:CD2	1:C:112:THR:CG2	2.64	0.80
1:D:275:GLU:O	3:D:603:NAI:H2A	1.82	0.80
1:C:272:THR:HG22	1:C:281:TRP:HD1	1.47	0.79
2:F:601:GLU:HA	3:F:604:NAI:H4N	1.65	0.79
1:D:413:VAL:HG22	1:D:430:ILE:HG13	1.64	0.79
1:C:126:LYS:HZ2	2:C:601:GLU:N	1.80	0.79
1:E:9:PHE:CE1	1:E:328:GLU:HG2	2.17	0.79
1:F:282:ASN:ND2	1:F:284:ASP:H	1.79	0.79
1:B:499:THR:HG21	1:E:64:PRO:HG2	1.64	0.79
1:D:91:GLY:HA3	1:D:125:ALA:O	1.81	0.79
1:E:281:TRP:CZ2	1:E:283:PRO:HG3	2.18	0.78
1:D:272:THR:HG21	1:D:317:VAL:HG11	1.66	0.78
1:C:258:HIS:HD2	1:C:261:ARG:NH1	1.81	0.78
1:F:271:ILE:HG13	1:F:272:THR:HG23	1.65	0.78
1:D:53:LYS:HE2	5:D:714:HOH:O	1.82	0.78
1:A:253:GLY:HA3	3:A:603:NAI:C5B	2.14	0.78
1:C:272:THR:HG22	1:C:281:TRP:CD1	2.18	0.78
1:F:258:HIS:HD2	1:F:261:ARG:HH11	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:HIS:HD2	1:B:261:ARG:HH11	1.32	0.78
1:D:282:ASN:ND2	1:D:284:ASP:H	1.82	0.78
1:D:3:ARG:HG3	1:D:4:GLU:H	1.46	0.78
1:D:396:ARG:HH21	1:F:456:THR:HG21	1.49	0.78
1:E:186:THR:HG22	1:E:187:ILE:N	1.99	0.78
1:E:91:GLY:HA3	1:E:125:ALA:O	1.84	0.78
1:F:272:THR:CG2	1:F:281:TRP:HD1	1.97	0.77
1:A:419:ARG:NH2	5:A:773:HOH:O	2.17	0.77
1:E:271:ILE:O	1:E:272:THR:HG23	1.84	0.77
1:D:126:LYS:HZ2	2:D:601:GLU:N	1.82	0.77
1:A:112:THR:HG22	1:A:124:GLY:HA3	1.64	0.77
1:C:75:ILE:H	1:C:75:ILE:HD13	1.47	0.77
2:C:601:GLU:C	3:C:604:NAI:H5N	2.05	0.77
1:A:9:PHE:CE1	1:A:328:GLU:HG2	2.19	0.76
1:E:82:HIS:HD2	1:E:112:THR:HG21	1.50	0.76
3:D:604:NAI:H4N	1:E:205:GLN:O	1.86	0.76
3:D:605:NAI:H52N	3:D:605:NAI:N1N	1.99	0.76
1:F:248:VAL:HB	1:F:272:THR:OG1	1.86	0.76
1:F:282:ASN:C	1:F:282:ASN:HD22	1.89	0.76
1:D:186:THR:HG22	1:D:187:ILE:N	2.01	0.76
1:C:501:THR:HG22	1:F:143:LYS:HD3	1.66	0.76
1:E:264:HIS:HD2	5:E:712:HOH:O	1.68	0.76
1:A:272:THR:HB	1:A:314:ILE:HD11	1.68	0.75
1:B:3:ARG:HG3	1:B:4:GLU:H	1.50	0.75
1:E:141:LEU:O	1:E:145:THR:HG23	1.85	0.75
1:A:253:GLY:CA	3:A:603:NAI:H52A	2.17	0.75
1:A:339:VAL:N	5:A:763:HOH:O	2.19	0.75
1:D:258:HIS:HD2	1:D:261:ARG:HH11	1.35	0.75
1:A:339:VAL:O	1:A:340:LYS:HG2	1.86	0.75
1:A:72:TRP:HB2	1:D:47:SER:HB3	1.67	0.75
1:E:258:HIS:HD2	1:E:261:ARG:HH11	1.33	0.75
1:C:248:VAL:HG12	1:C:319:CYS:SG	2.27	0.75
1:D:171:THR:HB	1:D:175:GLU:HG3	1.69	0.75
1:F:272:THR:HG22	1:F:281:TRP:CD1	2.17	0.74
1:C:219:VAL:HG22	1:C:373:LEU:HD13	1.67	0.74
1:A:258:HIS:HD2	1:A:261:ARG:NH1	1.85	0.74
1:A:482:TYR:O	1:A:486:ILE:HG13	1.87	0.74
1:A:349:ASN:ND2	3:A:603:NAI:H6N	2.02	0.74
1:A:64:PRO:HG2	1:D:499:THR:HG21	1.67	0.74
1:A:143:LYS:HD3	1:D:501:THR:HG22	1.68	0.74
1:C:82:HIS:HD2	1:C:112:THR:CG2	1.98	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:THR:CG2	1:D:317:VAL:HG11	2.18	0.74
1:C:272:THR:CG2	1:C:281:TRP:CD1	2.70	0.73
1:F:427:THR:HG22	1:F:429:PRO:HD3	1.70	0.73
1:C:499:THR:HG21	1:F:64:PRO:HG2	1.68	0.73
1:A:38:GLU:HG2	1:A:39:GLU:N	1.98	0.73
1:C:272:THR:HG21	1:C:281:TRP:HD1	1.52	0.73
1:E:272:THR:HG22	1:E:281:TRP:HA	1.71	0.73
1:A:82:HIS:HD2	1:A:112:THR:CG2	2.02	0.73
1:C:141:LEU:O	1:C:145:THR:HG23	1.89	0.73
1:D:294:PHE:CE2	1:D:298:HIS:CE1	2.76	0.73
1:D:9:PHE:CE1	1:D:328:GLU:HG2	2.23	0.73
1:E:271:ILE:O	1:E:272:THR:CG2	2.37	0.73
2:C:601:GLU:CA	3:C:604:NAI:H4N	2.16	0.73
1:F:282:ASN:HD21	1:F:284:ASP:HB2	1.52	0.73
1:A:396:ARG:HH21	1:B:456:THR:HG21	1.53	0.73
1:E:345:ALA:HB1	1:E:373:LEU:HD11	1.69	0.73
1:E:79:ARG:HD2	1:E:127:ALA:HB2	1.71	0.72
1:B:272:THR:CG2	1:B:281:TRP:HD1	2.02	0.72
1:A:186:THR:HG22	1:A:187:ILE:N	2.02	0.72
1:A:82:HIS:CD2	1:A:112:THR:CG2	2.72	0.72
3:A:604:NAI:H3D	3:A:604:NAI:C2N	2.20	0.72
2:F:601:GLU:CA	3:F:604:NAI:H4N	2.19	0.72
1:D:387:ASN:OD1	5:D:750:HOH:O	2.07	0.72
1:C:79:ARG:HD2	1:C:127:ALA:HB2	1.72	0.72
1:E:224:GLU:O	1:E:228:ASN:HB2	1.89	0.72
1:F:215:THR:HG21	3:F:604:NAI:C7N	2.20	0.72
1:B:24:VAL:CG1	1:B:483:VAL:HG13	2.19	0.71
1:A:258:HIS:CD2	1:A:261:ARG:HH11	2.00	0.71
1:F:91:GLY:HA3	1:F:125:ALA:O	1.91	0.71
1:B:82:HIS:CD2	1:B:112:THR:CG2	2.73	0.71
1:F:39:GLU:O	1:F:39:GLU:HG2	1.88	0.71
1:B:501:THR:HG22	1:E:143:LYS:HD3	1.71	0.71
1:C:271:ILE:O	1:C:272:THR:HG22	1.90	0.71
1:A:3:ARG:HG3	1:A:4:GLU:H	1.55	0.71
1:C:24:VAL:HG11	1:C:483:VAL:HG13	1.73	0.71
2:F:601:GLU:C	3:F:604:NAI:C5N	2.59	0.71
1:C:143:LYS:HD3	1:F:501:THR:HG22	1.73	0.71
4:C:602:GTP:H4'	4:C:602:GTP:H8	1.49	0.70
1:C:282:ASN:HD22	1:C:282:ASN:C	1.93	0.70
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.20	0.70
1:F:186:THR:HG22	1:F:187:ILE:HD13	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:THR:HB	1:A:314:ILE:CD1	2.22	0.70
1:B:272:THR:HB	1:B:280:ILE:O	1.91	0.70
1:C:24:VAL:CG1	1:C:483:VAL:HG13	2.22	0.70
1:C:457:MET:HA	1:C:457:MET:CE	2.21	0.70
1:C:275:GLU:HA	3:C:604:NAI:H2A	1.74	0.70
2:A:601:GLU:CA	3:A:603:NAI:H4N	2.22	0.70
1:B:392:VAL:HG13	1:C:386:LEU:HD21	1.73	0.70
1:F:303:GLY:H	1:F:309:ILE:HD11	1.57	0.70
1:C:171:THR:HB	1:C:175:GLU:HG3	1.74	0.70
1:C:37:THR:O	1:C:38:GLU:HB2	1.91	0.69
1:B:91:GLY:HA3	1:B:125:ALA:O	1.91	0.69
3:D:604:NAI:O7N	1:E:205:GLN:HA	1.91	0.69
1:C:9:PHE:CE1	1:C:328:GLU:HG2	2.27	0.69
1:E:275:GLU:HA	3:E:603:NAI:H2A	1.74	0.69
1:A:120:VAL:O	3:C:603:NAI:N6A	2.25	0.69
1:D:248:VAL:HG23	1:D:272:THR:O	1.92	0.69
1:D:457:MET:HA	1:D:457:MET:HE2	1.74	0.69
3:F:602:NAI:N1N	3:F:602:NAI:H52N	2.07	0.69
4:C:602:GTP:O1B	4:C:602:GTP:H5"	1.93	0.69
2:C:601:GLU:C	3:C:604:NAI:C5N	2.61	0.69
2:C:601:GLU:HA	3:C:604:NAI:C4N	2.21	0.69
1:F:9:PHE:CE1	1:F:328:GLU:HG2	2.28	0.69
2:F:601:GLU:C	3:F:604:NAI:H5N	2.13	0.69
2:A:601:GLU:C	3:A:603:NAI:C5N	2.61	0.68
3:D:604:NAI:H4N	1:E:205:GLN:C	2.14	0.68
1:E:271:ILE:HD11	1:E:319:CYS:HB3	1.76	0.68
2:A:601:GLU:C	3:A:603:NAI:H5N	2.14	0.68
1:F:422:GLY:HA3	5:F:722:HOH:O	1.91	0.68
1:B:272:THR:HG21	1:B:281:TRP:HD1	1.58	0.68
1:D:27:LYS:O	1:D:30:GLU:HB3	1.94	0.68
1:F:30:GLU:HG3	1:F:31:ASP:N	2.09	0.68
1:A:24:VAL:HG11	1:A:483:VAL:HG13	1.76	0.68
1:F:3:ARG:HG3	1:F:4:GLU:H	1.59	0.68
1:B:246:THR:HG22	1:B:320:ASP:H	1.59	0.68
1:F:423:LYS:N	1:F:423:LYS:HD3	2.07	0.68
1:E:3:ARG:HG3	1:E:4:GLU:H	1.58	0.68
1:E:271:ILE:C	1:E:272:THR:HG23	2.13	0.67
1:C:281:TRP:CZ2	1:C:283:PRO:HG3	2.28	0.67
1:B:412:SER:HA	1:C:433:THR:HG23	1.75	0.67
1:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.28	0.67
1:C:215:THR:HG21	3:C:604:NAI:C7N	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:PHE:CD1	1:C:75:ILE:HD11	2.30	0.67
1:A:112:THR:HG22	1:A:124:GLY:CA	2.24	0.67
1:B:141:LEU:O	1:B:145:THR:HG23	1.95	0.67
1:D:272:THR:HG21	1:D:317:VAL:CG1	2.24	0.67
1:B:271:ILE:O	1:B:272:THR:HG22	1.95	0.67
1:C:47:SER:HB3	1:F:72:TRP:HB2	1.77	0.67
1:F:452:GLY:O	1:F:456:THR:HG23	1.95	0.67
1:D:457:MET:HA	1:D:457:MET:CE	2.25	0.67
1:C:118:VAL:HG23	1:C:120:VAL:HG23	1.76	0.67
1:C:282:ASN:ND2	1:C:284:ASP:H	1.92	0.67
1:A:281:TRP:CZ2	1:A:283:PRO:HG3	2.30	0.67
1:D:44:ARG:NH1	1:D:494:ASN:HD21	1.91	0.67
1:B:281:TRP:CZ2	1:B:283:PRO:HG3	2.29	0.67
1:F:171:THR:HB	1:F:175:GLU:HG3	1.77	0.67
1:C:420:LYS:HB3	1:C:421:PHE:CD2	2.30	0.67
1:D:146:ARG:HG2	1:D:182:THR:HG21	1.77	0.66
1:A:91:GLY:HA3	1:A:125:ALA:O	1.95	0.66
1:B:282:ASN:HD22	1:B:282:ASN:C	1.98	0.66
2:E:601:GLU:C	3:E:603:NAI:H5N	2.15	0.66
1:C:501:THR:HA	5:F:741:HOH:O	1.96	0.66
1:D:282:ASN:HD22	1:D:282:ASN:C	1.97	0.66
1:B:258:HIS:HD2	1:B:261:ARG:NH1	1.94	0.66
1:F:423:LYS:H	1:F:423:LYS:HD3	1.60	0.66
4:C:602:GTP:C8	4:C:602:GTP:C4'	2.74	0.66
1:C:63:PHE:CE1	1:C:75:ILE:HD11	2.31	0.66
1:B:75:ILE:N	1:B:75:ILE:HD13	2.02	0.66
1:B:72:TRP:HB2	1:E:47:SER:HB3	1.78	0.66
1:D:75:ILE:HD13	1:D:75:ILE:H	1.59	0.66
1:F:141:LEU:O	1:F:145:THR:HG23	1.96	0.66
1:B:99:VAL:HA	1:B:103:GLU:OE1	1.95	0.66
1:B:387:ASN:ND2	3:C:605:NAI:H3D	2.10	0.65
1:C:476:ASP:OD2	1:C:479:THR:HG23	1.96	0.65
1:A:99:VAL:HA	1:A:103:GLU:OE1	1.96	0.65
1:E:282:ASN:C	1:E:282:ASN:HD22	1.97	0.65
1:D:226:PHE:C	1:D:228:ASN:H	1.97	0.65
3:A:604:NAI:H3D	3:A:604:NAI:H2N	1.79	0.65
1:C:38:GLU:HG2	1:C:39:GLU:N	2.11	0.65
1:C:346:GLU:OE1	1:C:352:THR:HG23	1.96	0.65
1:B:189:HIS:HE1	1:F:155:LYS:NZ	1.93	0.65
1:D:169:MET:HE1	3:D:603:NAI:H8A	1.79	0.65
1:D:79:ARG:HD2	1:D:127:ALA:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:THR:HG21	1:E:396:ARG:HH21	1.61	0.65
1:C:53:LYS:O	1:C:82:HIS:HE1	1.80	0.65
1:D:169:MET:HG2	3:D:603:NAI:O1N	1.96	0.65
1:D:282:ASN:HD21	1:D:284:ASP:HB2	1.62	0.64
1:E:126:LYS:NZ	2:E:601:GLU:N	2.44	0.64
1:E:346:GLU:OE1	1:E:352:THR:HG23	1.98	0.64
1:C:3:ARG:HG3	1:C:4:GLU:H	1.62	0.64
2:E:601:GLU:C	3:E:603:NAI:C5N	2.65	0.64
1:A:201:LYS:NZ	1:A:388:ASN:HD21	1.95	0.64
1:A:431:VAL:HG13	1:A:432:PRO:HD2	1.79	0.64
1:A:171:THR:HB	1:A:175:GLU:HG3	1.79	0.64
4:B:602:GTP:H5'	4:B:602:GTP:C8	2.32	0.64
1:D:275:GLU:C	3:D:603:NAI:C2A	2.61	0.64
3:A:604:NAI:C2N	3:A:604:NAI:C3D	2.72	0.64
1:E:86:ARG:NH1	3:F:602:NAI:H72N	1.96	0.64
1:B:63:PHE:CE1	1:B:75:ILE:HD11	2.33	0.64
1:A:189:HIS:HE1	1:E:155:LYS:NZ	1.96	0.64
1:E:186:THR:HG22	1:E:187:ILE:HD13	1.80	0.64
1:E:282:ASN:ND2	1:E:284:ASP:H	1.95	0.64
1:C:44:ARG:HH12	1:C:494:ASN:HD21	1.46	0.64
1:E:215:THR:HG21	3:E:603:NAI:C7N	2.28	0.63
1:A:282:ASN:ND2	1:A:284:ASP:H	1.96	0.63
1:D:271:ILE:HD11	1:D:319:CYS:HB3	1.80	0.63
1:D:86:ARG:NH1	3:D:604:NAI:O7N	2.31	0.63
1:D:133:PRO:HG2	1:D:170:SER:HB3	1.80	0.63
1:B:63:PHE:CD1	1:B:75:ILE:HD11	2.34	0.63
1:D:326:ALA:HB1	3:D:603:NAI:N7A	2.13	0.63
2:E:601:GLU:HA	3:E:603:NAI:H4N	1.81	0.63
1:D:294:PHE:CE2	1:D:298:HIS:ND1	2.66	0.63
1:D:19:ARG:HH11	1:D:19:ARG:CB	2.12	0.63
3:A:604:NAI:O2D	3:A:604:NAI:H2N	1.99	0.63
1:C:67:ARG:HD2	1:C:140:GLU:OE1	1.98	0.63
1:F:248:VAL:CB	1:F:272:THR:OG1	2.47	0.62
1:B:186:THR:HG22	1:B:187:ILE:HD13	1.80	0.62
1:B:248:VAL:HG23	1:B:314:ILE:HD11	1.79	0.62
1:F:186:THR:HG22	1:F:187:ILE:N	2.14	0.62
1:C:282:ASN:HD22	1:C:284:ASP:H	1.45	0.62
1:C:271:ILE:HD11	1:C:319:CYS:HB3	1.81	0.62
1:B:63:PHE:O	1:B:75:ILE:HD13	1.98	0.62
1:B:255:VAL:HG22	1:B:325:ALA:HB1	1.81	0.62
3:F:602:NAI:H4D	3:F:602:NAI:O2N	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:TRP:O	1:C:182:THR:HG23	1.99	0.62
1:E:44:ARG:NH1	1:E:494:ASN:HD21	1.92	0.62
1:F:476:ASP:OD2	1:F:479:THR:HG23	1.99	0.62
1:C:457:MET:HA	1:C:457:MET:HE2	1.82	0.62
1:D:112:THR:HG22	1:D:124:GLY:CA	2.25	0.62
1:A:24:VAL:CG1	1:A:483:VAL:HG13	2.30	0.62
1:E:333:LYS:HE2	1:E:355:GLU:HG2	1.81	0.62
1:E:339:VAL:HG21	1:E:360:PHE:HE2	1.65	0.62
1:A:349:ASN:HD21	3:A:603:NAI:H6N	1.64	0.62
1:D:146:ARG:HE	1:D:182:THR:HG22	1.65	0.62
1:A:65:ILE:HD13	1:D:501:THR:HG23	1.81	0.62
1:B:24:VAL:HG11	1:B:483:VAL:HG13	1.80	0.62
1:D:219:VAL:HG22	1:D:373:LEU:HD13	1.81	0.62
1:E:248:VAL:HB	1:E:272:THR:OG1	2.00	0.61
1:E:107:LEU:HB3	1:E:126:LYS:HG2	1.83	0.61
1:F:248:VAL:CG1	1:F:319:CYS:SG	2.88	0.61
1:C:172:GLY:H	1:C:175:GLU:HG2	1.64	0.61
1:A:501:THR:HG22	1:D:143:LYS:HD3	1.83	0.61
1:F:53:LYS:O	1:F:82:HIS:HE1	1.83	0.61
1:A:272:THR:CG2	1:A:281:TRP:HD1	2.14	0.61
3:A:604:NAI:H2A	1:B:85:HIS:NE2	2.16	0.61
1:E:275:GLU:HA	3:E:603:NAI:C2A	2.31	0.61
1:E:386:LEU:HD21	1:F:392:VAL:HG13	1.83	0.61
3:D:605:NAI:H3B	3:D:605:NAI:H8A	1.82	0.60
1:F:349:ASN:ND2	3:F:604:NAI:H6N	2.16	0.60
1:D:19:ARG:HB2	1:D:19:ARG:HH11	1.65	0.60
1:D:99:VAL:HA	1:D:103:GLU:OE1	2.00	0.60
1:C:96:SER:O	1:C:99:VAL:HG13	2.01	0.60
1:F:258:HIS:HD2	1:F:261:ARG:NH1	1.97	0.60
1:F:221:HIS:HE1	5:F:765:HOH:O	1.84	0.60
1:E:420:LYS:HB3	1:E:421:PHE:CD2	2.37	0.60
1:C:271:ILE:HG13	1:C:272:THR:CG2	2.27	0.60
1:C:91:GLY:HA3	1:C:125:ALA:O	2.02	0.60
1:C:64:PRO:HG2	1:F:499:THR:HG21	1.84	0.60
1:F:112:THR:HG22	1:F:124:GLY:CA	2.29	0.60
1:A:275:GLU:CA	3:A:603:NAI:H2A	2.32	0.60
1:D:476:ASP:CG	1:D:479:THR:HG23	2.21	0.60
1:B:67:ARG:HD2	1:B:140:GLU:OE1	2.01	0.60
1:B:282:ASN:ND2	1:B:284:ASP:H	2.00	0.60
1:D:141:LEU:O	1:D:145:THR:HG23	2.02	0.60
1:D:396:ARG:HH21	1:F:456:THR:CG2	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:THR:CG2	1:B:281:TRP:CD1	2.85	0.60
1:F:387:ASN:OD1	5:F:763:HOH:O	2.17	0.60
1:F:304:PHE:CD1	1:F:305:PRO:HD2	2.37	0.60
1:E:241:GLY:O	1:E:245:LYS:HD3	2.02	0.60
1:E:275:GLU:CA	3:E:603:NAI:H2A	2.32	0.60
1:B:226:PHE:C	1:B:228:ASN:H	2.05	0.60
1:F:178:TRP:O	1:F:182:THR:HG23	2.01	0.60
1:D:227:ILE:HG23	1:D:227:ILE:O	2.01	0.60
1:A:282:ASN:C	1:A:282:ASN:HD22	2.05	0.59
1:D:12:MET:HG3	1:D:354:PRO:HD3	1.84	0.59
1:A:37:THR:O	1:A:38:GLU:CB	2.51	0.59
1:E:112:THR:HG22	1:E:124:GLY:HA3	1.84	0.59
1:B:186:THR:CG2	1:B:187:ILE:N	2.58	0.59
1:E:37:THR:HA	1:E:41:LYS:HE3	1.84	0.59
1:E:86:ARG:NH1	3:F:602:NAI:N7N	2.51	0.59
1:E:67:ARG:HD2	1:E:140:GLU:OE1	2.02	0.59
2:B:601:GLU:C	3:B:603:NAI:C5N	2.71	0.59
1:A:427:THR:HG22	1:A:429:PRO:HD3	1.83	0.59
1:A:423:LYS:HD3	1:A:423:LYS:H	1.67	0.59
1:D:248:VAL:HG12	1:D:319:CYS:SG	2.43	0.59
2:E:601:GLU:CA	3:E:603:NAI:H4N	2.33	0.59
1:E:44:ARG:HH12	1:E:494:ASN:ND2	1.95	0.59
1:A:186:THR:HG22	1:A:187:ILE:H	1.67	0.59
1:A:53:LYS:O	1:A:82:HIS:HE1	1.85	0.58
1:E:186:THR:HG22	1:E:187:ILE:H	1.68	0.58
1:E:212:ILE:HG22	5:E:746:HOH:O	2.02	0.58
1:C:387:ASN:OD1	5:C:759:HOH:O	2.17	0.58
1:A:169:MET:HA	3:A:603:NAI:O1A	2.03	0.58
1:C:462:ARG:HA	1:C:465:MET:HE2	1.84	0.58
1:D:95:TYR:OH	1:D:145:THR:HB	2.03	0.58
1:B:64:PRO:HG2	1:E:499:THR:HG21	1.84	0.58
1:B:264:HIS:HD2	5:B:710:HOH:O	1.86	0.58
1:A:392:VAL:HG13	1:B:386:LEU:HD21	1.85	0.58
1:E:248:VAL:HG12	1:E:319:CYS:SG	2.44	0.58
1:D:409:LEU:HD23	1:D:409:LEU:C	2.24	0.58
1:C:112:THR:HG22	1:C:124:GLY:HA3	1.85	0.58
1:D:272:THR:CG2	1:D:281:TRP:CD1	2.73	0.58
1:C:95:TYR:OH	1:C:145:THR:HB	2.03	0.58
1:C:328:GLU:HG3	5:C:712:HOH:O	2.04	0.58
1:E:260:MET:HG2	1:E:288:PRO:HG3	1.85	0.58
1:D:142:GLU:OE2	1:D:146:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TRP:O	1:B:182:THR:HG23	2.03	0.58
1:B:215:THR:HG21	3:B:603:NAI:C7N	2.34	0.58
3:D:605:NAI:H8A	3:D:605:NAI:C3B	2.32	0.58
1:D:65:ILE:HG13	1:D:144:ILE:HG12	1.86	0.58
1:D:44:ARG:HH12	1:D:494:ASN:ND2	1.94	0.57
1:B:420:LYS:HB3	1:B:421:PHE:CD2	2.39	0.57
1:D:421:PHE:N	1:D:421:PHE:CD2	2.71	0.57
1:E:252:PHE:CZ	1:E:257:LEU:HD13	2.39	0.57
1:C:50:ARG:HD3	5:F:755:HOH:O	2.04	0.57
1:D:82:HIS:CD2	1:D:112:THR:CG2	2.87	0.57
1:C:72:TRP:HB2	1:F:47:SER:HB3	1.85	0.57
1:A:75:ILE:H	1:A:75:ILE:HD13	1.69	0.57
3:D:604:NAI:O7N	1:E:204:SER:O	2.23	0.57
1:B:248:VAL:HG12	1:B:319:CYS:SG	2.45	0.57
1:D:349:ASN:HD21	3:D:603:NAI:H6N	1.65	0.57
3:D:603:NAI:O1A	3:D:603:NAI:O1N	2.23	0.57
1:B:44:ARG:NH1	1:B:494:ASN:HD21	2.03	0.57
1:C:63:PHE:O	1:C:75:ILE:HD13	2.05	0.57
1:C:421:PHE:N	1:C:421:PHE:CD2	2.70	0.57
1:D:386:LEU:HD21	1:E:392:VAL:HG13	1.85	0.57
1:F:409:LEU:C	1:F:409:LEU:HD23	2.25	0.57
1:B:248:VAL:CG2	1:B:314:ILE:HD11	2.35	0.57
1:D:247:PHE:CZ	1:D:270:CYS:HB2	2.40	0.57
1:F:272:THR:CG2	1:F:317:VAL:HG11	2.29	0.57
1:D:258:HIS:HD2	1:D:261:ARG:NH1	2.01	0.57
1:E:86:ARG:HH11	3:F:602:NAI:H72N	1.52	0.57
1:E:275:GLU:OE1	3:E:603:NAI:H2B	2.05	0.56
1:D:178:TRP:O	1:D:182:THR:CG2	2.51	0.56
1:E:245:LYS:HD2	1:E:245:LYS:N	2.20	0.56
1:E:462:ARG:HA	1:E:465:MET:HE2	1.86	0.56
1:C:260:MET:HG2	1:C:288:PRO:HG3	1.87	0.56
1:A:282:ASN:HD22	1:A:284:ASP:H	1.52	0.56
1:D:217:ARG:NH2	4:D:602:GTP:O3G	2.38	0.56
1:A:419:ARG:CZ	5:A:773:HOH:O	2.51	0.56
1:F:294:PHE:CE2	1:F:305:PRO:HD3	2.40	0.56
1:A:141:LEU:O	1:A:145:THR:HG23	2.06	0.56
1:A:166:ALA:HB1	1:A:167:PRO:HD2	1.87	0.56
1:A:349:ASN:HD21	3:A:603:NAI:C6N	2.17	0.56
3:D:605:NAI:C6N	3:D:605:NAI:H52N	2.36	0.56
1:E:258:HIS:HD2	1:E:261:ARG:NH1	1.99	0.56
1:B:272:THR:HG22	1:B:281:TRP:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:GLU:OE2	1:E:478:ARG:NH2	2.38	0.56
1:F:217:ARG:HD3	5:F:765:HOH:O	2.06	0.56
1:F:339:VAL:O	1:F:340:LYS:HG2	2.05	0.56
3:A:603:NAI:O1A	3:A:603:NAI:O1N	2.23	0.56
1:C:282:ASN:HD21	1:C:284:ASP:HB2	1.71	0.56
1:F:44:ARG:HH12	1:F:494:ASN:HD21	1.52	0.56
1:B:112:THR:HG22	1:B:124:GLY:HA3	1.87	0.56
1:B:17:PHE:CD2	1:B:53:LYS:HD2	2.41	0.56
1:D:431:VAL:HG13	1:D:432:PRO:HD2	1.88	0.56
1:F:82:HIS:CD2	1:F:112:THR:CG2	2.84	0.55
3:D:605:NAI:N6A	1:F:120:VAL:O	2.39	0.55
1:C:271:ILE:C	1:C:272:THR:CG2	2.74	0.55
1:F:396:ARG:HG3	1:F:396:ARG:O	2.05	0.55
1:F:328:GLU:HG3	5:F:717:HOH:O	2.06	0.55
1:D:27:LYS:HD3	1:D:487:GLU:OE2	2.05	0.55
1:F:228:ASN:HD21	1:F:241:GLY:HA2	1.71	0.55
1:A:255:VAL:HG22	1:A:325:ALA:HB1	1.87	0.55
1:C:37:THR:HA	1:C:41:LYS:HE3	1.88	0.55
1:C:476:ASP:CG	1:C:479:THR:HG23	2.27	0.55
1:F:333:LYS:HE2	1:F:355:GLU:HG2	1.89	0.55
1:D:101:VAL:O	1:D:105:LYS:HG3	2.07	0.55
1:E:63:PHE:CE1	1:E:75:ILE:HD11	2.42	0.55
1:F:346:GLU:CD	1:F:478:ARG:HH22	2.10	0.55
1:E:248:VAL:CG2	1:E:249:VAL:N	2.70	0.55
1:D:141:LEU:O	1:D:145:THR:CG2	2.55	0.55
1:C:248:VAL:CG2	1:C:249:VAL:N	2.69	0.55
1:C:420:LYS:HB3	1:C:421:PHE:CE2	2.42	0.55
1:B:241:GLY:O	1:B:245:LYS:HD3	2.06	0.55
2:D:601:GLU:C	3:D:603:NAI:C5N	2.75	0.55
1:B:470:LYS:HD3	1:B:471:TYR:CE1	2.41	0.55
1:D:423:LYS:HE2	1:D:423:LYS:H	1.72	0.55
1:D:349:ASN:HD21	3:D:603:NAI:C6N	2.20	0.55
1:C:349:ASN:ND2	3:C:604:NAI:H6N	2.22	0.55
1:C:44:ARG:NH1	1:C:494:ASN:HD21	2.04	0.55
1:E:35:ARG:C	1:E:37:THR:H	2.11	0.55
1:B:211:ARG:HD2	1:B:211:ARG:O	2.07	0.54
1:A:178:TRP:O	1:A:182:THR:HG23	2.06	0.54
1:D:186:THR:HG22	1:D:187:ILE:HD13	1.88	0.54
3:D:605:NAI:C2A	1:F:85:HIS:HE2	2.21	0.54
1:D:19:ARG:CG	1:D:19:ARG:HH11	2.19	0.54
1:A:462:ARG:HA	1:A:465:MET:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:462:ARG:HA	1:F:465:MET:HE2	1.89	0.54
1:D:316:GLU:OE1	1:D:338:ARG:HD2	2.08	0.54
1:D:349:ASN:ND2	3:D:603:NAI:C6N	2.68	0.54
1:A:275:GLU:C	3:A:603:NAI:C2A	2.76	0.54
5:A:772:HOH:O	1:B:456:THR:HG22	2.07	0.54
1:A:16:PHE:CD2	1:A:478:ARG:HD3	2.41	0.54
1:E:353:THR:HB	1:E:354:PRO:HD2	1.88	0.54
1:B:155:LYS:NZ	1:F:189:HIS:HE1	2.06	0.54
1:B:36:GLU:O	1:B:38:GLU:HG2	2.08	0.54
1:D:496:ALA:HB2	1:E:205:GLN:OE1	2.07	0.54
1:C:75:ILE:N	1:C:75:ILE:HD13	2.20	0.54
1:C:241:GLY:O	1:C:245:LYS:HD3	2.07	0.54
2:A:601:GLU:O	3:A:603:NAI:H5N	2.08	0.54
1:D:53:LYS:O	1:D:82:HIS:HE1	1.91	0.54
1:A:501:THR:HG21	1:D:66:ARG:H	1.73	0.54
1:B:166:ALA:HB1	1:B:167:PRO:HD2	1.90	0.54
1:A:396:ARG:O	1:A:396:ARG:HG3	2.06	0.54
1:B:421:PHE:CD2	1:B:421:PHE:N	2.74	0.54
1:B:233:MET:HE2	1:B:236:LEU:HD12	1.90	0.54
1:D:276:SER:HA	3:D:603:NAI:C2A	2.38	0.54
1:E:44:ARG:NH1	1:E:494:ASN:ND2	2.55	0.54
1:E:133:PRO:HG2	1:E:170:SER:HB3	1.90	0.54
1:E:3:ARG:HG3	1:E:4:GLU:N	2.23	0.54
1:E:421:PHE:CD2	1:E:421:PHE:N	2.75	0.54
1:A:56:ASN:N	1:A:56:ASN:HD22	2.05	0.54
1:B:35:ARG:C	1:B:37:THR:H	2.10	0.53
1:D:103:GLU:O	1:D:107:LEU:HD22	2.07	0.53
1:B:392:VAL:CG1	1:C:386:LEU:HD21	2.37	0.53
1:A:356:ALA:O	1:A:360:PHE:CD1	2.60	0.53
1:F:255:VAL:HG22	1:F:325:ALA:HB1	1.90	0.53
1:B:171:THR:HB	1:B:175:GLU:HG3	1.90	0.53
1:D:248:VAL:CG2	1:D:249:VAL:N	2.71	0.53
1:C:275:GLU:HA	3:C:604:NAI:C2A	2.38	0.53
1:D:413:VAL:CG2	1:D:430:ILE:HG13	2.38	0.53
1:C:141:LEU:O	1:C:145:THR:CG2	2.55	0.53
1:F:142:GLU:OE2	1:F:146:ARG:NH1	2.41	0.53
1:C:132:ASN:C	1:C:132:ASN:HD22	2.11	0.53
1:B:354:PRO:HG2	5:B:739:HOH:O	2.07	0.53
1:F:61:LEU:HD11	1:F:148:PHE:CE1	2.44	0.53
2:D:601:GLU:CA	3:D:603:NAI:H4N	2.38	0.53
1:F:282:ASN:ND2	1:F:284:ASP:HB2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MET:HA	3:B:603:NAI:O1N	2.08	0.53
1:D:388:ASN:HA	3:D:605:NAI:H3D	1.91	0.53
1:D:433:THR:HG23	1:E:412:SER:HA	1.90	0.53
1:A:457:MET:CE	1:A:457:MET:HA	2.38	0.53
2:B:601:GLU:C	3:B:603:NAI:H5N	2.29	0.53
1:E:282:ASN:HD22	1:E:284:ASP:H	1.55	0.53
1:D:275:GLU:OE1	3:D:603:NAI:H2B	2.08	0.53
1:F:282:ASN:C	1:F:282:ASN:ND2	2.61	0.53
1:A:186:THR:HG22	1:A:187:ILE:HD13	1.91	0.53
1:B:282:ASN:C	1:B:282:ASN:ND2	2.61	0.53
1:F:476:ASP:CG	1:F:479:THR:HG23	2.30	0.53
1:B:146:ARG:HG2	1:B:182:THR:HG21	1.89	0.53
1:A:133:PRO:HG2	1:A:170:SER:HB3	1.89	0.53
1:B:271:ILE:HG13	1:B:272:THR:HG23	1.90	0.53
1:F:303:GLY:N	1:F:309:ILE:HD11	2.22	0.53
1:D:25:GLU:O	1:D:29:VAL:HG23	2.09	0.53
1:D:35:ARG:C	1:D:37:THR:H	2.12	0.53
1:C:272:THR:OG1	1:C:314:ILE:HD11	2.09	0.52
1:E:275:GLU:CA	3:E:603:NAI:C2A	2.87	0.52
1:A:189:HIS:HE1	1:E:155:LYS:HZ3	1.56	0.52
1:E:354:PRO:HG2	5:E:729:HOH:O	2.08	0.52
1:D:339:VAL:O	1:D:340:LYS:HG2	2.08	0.52
1:B:132:ASN:C	1:B:132:ASN:HD22	2.13	0.52
1:A:91:GLY:O	1:A:165:PRO:HA	2.09	0.52
1:B:238:MET:HE1	1:B:245:LYS:HZ3	1.73	0.52
5:A:749:HOH:O	1:D:500:PHE:HE2	1.91	0.52
1:B:345:ALA:HB1	1:B:373:LEU:HD11	1.91	0.52
1:C:248:VAL:HG22	1:C:249:VAL:N	2.24	0.52
1:E:258:HIS:CD2	1:E:261:ARG:HH11	2.22	0.52
1:F:89:CYS:HB3	1:F:125:ALA:HB2	1.92	0.52
1:C:171:THR:CB	1:C:175:GLU:HG3	2.38	0.52
1:A:348:ALA:HA	3:A:603:NAI:H1D	1.91	0.52
1:A:349:ASN:ND2	3:A:603:NAI:C6N	2.71	0.52
1:C:272:THR:OG1	1:C:314:ILE:CD1	2.58	0.52
1:B:246:THR:HG21	5:B:741:HOH:O	2.09	0.52
1:B:501:THR:HG23	1:E:65:ILE:HD13	1.92	0.52
1:A:111:MET:HE1	1:A:378:VAL:CG1	2.40	0.52
1:D:114:LYS:HE2	1:D:374:ASN:OD1	2.09	0.52
1:F:67:ARG:HD2	1:F:140:GLU:OE1	2.08	0.52
1:B:9:PHE:HE1	1:B:328:GLU:HG2	1.73	0.52
1:E:435:GLU:H	1:E:435:GLU:CD	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ARG:HH22	1:D:494:ASN:ND2	2.08	0.52
1:B:12:MET:HG3	1:B:354:PRO:HD3	1.91	0.52
2:D:601:GLU:HA	3:D:603:NAI:H4N	1.91	0.51
1:D:126:LYS:NZ	2:D:601:GLU:N	2.57	0.51
1:D:44:ARG:NH1	1:D:494:ASN:ND2	2.55	0.51
1:B:189:HIS:HE1	1:F:155:LYS:HZ3	1.57	0.51
1:D:269:LYS:HD3	1:D:284:ASP:O	2.10	0.51
1:B:201:LYS:NZ	1:B:388:ASN:HD21	2.09	0.51
1:F:96:SER:O	1:F:99:VAL:HG13	2.10	0.51
3:F:602:NAI:C6N	3:F:602:NAI:H52N	2.40	0.51
1:B:142:GLU:OE2	1:B:146:ARG:NH1	2.44	0.51
1:B:201:LYS:HZ1	1:B:388:ASN:HD21	1.59	0.51
1:E:272:THR:HG22	1:E:281:TRP:CD1	2.40	0.51
1:F:281:TRP:CZ2	1:F:283:PRO:HG3	2.46	0.51
1:D:185:SER:HB3	1:F:500:PHE:CE2	2.45	0.51
1:A:27:LYS:O	1:A:30:GLU:HB3	2.10	0.51
1:D:248:VAL:HG22	1:D:249:VAL:N	2.25	0.51
1:D:215:THR:HG21	3:D:603:NAI:C7N	2.41	0.51
1:C:248:VAL:CG1	1:C:319:CYS:SG	2.98	0.51
1:A:96:SER:O	1:A:99:VAL:HG13	2.10	0.51
1:A:501:THR:HG23	1:D:65:ILE:HD13	1.93	0.51
1:B:178:TRP:O	1:B:182:THR:CG2	2.59	0.51
1:A:142:GLU:OE2	1:A:146:ARG:NH1	2.43	0.51
1:B:201:LYS:HZ1	1:B:388:ASN:ND2	2.08	0.51
1:A:248:VAL:HB	1:A:272:THR:OG1	2.10	0.51
1:E:271:ILE:HG13	1:E:272:THR:HG23	1.91	0.51
1:B:470:LYS:HG2	1:B:470:LYS:O	2.09	0.51
1:F:61:LEU:HD11	1:F:148:PHE:HE1	1.75	0.51
1:A:211:ARG:HD2	1:A:211:ARG:O	2.10	0.51
1:A:272:THR:HG21	1:A:317:VAL:CG2	2.22	0.51
1:F:248:VAL:CG2	1:F:272:THR:OG1	2.59	0.51
1:C:186:THR:CG2	1:C:187:ILE:N	2.62	0.51
1:C:72:TRP:HB2	1:F:47:SER:CB	2.40	0.51
1:B:72:TRP:HB2	1:E:47:SER:CB	2.41	0.51
1:A:112:THR:HG22	1:A:124:GLY:N	2.26	0.51
1:D:476:ASP:OD2	1:D:479:THR:HG23	2.09	0.51
1:F:258:HIS:CD2	1:F:261:ARG:HH11	2.21	0.51
1:F:186:THR:HG22	1:F:187:ILE:H	1.74	0.51
1:B:482:TYR:O	1:B:486:ILE:HG13	2.10	0.51
1:A:260:MET:HE2	1:A:288:PRO:HG3	1.93	0.51
1:D:427:THR:HG23	1:D:429:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:HIS:HE1	1:D:155:LYS:NZ	2.09	0.51
1:C:409:LEU:C	1:C:409:LEU:HD23	2.31	0.51
1:C:275:GLU:CA	3:C:604:NAI:H2A	2.41	0.50
1:A:47:SER:CB	1:D:72:TRP:HB2	2.34	0.50
1:F:201:LYS:NZ	1:F:388:ASN:HD21	2.09	0.50
2:F:601:GLU:OXT	3:F:604:NAI:C5N	2.59	0.50
1:B:20:GLY:O	1:B:24:VAL:HG22	2.11	0.50
1:C:142:GLU:OE2	1:C:146:ARG:NH1	2.44	0.50
1:C:427:THR:CG2	1:C:429:PRO:HD3	2.41	0.50
1:F:27:LYS:HD3	1:F:487:GLU:OE2	2.11	0.50
1:E:334:SER:O	1:E:337:PRO:HD2	2.11	0.50
1:F:336:ALA:N	1:F:337:PRO:CD	2.74	0.50
3:F:604:NAI:O1A	3:F:604:NAI:O1N	2.30	0.50
3:D:605:NAI:C5D	3:D:605:NAI:N1N	2.71	0.50
1:F:346:GLU:OE2	1:F:478:ARG:NH2	2.43	0.50
1:A:146:ARG:HG2	1:A:182:THR:HG21	1.94	0.50
1:E:303:GLY:H	1:E:309:ILE:HD11	1.77	0.50
1:E:90:LYS:HD3	1:E:122:PHE:CE1	2.46	0.50
1:D:245:LYS:HD2	1:D:245:LYS:N	2.26	0.50
1:F:435:GLU:H	1:F:435:GLU:CD	2.15	0.50
1:E:219:VAL:HA	1:E:373:LEU:HD22	1.93	0.50
1:B:420:LYS:HD2	1:B:421:PHE:HE2	1.76	0.50
1:F:79:ARG:HD2	1:F:127:ALA:HB2	1.93	0.50
1:B:435:GLU:CD	1:B:435:GLU:H	2.15	0.50
1:E:271:ILE:C	1:E:272:THR:CG2	2.79	0.50
1:D:248:VAL:HB	1:D:272:THR:OG1	2.11	0.50
1:F:246:THR:HG22	1:F:320:ASP:H	1.76	0.50
1:B:271:ILE:C	1:B:272:THR:CG2	2.80	0.50
1:A:284:ASP:HB3	5:A:759:HOH:O	2.12	0.50
1:E:274:GLY:O	3:E:603:NAI:H2A	2.12	0.50
1:D:258:HIS:CD2	1:D:261:ARG:HD3	2.47	0.50
1:E:65:ILE:HG13	1:E:144:ILE:HG12	1.93	0.50
1:E:282:ASN:HD21	1:E:284:ASP:HB2	1.75	0.50
1:C:303:GLY:H	1:C:309:ILE:HD11	1.75	0.50
1:C:201:LYS:HZ1	1:C:388:ASN:HD21	1.59	0.50
1:B:34:THR:HG22	1:B:37:THR:N	2.27	0.50
1:D:479:THR:O	1:D:483:VAL:HG23	2.12	0.50
1:B:275:GLU:HB2	1:B:301:ILE:HD11	1.93	0.50
1:E:275:GLU:HB2	1:E:301:ILE:HD11	1.94	0.50
1:F:146:ARG:NH2	1:F:181:ASP:OD2	2.45	0.50
1:A:257:LEU:O	1:A:260:MET:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LYS:NZ	1:C:388:ASN:HD21	2.09	0.50
1:A:456:THR:HG21	1:C:396:ARG:HH21	1.76	0.50
1:C:336:ALA:N	1:C:337:PRO:CD	2.75	0.50
1:B:229:GLU:OE2	1:B:229:GLU:HA	2.12	0.50
1:A:271:ILE:HD11	1:A:319:CYS:HB3	1.94	0.49
1:A:275:GLU:HA	3:A:603:NAI:H2A	1.94	0.49
3:A:603:NAI:H2B	3:A:603:NAI:N3A	2.27	0.49
1:C:271:ILE:C	1:C:272:THR:HG22	2.33	0.49
1:E:452:GLY:O	1:E:456:THR:HG23	2.11	0.49
1:A:303:GLY:H	1:A:309:ILE:HD11	1.77	0.49
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.76	0.49
1:A:35:ARG:C	1:A:37:THR:H	2.16	0.49
1:C:133:PRO:HG2	1:C:170:SER:HB3	1.94	0.49
1:B:246:THR:CG2	1:B:319:CYS:HA	2.42	0.49
1:F:233:MET:HE2	1:F:233:MET:HA	1.94	0.49
1:B:53:LYS:O	1:B:82:HIS:HE1	1.95	0.49
1:E:282:ASN:C	1:E:282:ASN:ND2	2.65	0.49
1:C:452:GLY:O	1:C:456:THR:CG2	2.61	0.49
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.77	0.49
1:A:353:THR:HB	1:A:354:PRO:HD2	1.93	0.49
1:D:281:TRP:O	1:D:307:ALA:HB1	2.13	0.49
1:E:107:LEU:CB	1:E:126:LYS:HG2	2.42	0.49
1:F:275:GLU:CA	3:F:604:NAI:H2A	2.42	0.49
1:F:452:GLY:O	1:F:456:THR:CG2	2.60	0.49
1:B:282:ASN:HD22	1:B:283:PRO:N	2.10	0.49
1:E:396:ARG:O	1:E:396:ARG:HG3	2.12	0.49
1:A:239:THR:O	1:A:245:LYS:HE3	2.11	0.49
1:E:445:GLU:O	1:E:449:VAL:HG23	2.12	0.49
1:A:319:CYS:O	1:A:341:ALA:HA	2.12	0.49
1:C:169:MET:O	1:C:170:SER:HB2	2.12	0.49
1:E:156:GLY:HA2	5:E:713:HOH:O	2.12	0.49
1:D:257:LEU:O	1:D:257:LEU:HD12	2.12	0.49
1:C:258:HIS:CD2	1:C:261:ARG:NH1	2.68	0.49
1:A:388:ASN:HA	3:A:604:NAI:O2D	2.11	0.49
1:B:3:ARG:HG3	1:B:4:GLU:N	2.24	0.49
1:D:226:PHE:O	1:D:228:ASN:N	2.46	0.49
1:E:339:VAL:O	1:E:340:LYS:HG2	2.12	0.49
1:B:44:ARG:HH12	1:B:494:ASN:HD21	1.60	0.49
1:A:56:ASN:N	1:A:56:ASN:ND2	2.60	0.49
1:A:336:ALA:N	1:A:337:PRO:CD	2.76	0.49
1:D:132:ASN:C	1:D:132:ASN:HD22	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:MET:HE1	1:E:378:VAL:CG1	2.43	0.49
1:F:422:GLY:O	1:F:423:LYS:C	2.50	0.49
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.43	0.49
1:E:37:THR:O	1:E:38:GLU:CB	2.61	0.49
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.78	0.49
1:C:452:GLY:O	1:C:456:THR:HG22	2.13	0.49
1:F:219:VAL:HG22	1:F:373:LEU:HD13	1.95	0.49
1:C:257:LEU:O	1:C:257:LEU:HD12	2.13	0.49
1:B:113:TYR:O	1:B:117:VAL:HG23	2.13	0.49
1:F:12:MET:HG3	1:F:354:PRO:HD3	1.95	0.49
1:C:271:ILE:CG1	1:C:272:THR:HG23	2.34	0.49
1:E:226:PHE:C	1:E:228:ASN:H	2.14	0.49
1:D:326:ALA:HB1	3:D:603:NAI:C8A	2.43	0.49
1:E:82:HIS:CD2	1:E:112:THR:CG2	2.83	0.49
1:E:169:MET:HG2	3:E:603:NAI:O1N	2.12	0.49
1:A:282:ASN:HD22	1:A:283:PRO:N	2.11	0.48
1:A:281:TRP:HB2	1:A:310:TYR:HB2	1.94	0.48
1:F:14:GLU:HG2	1:F:53:LYS:HZ2	1.77	0.48
1:A:412:SER:HA	1:B:433:THR:HG23	1.94	0.48
1:A:248:VAL:HG12	1:A:319:CYS:SG	2.52	0.48
1:D:281:TRP:CH2	1:D:283:PRO:HG3	2.47	0.48
1:F:34:THR:O	1:F:37:THR:HB	2.13	0.48
1:B:271:ILE:O	1:B:272:THR:CG2	2.60	0.48
1:C:66:ARG:HB2	1:C:72:TRP:CZ3	2.48	0.48
1:E:211:ARG:HD2	1:E:211:ARG:O	2.13	0.48
1:D:324:PRO:HD2	1:D:345:ALA:O	2.13	0.48
1:D:47:SER:O	1:D:51:ILE:HG13	2.14	0.48
1:F:479:THR:O	1:F:483:VAL:HG23	2.13	0.48
1:E:142:GLU:CG	1:E:146:ARG:HH11	2.26	0.48
1:D:378:VAL:HG13	2:D:601:GLU:HG3	1.94	0.48
1:C:132:ASN:HD22	1:C:133:PRO:N	2.10	0.48
1:A:201:LYS:HZ3	1:A:388:ASN:HD21	1.61	0.48
1:C:24:VAL:HG13	1:C:483:VAL:HG13	1.95	0.48
3:C:605:NAI:H2B	3:C:605:NAI:H8A	1.62	0.48
1:F:434:ALA:HB3	1:F:435:GLU:OE1	2.13	0.48
1:D:388:ASN:HA	3:D:605:NAI:C3D	2.44	0.48
1:D:239:THR:O	1:D:245:LYS:HE3	2.12	0.48
2:B:601:GLU:HA	3:B:603:NAI:C5N	2.42	0.48
1:B:258:HIS:CD2	1:B:261:ARG:HH11	2.22	0.48
1:F:46:ARG:HB3	5:F:711:HOH:O	2.13	0.48
1:D:413:VAL:O	1:D:417:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:PHE:C	1:D:228:ASN:N	2.62	0.48
1:B:227:ILE:HD12	1:B:343:ILE:CD1	2.43	0.48
1:C:47:SER:CB	1:F:72:TRP:HB2	2.43	0.48
1:D:452:GLY:O	1:D:456:THR:HG23	2.13	0.48
1:E:14:GLU:O	1:E:17:PHE:HB3	2.13	0.48
1:A:189:HIS:CE1	1:E:155:LYS:NZ	2.80	0.48
1:D:420:LYS:HB3	1:D:421:PHE:CD2	2.49	0.48
1:A:241:GLY:O	1:A:245:LYS:HD3	2.14	0.48
1:D:281:TRP:HB2	1:D:310:TYR:HB2	1.94	0.48
1:F:246:THR:CG2	1:F:319:CYS:HA	2.43	0.48
1:D:85:HIS:O	3:D:604:NAI:N7N	2.47	0.48
1:C:413:VAL:O	1:C:417:LEU:HG	2.14	0.48
1:F:107:LEU:HB2	1:F:126:LYS:HG2	1.96	0.48
1:B:90:LYS:HD3	1:B:122:PHE:CE1	2.49	0.48
1:F:248:VAL:CG2	1:F:249:VAL:N	2.76	0.47
1:C:272:THR:HG21	1:C:281:TRP:CD1	2.40	0.47
1:F:275:GLU:C	3:F:604:NAI:H2A	2.34	0.47
1:C:281:TRP:HB2	1:C:310:TYR:HB2	1.96	0.47
1:A:246:THR:N	1:A:320:ASP:OD2	2.46	0.47
1:D:169:MET:HA	3:D:603:NAI:O1N	2.14	0.47
1:B:336:ALA:N	1:B:337:PRO:CD	2.77	0.47
1:A:247:PHE:CZ	1:A:270:CYS:HB2	2.50	0.47
1:C:65:ILE:HG13	1:C:144:ILE:HG12	1.97	0.47
1:E:281:TRP:HB2	1:E:310:TYR:HB2	1.95	0.47
1:F:248:VAL:HG13	1:F:322:LEU:HD12	1.95	0.47
1:C:107:LEU:HB3	1:C:126:LYS:HG2	1.95	0.47
1:D:238:MET:HE3	1:D:320:ASP:HB3	1.95	0.47
1:F:153:ALA:HB1	1:F:187:ILE:HG13	1.95	0.47
1:F:387:ASN:O	1:F:387:ASN:ND2	2.48	0.47
1:A:433:THR:HG23	1:C:412:SER:HA	1.95	0.47
1:E:236:LEU:HD22	1:E:342:LYS:HD2	1.96	0.47
1:A:92:GLY:HA2	1:A:166:ALA:O	2.15	0.47
1:F:133:PRO:HG2	1:F:170:SER:HB3	1.96	0.47
1:C:178:TRP:O	1:C:182:THR:CG2	2.62	0.47
1:A:431:VAL:HG13	1:A:432:PRO:CD	2.44	0.47
1:F:316:GLU:OE1	1:F:338:ARG:HD2	2.15	0.47
1:A:215:THR:HG21	3:A:603:NAI:C7N	2.45	0.47
2:F:601:GLU:O	3:F:604:NAI:H5N	2.14	0.47
3:D:605:NAI:C8A	3:D:605:NAI:C3B	2.92	0.47
1:F:186:THR:HG22	1:F:187:ILE:CD1	2.43	0.47
1:E:38:GLU:O	1:E:39:GLU:OE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:LEU:HD23	1:D:409:LEU:O	2.14	0.47
1:E:479:THR:O	1:E:483:VAL:HG23	2.15	0.47
1:E:5:ASP:O	1:E:332:THR:HG22	2.14	0.47
1:A:10:PHE:HA	1:A:106:ALA:HB2	1.97	0.47
1:F:260:MET:HG2	1:F:288:PRO:HG3	1.96	0.47
1:A:155:LYS:NZ	1:E:189:HIS:HE1	2.13	0.47
1:D:186:THR:HG22	1:D:187:ILE:CD1	2.45	0.47
1:B:126:LYS:HZ1	2:B:601:GLU:N	2.13	0.47
1:A:186:THR:CG2	1:A:187:ILE:N	2.71	0.47
1:C:66:ARG:H	1:F:501:THR:HG21	1.80	0.47
1:B:226:PHE:C	1:B:228:ASN:N	2.69	0.47
1:F:107:LEU:HG	1:F:126:LYS:HE2	1.96	0.47
1:F:362:GLU:C	1:F:364:ASN:H	2.18	0.47
1:B:16:PHE:CD2	1:B:478:ARG:HD3	2.50	0.47
1:B:30:GLU:HG3	1:B:31:ASP:N	2.30	0.47
1:A:112:THR:HG22	1:A:124:GLY:H	1.79	0.47
3:A:604:NAI:O2D	3:A:604:NAI:C2N	2.63	0.47
1:A:332:THR:HG22	1:A:353:THR:CG2	2.44	0.47
2:C:601:GLU:O	3:C:604:NAI:H5N	2.15	0.46
1:E:111:MET:CE	1:E:378:VAL:HG11	2.46	0.46
1:A:340:LYS:N	5:A:763:HOH:O	2.16	0.46
1:B:189:HIS:CE1	1:F:155:LYS:NZ	2.80	0.46
1:E:346:GLU:CD	1:E:478:ARG:HH22	2.18	0.46
1:E:94:ARG:NH1	1:E:103:GLU:OE2	2.47	0.46
1:E:201:LYS:HZ1	1:E:388:ASN:ND2	2.14	0.46
1:F:211:ARG:HD2	1:F:211:ARG:O	2.15	0.46
1:A:217:ARG:HD3	5:A:744:HOH:O	2.14	0.46
1:E:178:TRP:O	1:E:182:THR:CG2	2.63	0.46
1:F:37:THR:O	1:F:38:GLU:CG	2.57	0.46
1:D:153:ALA:HB1	1:D:187:ILE:HG13	1.96	0.46
1:D:3:ARG:HG3	1:D:4:GLU:N	2.24	0.46
1:C:384:GLU:O	1:C:387:ASN:HB3	2.15	0.46
1:A:387:ASN:OD1	5:A:724:HOH:O	2.20	0.46
1:C:346:GLU:HG2	1:C:351:PRO:HG2	1.96	0.46
1:D:103:GLU:HG2	1:D:107:LEU:CD2	2.45	0.46
1:F:387:ASN:C	1:F:387:ASN:ND2	2.68	0.46
1:A:332:THR:HG22	1:A:353:THR:HG23	1.98	0.46
1:C:12:MET:HG3	1:C:354:PRO:HD3	1.97	0.46
1:C:323:ILE:O	1:C:323:ILE:HG22	2.15	0.46
1:F:141:LEU:O	1:F:145:THR:CG2	2.63	0.46
1:A:162:VAL:HG22	1:C:190:TYR:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:VAL:CG2	1:D:272:THR:OG1	2.63	0.46
1:F:248:VAL:HG23	1:F:272:THR:OG1	2.16	0.46
3:C:605:NAI:C2N	3:C:605:NAI:O2D	2.63	0.46
3:F:602:NAI:N1N	3:F:602:NAI:C5D	2.78	0.46
1:B:420:LYS:HD2	1:B:421:PHE:CE2	2.50	0.46
1:D:34:THR:HB	1:D:41:LYS:HE2	1.98	0.46
1:B:263:LEU:HD11	1:B:323:ILE:HD11	1.98	0.46
1:F:65:ILE:HG12	1:F:75:ILE:HD11	1.98	0.46
1:D:269:LYS:HA	5:D:711:HOH:O	2.14	0.46
1:F:261:ARG:HH22	4:F:603:GTP:H1'	1.80	0.46
1:C:85:HIS:NE2	3:C:605:NAI:H2A	2.30	0.46
1:D:410:LEU:HD12	1:D:410:LEU:HA	1.65	0.46
3:B:603:NAI:O1N	3:B:603:NAI:O1A	2.33	0.46
1:D:282:ASN:ND2	1:D:282:ASN:C	2.69	0.46
1:D:276:SER:N	3:D:603:NAI:C2A	2.79	0.46
1:B:361:LEU:HA	1:B:361:LEU:HD23	1.82	0.46
1:E:201:LYS:NZ	1:E:388:ASN:HD21	2.13	0.46
1:A:19:ARG:HG2	1:A:479:THR:HG21	1.97	0.46
1:E:115:CYS:HB3	1:E:120:VAL:O	2.17	0.46
1:A:470:LYS:HD3	1:A:471:TYR:CE1	2.51	0.45
2:D:601:GLU:O	3:D:603:NAI:H5N	2.15	0.45
1:E:346:GLU:HG2	1:E:351:PRO:HG2	1.96	0.45
1:C:65:ILE:HA	1:C:65:ILE:HD13	1.78	0.45
1:A:315:LEU:HD13	1:A:331:LEU:CD1	2.46	0.45
1:E:132:ASN:HD22	1:E:134:LYS:H	1.64	0.45
1:F:423:LYS:O	1:F:424:HIS:C	2.55	0.45
1:C:427:THR:HG22	1:C:429:PRO:HD3	1.99	0.45
1:F:247:PHE:CZ	1:F:270:CYS:HB2	2.51	0.45
1:A:308:LYS:O	1:A:310:TYR:N	2.49	0.45
1:F:275:GLU:C	3:F:604:NAI:C2A	2.84	0.45
1:D:19:ARG:CG	1:D:19:ARG:NH1	2.76	0.45
1:E:336:ALA:N	1:E:337:PRO:CD	2.79	0.45
1:D:38:GLU:O	1:D:39:GLU:OE2	2.35	0.45
1:E:30:GLU:HG3	1:E:31:ASP:N	2.31	0.45
1:A:132:ASN:HD22	1:A:133:PRO:HD2	1.81	0.45
1:F:35:ARG:C	1:F:37:THR:H	2.19	0.45
1:C:239:THR:O	1:C:245:LYS:HE3	2.15	0.45
1:E:291:LEU:HD23	1:E:291:LEU:HA	1.80	0.45
2:B:601:GLU:CB	3:B:603:NAI:H4N	2.46	0.45
1:D:239:THR:HG23	1:D:245:LYS:HE3	1.99	0.45
1:D:192:ILE:HD11	1:F:385:TRP:CZ2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:MET:HG2	3:C:604:NAI:H52N	1.98	0.45
1:A:169:MET:O	1:A:170:SER:HB2	2.16	0.45
1:D:246:THR:HG23	1:D:320:ASP:H	1.81	0.45
1:A:201:LYS:HZ1	1:A:388:ASN:HD21	1.61	0.45
1:A:189:HIS:CE1	1:E:155:LYS:HZ1	2.33	0.45
1:E:211:ARG:HD3	1:E:380:VAL:HG12	1.99	0.45
1:B:221:HIS:HE1	5:B:758:HOH:O	1.99	0.45
1:E:91:GLY:O	1:E:165:PRO:HA	2.17	0.45
1:F:132:ASN:C	1:F:132:ASN:HD22	2.19	0.45
1:C:378:VAL:HG13	2:C:601:GLU:HG3	1.99	0.45
3:F:602:NAI:C4D	3:F:602:NAI:O2N	2.65	0.45
1:F:99:VAL:HA	1:F:103:GLU:OE1	2.17	0.45
1:A:19:ARG:HG2	1:A:479:THR:CG2	2.47	0.45
1:A:252:PHE:CZ	1:A:291:LEU:HD13	2.52	0.45
1:E:304:PHE:CD1	1:E:305:PRO:HD2	2.52	0.45
1:B:287:ASP:HA	1:B:288:PRO:HD3	1.82	0.45
1:C:132:ASN:ND2	1:C:134:LYS:H	2.15	0.45
1:D:146:ARG:NE	1:D:182:THR:HG22	2.32	0.45
1:E:356:ALA:O	1:E:360:PHE:CD1	2.70	0.45
1:A:423:LYS:HD3	1:A:423:LYS:N	2.32	0.45
1:B:65:ILE:HD13	1:E:501:THR:HG23	1.97	0.44
1:B:409:LEU:O	1:B:412:SER:HB2	2.16	0.44
1:F:146:ARG:HG2	1:F:182:THR:HG21	1.98	0.44
1:D:315:LEU:HD13	1:D:331:LEU:CD1	2.47	0.44
1:E:275:GLU:C	3:E:603:NAI:C2A	2.85	0.44
1:F:427:THR:CG2	1:F:429:PRO:HD3	2.42	0.44
1:C:172:GLY:H	1:C:175:GLU:CG	2.30	0.44
1:B:227:ILE:HG22	1:B:228:ASN:HB2	2.00	0.44
1:E:255:VAL:CG1	3:E:603:NAI:O5D	2.65	0.44
1:A:339:VAL:O	1:A:340:LYS:CG	2.63	0.44
1:F:169:MET:HG2	3:F:604:NAI:O1N	2.17	0.44
1:E:132:ASN:HD22	1:E:132:ASN:C	2.20	0.44
1:B:363:ARG:NH2	5:B:761:HOH:O	2.03	0.44
1:D:346:GLU:OE2	1:D:478:ARG:NH2	2.50	0.44
1:C:253:GLY:HA3	3:C:604:NAI:O5B	2.17	0.44
1:A:255:VAL:HG13	3:A:603:NAI:O5D	2.17	0.44
1:E:89:CYS:HB3	1:E:125:ALA:HB2	1.99	0.44
1:A:85:HIS:NE2	3:C:603:NAI:H2A	2.31	0.44
1:E:37:THR:O	1:E:38:GLU:CG	2.65	0.44
1:C:246:THR:HG22	1:C:320:ASP:OD2	2.18	0.44
1:B:350:GLY:N	1:B:351:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ARG:HD2	1:B:127:ALA:HB2	1.99	0.44
1:E:310:TYR:HE1	1:E:312:GLY:O	2.01	0.44
1:E:132:ASN:ND2	1:E:134:LYS:H	2.15	0.44
1:D:38:GLU:HB3	1:D:39:GLU:H	1.60	0.44
1:D:308:LYS:N	1:D:308:LYS:HD2	2.32	0.44
1:F:281:TRP:CB	1:F:310:TYR:HB2	2.48	0.44
1:A:82:HIS:CD2	1:A:112:THR:HG23	2.52	0.44
1:D:186:THR:CG2	1:D:187:ILE:N	2.72	0.44
1:C:201:LYS:HZ1	1:C:388:ASN:ND2	2.16	0.44
1:B:491:ARG:HD2	5:B:768:HOH:O	2.18	0.44
1:D:171:THR:CB	1:D:175:GLU:HG3	2.43	0.44
1:B:246:THR:CG2	1:B:320:ASP:H	2.28	0.44
1:B:412:SER:HA	1:C:433:THR:CG2	2.44	0.44
1:D:44:ARG:NH2	1:D:494:ASN:ND2	2.66	0.44
3:D:605:NAI:C2N	3:D:605:NAI:H52N	2.48	0.44
1:B:238:MET:CE	1:B:245:LYS:NZ	2.81	0.44
1:F:486:ILE:O	1:F:487:GLU:C	2.55	0.44
1:F:65:ILE:HD13	1:F:65:ILE:HA	1.84	0.44
1:A:19:ARG:HB2	1:A:19:ARG:HH11	1.82	0.44
1:D:214:ALA:HB1	1:D:380:VAL:HG21	1.99	0.44
1:B:14:GLU:HB3	1:B:53:LYS:NZ	2.33	0.44
1:E:112:THR:HB	1:E:124:GLY:H	1.82	0.44
1:F:63:PHE:CE1	1:F:75:ILE:HD11	2.52	0.44
1:A:113:TYR:O	1:A:117:VAL:HG23	2.18	0.44
1:C:500:PHE:HD2	1:C:500:PHE:H	1.66	0.44
1:B:34:THR:O	1:B:37:THR:HB	2.18	0.43
1:C:245:LYS:HD2	1:C:245:LYS:N	2.32	0.43
1:D:340:LYS:H	1:D:363:ARG:HH22	1.66	0.43
1:A:229:GLU:OE2	1:A:229:GLU:HA	2.18	0.43
1:B:118:VAL:O	1:B:119:ASP:HB2	2.18	0.43
1:E:248:VAL:HG22	1:E:249:VAL:N	2.33	0.43
1:B:501:THR:HG21	1:E:66:ARG:H	1.82	0.43
1:C:346:GLU:HG2	1:C:351:PRO:CG	2.48	0.43
1:B:28:LEU:O	1:B:32:LEU:HB2	2.17	0.43
1:D:205:GLN:OE1	1:F:496:ALA:HB2	2.17	0.43
1:F:166:ALA:HB1	1:F:167:PRO:HD2	1.99	0.43
2:E:601:GLU:O	3:E:603:NAI:H5N	2.18	0.43
1:D:313:SER:HB3	1:D:316:GLU:HG3	1.99	0.43
1:A:448:ILE:HA	1:A:448:ILE:HD13	1.86	0.43
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.90	0.43
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:HG13	1:A:322:LEU:HD12	2.01	0.43
1:E:248:VAL:HG23	1:E:314:ILE:HD11	1.99	0.43
1:C:186:THR:HG22	1:C:187:ILE:HD13	2.01	0.43
1:A:201:LYS:HZ1	1:A:388:ASN:ND2	2.16	0.43
1:E:178:TRP:O	1:E:182:THR:HG23	2.18	0.43
1:A:95:TYR:OH	1:A:145:THR:HB	2.18	0.43
1:C:189:HIS:HE1	1:D:155:LYS:HZ3	1.66	0.43
1:F:361:LEU:HD23	1:F:361:LEU:HA	1.79	0.43
1:D:314:ILE:HG13	1:D:314:ILE:O	2.18	0.43
1:A:258:HIS:CD2	1:A:261:ARG:NH1	2.73	0.43
1:C:222:GLY:HA3	1:C:373:LEU:HD23	2.00	0.43
1:B:420:LYS:HB3	1:B:421:PHE:CE2	2.53	0.43
1:C:142:GLU:O	1:C:146:ARG:HG3	2.19	0.43
1:A:354:PRO:O	1:A:357:ASP:HB2	2.18	0.43
1:A:440:ILE:HA	1:A:440:ILE:HD12	1.88	0.43
1:E:274:GLY:C	3:E:603:NAI:H2A	2.39	0.43
1:F:91:GLY:O	1:F:165:PRO:HA	2.18	0.43
1:E:201:LYS:HZ1	1:E:388:ASN:HD21	1.66	0.43
1:A:387:ASN:ND2	1:A:387:ASN:C	2.72	0.43
1:C:84:GLN:HB2	1:C:84:GLN:HE21	1.48	0.43
1:D:308:LYS:O	1:D:310:TYR:N	2.52	0.43
1:C:349:ASN:HD21	3:C:604:NAI:H6N	1.82	0.43
1:D:85:HIS:NE2	3:D:604:NAI:N1A	2.64	0.43
1:C:63:PHE:CD1	1:C:147:ARG:HG2	2.54	0.43
1:E:373:LEU:HA	1:E:373:LEU:HD23	1.84	0.43
1:B:24:VAL:HG13	1:B:483:VAL:HG13	2.01	0.43
1:E:420:LYS:HB3	1:E:421:PHE:CE2	2.52	0.43
1:B:346:GLU:OE2	1:B:478:ARG:NH2	2.52	0.43
1:F:63:PHE:CZ	1:F:75:ILE:HG13	2.54	0.43
1:F:169:MET:HA	3:F:604:NAI:O1N	2.19	0.43
1:A:24:VAL:HG13	1:A:483:VAL:HG22	2.00	0.43
1:A:238:MET:HE3	1:A:320:ASP:HB3	2.01	0.43
1:E:410:LEU:HA	1:E:410:LEU:HD12	1.70	0.43
1:E:27:LYS:HD3	1:E:487:GLU:OE2	2.18	0.43
1:F:248:VAL:HG22	1:F:249:VAL:N	2.33	0.43
1:E:255:VAL:HG22	1:E:325:ALA:HB1	2.00	0.43
2:F:601:GLU:OXT	3:F:604:NAI:H5N	2.18	0.43
1:E:9:PHE:O	1:E:13:VAL:HG23	2.19	0.43
1:E:65:ILE:HD13	1:E:65:ILE:HA	1.88	0.43
1:F:388:ASN:HA	3:F:602:NAI:H6N	1.99	0.43
1:B:90:LYS:HD2	1:B:164:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:THR:CG2	1:F:320:ASP:H	2.32	0.42
1:E:226:PHE:C	1:E:228:ASN:N	2.73	0.42
1:B:363:ARG:HD2	5:B:760:HOH:O	2.18	0.42
1:C:370:ASP:O	1:C:372:TYR:N	2.52	0.42
1:C:281:TRP:HB2	1:C:310:TYR:CD2	2.54	0.42
1:F:14:GLU:HG2	1:F:53:LYS:NZ	2.33	0.42
1:B:75:ILE:CD1	1:B:75:ILE:N	2.76	0.42
1:A:103:GLU:O	1:A:107:LEU:HD22	2.20	0.42
1:A:281:TRP:CB	1:A:310:TYR:HB2	2.49	0.42
1:B:38:GLU:HG3	1:B:40:GLN:N	2.18	0.42
1:B:272:THR:OG1	1:B:314:ILE:CD1	2.67	0.42
1:D:227:ILE:HD12	1:D:343:ILE:CD1	2.49	0.42
1:A:63:PHE:CE1	1:A:75:ILE:HD11	2.54	0.42
1:D:185:SER:HB3	1:F:500:PHE:HE2	1.84	0.42
1:A:222:GLY:HA3	1:A:373:LEU:CD2	2.50	0.42
1:E:443:ALA:HB2	1:F:401:TYR:CE2	2.55	0.42
1:E:500:PHE:HB3	1:F:146:ARG:HE	1.85	0.42
1:D:361:LEU:HD23	1:D:361:LEU:HA	1.84	0.42
1:E:457:MET:HA	1:E:457:MET:CE	2.49	0.42
1:B:205:GLN:OE1	1:C:496:ALA:HB2	2.20	0.42
1:F:281:TRP:HB3	1:F:310:TYR:HB2	2.02	0.42
1:C:182:THR:O	1:C:186:THR:HB	2.19	0.42
1:F:95:TYR:OH	1:F:145:THR:HB	2.20	0.42
1:E:287:ASP:HA	1:E:288:PRO:HD3	1.85	0.42
1:F:355:GLU:O	1:F:359:ILE:HG12	2.19	0.42
1:D:150:MET:O	1:D:154:LYS:HG3	2.19	0.42
1:B:440:ILE:HA	1:B:440:ILE:HD12	1.83	0.42
1:D:201:LYS:NZ	1:D:388:ASN:HD21	2.17	0.42
1:C:87:THR:HB	1:C:88:PRO:HA	2.01	0.42
1:E:175:GLU:H	1:E:175:GLU:CD	2.23	0.42
1:F:342:LYS:HD3	1:F:342:LYS:HA	1.92	0.42
1:E:152:LEU:HA	1:E:152:LEU:HD23	1.81	0.42
2:D:601:GLU:C	3:D:603:NAI:H5N	2.39	0.42
1:D:91:GLY:O	1:D:165:PRO:HA	2.20	0.42
1:D:294:PHE:CD2	1:D:298:HIS:CE1	3.08	0.42
1:B:452:GLY:O	1:B:456:THR:HG23	2.19	0.42
1:B:245:LYS:HD2	1:B:245:LYS:N	2.34	0.42
1:E:342:LYS:HA	1:E:342:LYS:HD3	1.82	0.42
1:A:387:ASN:HD22	1:A:387:ASN:C	2.22	0.42
2:E:601:GLU:OXT	3:E:603:NAI:C5N	2.67	0.42
1:C:35:ARG:C	1:C:37:THR:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLY:O	1:B:165:PRO:HA	2.20	0.42
1:A:85:HIS:CE1	5:A:726:HOH:O	2.72	0.42
1:F:409:LEU:O	1:F:409:LEU:HD23	2.20	0.42
1:A:30:GLU:HG3	1:A:31:ASP:N	2.33	0.42
1:A:282:ASN:HD21	1:A:284:ASP:HB2	1.85	0.42
1:A:258:HIS:CD2	1:A:261:ARG:HD3	2.55	0.42
1:E:169:MET:HA	3:E:603:NAI:O1A	2.19	0.42
1:B:248:VAL:CG1	1:B:319:CYS:SG	3.08	0.42
1:D:94:ARG:O	1:D:128:GLY:HA2	2.19	0.42
1:D:342:LYS:HD3	1:D:342:LYS:HA	1.80	0.42
1:B:107:LEU:HB3	1:B:126:LYS:HD3	2.01	0.42
1:E:281:TRP:CH2	1:E:283:PRO:HG3	2.54	0.42
1:F:261:ARG:NH2	4:F:603:GTP:H1'	2.34	0.42
1:D:75:ILE:HD13	1:D:75:ILE:N	2.30	0.42
1:B:189:HIS:CE1	1:F:155:LYS:HZ1	2.38	0.42
1:A:260:MET:HG2	1:A:288:PRO:HG3	2.01	0.42
1:E:238:MET:HE1	1:E:245:LYS:HZ3	1.85	0.41
1:A:75:ILE:N	1:A:75:ILE:HD13	2.35	0.41
1:D:69:ASP:OD2	1:D:69:ASP:C	2.58	0.41
1:D:319:CYS:O	1:D:341:ALA:HA	2.20	0.41
3:D:604:NAI:C4N	1:E:205:GLN:O	2.64	0.41
1:F:94:ARG:HG3	1:F:169:MET:HB2	2.01	0.41
1:D:30:GLU:HG3	1:D:31:ASP:N	2.34	0.41
1:A:245:LYS:N	1:A:245:LYS:HD2	2.36	0.41
1:E:433:THR:HG23	1:F:412:SER:HA	2.01	0.41
1:A:491:ARG:HG3	1:A:495:GLU:OE2	2.20	0.41
1:B:410:LEU:HD12	1:B:410:LEU:HA	1.91	0.41
1:E:362:GLU:C	1:E:364:ASN:H	2.24	0.41
1:D:276:SER:N	3:D:603:NAI:H2A	2.31	0.41
1:E:349:ASN:ND2	3:E:603:NAI:H6N	2.36	0.41
1:A:85:HIS:HE1	5:A:726:HOH:O	2.03	0.41
1:B:227:ILE:CD1	1:B:343:ILE:HD12	2.50	0.41
1:D:200:GLY:HA2	1:D:211:ARG:HG2	2.03	0.41
1:D:282:ASN:HD22	1:D:283:PRO:N	2.17	0.41
1:C:282:ASN:HD22	1:C:283:PRO:N	2.19	0.41
1:D:85:HIS:CE1	5:D:725:HOH:O	2.74	0.41
1:F:169:MET:HG2	3:F:604:NAI:H52N	2.03	0.41
3:C:603:NAI:O5B	3:C:603:NAI:O1N	2.39	0.41
3:C:603:NAI:PA	3:C:603:NAI:H3B	2.60	0.41
1:F:201:LYS:HZ1	1:F:388:ASN:HD21	1.69	0.41
1:F:304:PHE:HA	1:F:305:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:HIS:O	1:C:225:ASN:ND2	2.53	0.41
1:F:239:THR:O	1:F:245:LYS:HE3	2.20	0.41
1:A:349:ASN:ND2	3:A:603:NAI:H2D	2.36	0.41
1:C:187:ILE:HG12	1:C:187:ILE:H	1.58	0.41
1:E:38:GLU:HB3	1:E:39:GLU:H	1.48	0.41
1:A:142:GLU:HA	1:A:178:TRP:CE3	2.55	0.41
1:F:354:PRO:HG2	5:F:725:HOH:O	2.21	0.41
1:B:196:ALA:HB1	1:B:385:TRP:CD1	2.56	0.41
1:A:317:VAL:O	5:A:762:HOH:O	2.21	0.41
1:B:35:ARG:O	1:B:37:THR:HG22	2.21	0.41
1:C:66:ARG:H	1:F:501:THR:CG2	2.34	0.41
1:A:427:THR:CG2	1:A:429:PRO:HD3	2.49	0.41
1:B:391:HIS:HE1	5:B:734:HOH:O	2.04	0.41
1:A:372:TYR:OH	1:A:461:ALA:HB2	2.19	0.41
1:D:436:PHE:CZ	1:E:409:LEU:HD12	2.55	0.41
1:D:477:LEU:HD23	1:D:477:LEU:HA	1.84	0.41
1:B:417:LEU:HA	1:B:417:LEU:HD23	1.84	0.41
1:E:248:VAL:CG1	1:E:319:CYS:SG	3.08	0.41
1:F:308:LYS:O	1:F:310:TYR:N	2.54	0.41
1:C:282:ASN:C	1:C:282:ASN:ND2	2.66	0.41
1:B:37:THR:O	1:B:38:GLU:HB3	2.21	0.41
1:C:222:GLY:HA3	1:C:373:LEU:CD2	2.50	0.41
1:E:345:ALA:HB1	1:E:373:LEU:CD1	2.44	0.41
1:B:30:GLU:C	1:B:32:LEU:H	2.24	0.41
1:E:147:ARG:NH2	5:E:701:HOH:O	2.54	0.41
1:D:253:GLY:HA3	3:D:603:NAI:O5B	2.21	0.41
1:C:126:LYS:HD2	1:C:126:LYS:HA	1.87	0.41
1:C:132:ASN:HD22	1:C:133:PRO:CD	2.34	0.41
1:D:414:GLN:HB2	1:D:430:ILE:HG12	2.02	0.41
1:F:423:LYS:O	1:F:425:GLY:N	2.54	0.41
1:F:146:ARG:HE	1:F:182:THR:HG22	1.84	0.41
1:E:458:GLU:OE2	1:E:462:ARG:HD3	2.21	0.41
1:C:287:ASP:HA	1:C:288:PRO:HD3	1.82	0.41
1:B:155:LYS:HZ3	1:F:189:HIS:HE1	1.67	0.41
1:A:111:MET:HE1	1:A:378:VAL:HG11	2.03	0.41
1:A:111:MET:HE1	1:A:378:VAL:HG13	2.03	0.41
1:A:287:ASP:HA	1:A:288:PRO:HD3	1.83	0.41
1:A:219:VAL:HG13	1:A:373:LEU:HD11	2.03	0.41
1:A:318:ASP:HA	1:A:340:LYS:HG3	2.03	0.41
1:B:392:VAL:N	3:C:605:NAI:O3D	2.54	0.41
1:D:19:ARG:NH1	1:D:19:ARG:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:GLY:O	1:F:24:VAL:HG22	2.20	0.41
1:E:37:THR:O	1:E:38:GLU:HG3	2.20	0.41
1:D:346:GLU:CD	1:D:478:ARG:HH22	2.25	0.41
1:E:410:LEU:HG	1:E:430:ILE:HG22	2.03	0.41
1:C:342:LYS:HD3	1:C:342:LYS:HA	1.89	0.41
1:C:406:ASN:ND2	5:C:726:HOH:O	2.54	0.41
1:E:417:LEU:HB3	1:E:428:ILE:HD12	2.03	0.41
1:C:17:PHE:CE1	1:C:486:ILE:HG12	2.56	0.41
1:E:111:MET:HB3	1:E:111:MET:HE2	1.91	0.41
1:E:378:VAL:HG13	2:E:601:GLU:HG3	2.03	0.41
1:F:171:THR:CB	1:F:175:GLU:HG3	2.49	0.41
1:F:346:GLU:OE1	1:F:352:THR:HG23	2.21	0.41
1:C:30:GLU:HG3	1:C:31:ASP:N	2.34	0.41
1:C:374:ASN:OD1	1:C:374:ASN:C	2.60	0.41
2:C:601:GLU:HA	3:C:604:NAI:C5N	2.51	0.40
1:F:201:LYS:HZ1	1:F:388:ASN:ND2	2.19	0.40
1:E:86:ARG:HD3	3:F:602:NAI:N7N	2.36	0.40
1:F:44:ARG:NH1	1:F:494:ASN:HD21	2.15	0.40
1:F:257:LEU:HD12	1:F:257:LEU:O	2.21	0.40
1:F:269:LYS:HE3	1:F:269:LYS:HB2	1.89	0.40
1:F:371:LEU:HA	1:F:371:LEU:HD23	1.72	0.40
1:D:17:PHE:CD2	1:D:53:LYS:HD2	2.57	0.40
1:B:65:ILE:HD13	1:B:65:ILE:HA	1.81	0.40
1:D:450:HIS:CE1	4:D:602:GTP:O1B	2.74	0.40
1:F:141:LEU:HA	1:F:141:LEU:HD23	1.92	0.40
1:E:339:VAL:HG21	1:E:360:PHE:CE2	2.52	0.40
1:E:110:LEU:HA	1:E:110:LEU:HD23	1.90	0.40
1:A:361:LEU:HD23	1:A:361:LEU:HA	1.64	0.40
1:B:192:ILE:HD11	1:C:389:LEU:HD11	2.03	0.40
1:A:72:TRP:CD1	1:D:47:SER:HB3	2.56	0.40
1:B:272:THR:HG22	1:B:281:TRP:CD1	2.56	0.40
1:D:96:SER:O	1:D:99:VAL:HG13	2.21	0.40
1:B:227:ILE:HG23	1:B:227:ILE:O	2.21	0.40
1:B:64:PRO:HB3	1:E:51:ILE:HD13	2.02	0.40
1:F:44:ARG:NH1	1:F:494:ASN:ND2	2.70	0.40
1:C:146:ARG:NH2	1:C:181:ASP:OD2	2.54	0.40
1:A:333:LYS:HE3	1:A:333:LYS:HB3	1.91	0.40
1:E:10:PHE:HA	1:E:106:ALA:HB2	2.04	0.40
1:C:36:GLU:O	1:C:37:THR:C	2.60	0.40
1:A:153:ALA:HB1	1:A:187:ILE:HG13	2.04	0.40
1:C:421:PHE:O	1:C:422:GLY:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:THR:HA	1:D:41:LYS:HE3	2.04	0.40
1:A:246:THR:HG22	1:A:320:ASP:H	1.85	0.40
1:A:333:LYS:HE2	1:A:355:GLU:HG2	2.02	0.40
1:C:339:VAL:O	1:C:341:ALA:N	2.54	0.40
1:E:316:GLU:OE1	1:E:338:ARG:HD2	2.22	0.40
1:D:336:ALA:N	1:D:337:PRO:CD	2.84	0.40
1:F:218:GLY:HA3	5:F:766:HOH:O	2.20	0.40
1:A:275:GLU:C	3:A:603:NAI:H2A	2.41	0.40
1:E:213:SER:HB3	1:E:258:HIS:CD2	2.56	0.40
1:C:61:LEU:C	1:C:61:LEU:HD12	2.41	0.40
1:E:84:GLN:HE21	1:E:84:GLN:HB2	1.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	458 (92%)	31 (6%)	10 (2%)	9 11
1	B	499/501 (100%)	461 (92%)	30 (6%)	8 (2%)	12 16
1	C	499/501 (100%)	468 (94%)	21 (4%)	10 (2%)	9 11
1	D	499/501 (100%)	460 (92%)	28 (6%)	11 (2%)	8 9
1	E	499/501 (100%)	462 (93%)	30 (6%)	7 (1%)	14 19
1	F	499/501 (100%)	468 (94%)	23 (5%)	8 (2%)	12 16
All	All	2994/3006 (100%)	2777 (93%)	163 (5%)	54 (2%)	11 13

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG

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Mol	Chain	Res	Type
1	A	38	GLU
1	B	38	GLU
1	B	422	GLY
1	C	38	GLU
1	C	371	LEU
1	C	422	GLY
1	D	38	GLU
1	D	309	ILE
1	D	422	GLY
1	E	38	GLU
1	E	422	GLY
1	F	424	HIS
1	A	37	THR
1	A	309	ILE
1	A	422	GLY
1	A	424	HIS
1	B	3	ARG
1	B	30	GLU
1	C	3	ARG
1	C	37	THR
1	D	3	ARG
1	D	30	GLU
1	D	498	VAL
1	E	3	ARG
1	E	309	ILE
1	F	3	ARG
1	F	30	GLU
1	F	38	GLU
1	F	309	ILE
1	F	363	ARG
1	A	30	GLU
1	C	30	GLU
1	C	340	LYS
1	D	371	LEU
1	E	173	GLU
1	A	36	GLU
1	A	371	LEU
1	A	498	VAL
1	B	36	GLU
1	B	371	LEU
1	C	309	ILE
1	D	36	GLU

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Mol	Chain	Res	Type
1	D	173	GLU
1	E	36	GLU
1	F	423	LYS
1	B	340	LYS
1	B	498	VAL
1	C	498	VAL
1	D	227	ILE
1	D	165	PRO
1	E	498	VAL
1	F	422	GLY
1	C	317	VAL

5.3.2 Protein sidechains (i)

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	420/420 (100%)	375 (89%)	45 (11%)	8	11
1	B	420/420 (100%)	376 (90%)	44 (10%)	8	12
1	C	420/420 (100%)	373 (89%)	47 (11%)	7	10
1	D	420/420 (100%)	376 (90%)	44 (10%)	8	12
1	E	420/420 (100%)	377 (90%)	43 (10%)	9	13
1	F	420/420 (100%)	375 (89%)	45 (11%)	8	11
All	All	2520/2520 (100%)	2252 (89%)	268 (11%)	8	12

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	35	ARG
1	A	65	ILE
1	A	75	ILE
1	A	84	GLN
1	A	102	ASP
1	A	107	LEU

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Mol	Chain	Res	Type
1	A	112	THR
1	A	132	ASN
1	A	145	THR
1	A	162	VAL
1	A	175	GLU
1	A	182	THR
1	A	187	ILE
1	A	215	THR
1	A	239	THR
1	A	245	LYS
1	A	246	THR
1	A	249	VAL
1	A	255	VAL
1	A	277	ASP
1	A	282	ASN
1	A	291	LEU
1	A	328	GLU
1	A	331	LEU
1	A	340	LYS
1	A	352	THR
1	A	361	LEU
1	A	363	ARG
1	A	364	ASN
1	A	373	LEU
1	A	378	VAL
1	A	381	SER
1	A	386	LEU
1	A	387	ASN
1	A	392	VAL
1	A	396	ARG
1	A	410	LEU
1	A	413	VAL
1	A	423	LYS
1	A	427	THR
1	A	437	GLN
1	A	456	THR
1	A	460	SER
1	A	469	MET
1	B	19	ARG
1	B	35	ARG
1	B	65	ILE
1	B	75	ILE

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Mol	Chain	Res	Type
1	B	79	ARG
1	B	84	GLN
1	B	102	ASP
1	B	107	LEU
1	B	112	THR
1	B	132	ASN
1	B	145	THR
1	B	162	VAL
1	B	182	THR
1	B	187	ILE
1	B	215	THR
1	B	228	ASN
1	B	239	THR
1	B	245	LYS
1	B	246	THR
1	B	248	VAL
1	B	249	VAL
1	B	255	VAL
1	B	282	ASN
1	B	291	LEU
1	B	328	GLU
1	B	331	LEU
1	B	332	THR
1	B	338	ARG
1	B	352	THR
1	B	361	LEU
1	B	363	ARG
1	B	364	ASN
1	B	373	LEU
1	B	378	VAL
1	B	386	LEU
1	B	387	ASN
1	B	392	VAL
1	B	410	LEU
1	B	413	VAL
1	B	427	THR
1	B	437	GLN
1	B	438	ASP
1	B	456	THR
1	B	469	MET
1	C	19	ARG
1	C	24	VAL

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Mol	Chain	Res	Type
1	C	35	ARG
1	C	65	ILE
1	C	75	ILE
1	C	79	ARG
1	C	84	GLN
1	C	96	SER
1	C	99	VAL
1	C	102	ASP
1	C	107	LEU
1	C	112	THR
1	C	132	ASN
1	C	145	THR
1	C	162	VAL
1	C	175	GLU
1	C	182	THR
1	C	215	THR
1	C	227	ILE
1	C	239	THR
1	C	245	LYS
1	C	249	VAL
1	C	255	VAL
1	C	272	THR
1	C	279	SER
1	C	282	ASN
1	C	291	LEU
1	C	328	GLU
1	C	331	LEU
1	C	352	THR
1	C	361	LEU
1	C	364	ASN
1	C	371	LEU
1	C	373	LEU
1	C	378	VAL
1	C	386	LEU
1	C	392	VAL
1	C	402	GLU
1	C	410	LEU
1	C	413	VAL
1	C	421	PHE
1	C	427	THR
1	C	431	VAL
1	C	438	ASP

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Mol	Chain	Res	Type
1	C	456	THR
1	C	469	MET
1	C	479	THR
1	D	19	ARG
1	D	34	THR
1	D	35	ARG
1	D	38	GLU
1	D	60	SER
1	D	61	LEU
1	D	65	ILE
1	D	75	ILE
1	D	79	ARG
1	D	84	GLN
1	D	96	SER
1	D	102	ASP
1	D	107	LEU
1	D	112	THR
1	D	132	ASN
1	D	145	THR
1	D	162	VAL
1	D	175	GLU
1	D	182	THR
1	D	215	THR
1	D	228	ASN
1	D	249	VAL
1	D	255	VAL
1	D	282	ASN
1	D	291	LEU
1	D	295	LYS
1	D	331	LEU
1	D	352	THR
1	D	364	ASN
1	D	371	LEU
1	D	373	LEU
1	D	378	VAL
1	D	381	SER
1	D	386	LEU
1	D	392	VAL
1	D	396	ARG
1	D	402	GLU
1	D	410	LEU
1	D	427	THR

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Mol	Chain	Res	Type
1	D	438	ASP
1	D	456	THR
1	D	460	SER
1	D	469	MET
1	D	479	THR
1	E	19	ARG
1	E	24	VAL
1	E	35	ARG
1	E	65	ILE
1	E	75	ILE
1	E	79	ARG
1	E	84	GLN
1	E	96	SER
1	E	102	ASP
1	E	107	LEU
1	E	112	THR
1	E	132	ASN
1	E	145	THR
1	E	162	VAL
1	E	182	THR
1	E	187	ILE
1	E	215	THR
1	E	228	ASN
1	E	239	THR
1	E	245	LYS
1	E	248	VAL
1	E	249	VAL
1	E	255	VAL
1	E	282	ASN
1	E	291	LEU
1	E	295	LYS
1	E	331	LEU
1	E	332	THR
1	E	352	THR
1	E	361	LEU
1	E	364	ASN
1	E	371	LEU
1	E	373	LEU
1	E	378	VAL
1	E	386	LEU
1	E	392	VAL
1	E	410	LEU

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Mol	Chain	Res	Type
1	E	412	SER
1	E	423	LYS
1	E	427	THR
1	E	437	GLN
1	E	456	THR
1	E	469	MET
1	F	19	ARG
1	F	24	VAL
1	F	35	ARG
1	F	39	GLU
1	F	47	SER
1	F	75	ILE
1	F	84	GLN
1	F	96	SER
1	F	102	ASP
1	F	112	THR
1	F	132	ASN
1	F	145	THR
1	F	162	VAL
1	F	175	GLU
1	F	182	THR
1	F	187	ILE
1	F	212	ILE
1	F	215	THR
1	F	239	THR
1	F	246	THR
1	F	282	ASN
1	F	291	LEU
1	F	331	LEU
1	F	340	LYS
1	F	352	THR
1	F	363	ARG
1	F	364	ASN
1	F	371	LEU
1	F	373	LEU
1	F	378	VAL
1	F	381	SER
1	F	386	LEU
1	F	392	VAL
1	F	396	ARG
1	F	410	LEU
1	F	413	VAL

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Mol	Chain	Res	Type
1	F	423	LYS
1	F	427	THR
1	F	437	GLN
1	F	438	ASP
1	F	441	SER
1	F	456	THR
1	F	460	SER
1	F	469	MET
1	F	479	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	82	HIS
1	A	84	GLN
1	A	132	ASN
1	A	189	HIS
1	A	228	ASN
1	A	254	ASN
1	A	258	HIS
1	A	282	ASN
1	A	298	HIS
1	A	349	ASN
1	A	387	ASN
1	A	388	ASN
1	A	406	ASN
1	A	450	HIS
1	A	494	ASN
1	B	56	ASN
1	B	82	HIS
1	B	84	GLN
1	B	132	ASN
1	B	189	HIS
1	B	254	ASN
1	B	258	HIS
1	B	282	ASN
1	B	387	ASN
1	B	388	ASN
1	B	406	ASN
1	B	408	HIS
1	B	424	HIS

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Mol	Chain	Res	Type
1	B	494	ASN
1	C	56	ASN
1	C	82	HIS
1	C	84	GLN
1	C	132	ASN
1	C	189	HIS
1	C	258	HIS
1	C	282	ASN
1	C	364	ASN
1	C	387	ASN
1	C	388	ASN
1	C	406	ASN
1	C	437	GLN
1	C	494	ASN
1	D	56	ASN
1	D	82	HIS
1	D	84	GLN
1	D	132	ASN
1	D	189	HIS
1	D	228	ASN
1	D	254	ASN
1	D	258	HIS
1	D	282	ASN
1	D	364	ASN
1	D	387	ASN
1	D	406	ASN
1	D	450	HIS
1	D	494	ASN
1	E	56	ASN
1	E	82	HIS
1	E	84	GLN
1	E	132	ASN
1	E	189	HIS
1	E	195	HIS
1	E	228	ASN
1	E	258	HIS
1	E	282	ASN
1	E	387	ASN
1	E	388	ASN
1	E	406	ASN
1	E	437	GLN
1	E	494	ASN

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Mol	Chain	Res	Type
1	F	56	ASN
1	F	82	HIS
1	F	84	GLN
1	F	132	ASN
1	F	189	HIS
1	F	228	ASN
1	F	254	ASN
1	F	258	HIS
1	F	282	ASN
1	F	387	ASN
1	F	388	ASN
1	F	406	ASN
1	F	424	HIS
1	F	437	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

24 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	601	-	3,9,9	0.40	0	2,11,11	0.22	0
4	GTP	A	602	-	25,34,34	2.26	4 (16%)	34,54,54	1.82	7 (20%)
3	NAI	A	603	-	38,48,48	3.66	15 (39%)	48,73,73	2.44	17 (35%)
3	NAI	A	604	-	38,48,48	3.87	14 (36%)	48,73,73	2.84	15 (31%)
2	GLU	B	601	-	3,9,9	0.51	0	2,11,11	0.47	0
4	GTP	B	602	-	25,34,34	2.17	4 (16%)	34,54,54	2.08	8 (23%)
3	NAI	B	603	-	38,48,48	3.43	15 (39%)	48,73,73	2.37	13 (27%)
2	GLU	C	601	-	3,9,9	0.49	0	2,11,11	0.31	0
4	GTP	C	602	-	25,34,34	2.18	4 (16%)	34,54,54	2.54	12 (35%)
3	NAI	C	603	-	38,48,48	3.63	14 (36%)	48,73,73	2.86	13 (27%)
3	NAI	C	604	-	38,48,48	3.64	14 (36%)	48,73,73	2.22	12 (25%)
3	NAI	C	605	-	38,48,48	3.76	13 (34%)	48,73,73	2.69	16 (33%)
2	GLU	D	601	-	3,9,9	0.44	0	2,11,11	0.11	0
4	GTP	D	602	-	25,34,34	2.23	5 (20%)	34,54,54	2.44	11 (32%)
3	NAI	D	603	-	38,48,48	3.58	14 (36%)	48,73,73	2.27	11 (22%)
3	NAI	D	604	-	38,48,48	3.98	16 (42%)	48,73,73	2.83	16 (33%)
3	NAI	D	605	-	38,48,48	3.88	14 (36%)	48,73,73	2.68	11 (22%)
2	GLU	E	601	-	3,9,9	0.35	0	2,11,11	0.02	0
4	GTP	E	602	-	25,34,34	2.22	4 (16%)	34,54,54	2.05	7 (20%)
3	NAI	E	603	-	38,48,48	3.61	15 (39%)	48,73,73	2.08	13 (27%)
2	GLU	F	601	-	3,9,9	0.31	0	2,11,11	0.09	0
3	NAI	F	602	-	38,48,48	3.90	15 (39%)	48,73,73	2.76	14 (29%)
4	GTP	F	603	-	25,34,34	2.17	6 (24%)	34,54,54	2.51	12 (35%)
3	NAI	F	604	-	38,48,48	3.59	14 (36%)	48,73,73	2.32	16 (33%)

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	601	-	-	0/3/9/9	0/0/0/0
4	GTP	A	602	-	-	0/18/38/38	0/3/3/3
3	NAI	A	603	-	3/3/13/16	0/25/72/72	0/5/5/5
3	NAI	A	604	-	1/1/13/16	0/25/72/72	0/5/5/5
2	GLU	B	601	-	-	0/3/9/9	0/0/0/0
4	GTP	B	602	-	-	0/18/38/38	0/3/3/3
3	NAI	B	603	-	1/1/13/16	0/25/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	C	601	-	-	0/3/9/9	0/0/0/0
4	GTP	C	602	-	1/1/7/7	0/18/38/38	0/3/3/3
3	NAI	C	603	-	1/1/13/16	0/25/72/72	0/5/5/5
3	NAI	C	604	-	2/2/13/16	0/25/72/72	0/5/5/5
3	NAI	C	605	-	1/1/13/16	0/25/72/72	0/5/5/5
2	GLU	D	601	-	-	0/3/9/9	0/0/0/0
4	GTP	D	602	-	2/2/7/7	0/18/38/38	0/3/3/3
3	NAI	D	603	-	2/2/13/16	0/25/72/72	0/5/5/5
3	NAI	D	604	-	-	0/25/72/72	0/5/5/5
3	NAI	D	605	-	2/2/13/16	0/25/72/72	0/5/5/5
2	GLU	E	601	-	-	0/3/9/9	0/0/0/0
4	GTP	E	602	-	-	0/18/38/38	0/3/3/3
3	NAI	E	603	-	2/2/13/16	0/25/72/72	0/5/5/5
2	GLU	F	601	-	-	0/3/9/9	0/0/0/0
3	NAI	F	602	-	-	1/25/72/72	0/5/5/5
4	GTP	F	603	-	1/1/7/7	0/18/38/38	0/3/3/3
3	NAI	F	604	-	1/1/13/16	0/25/72/72	0/5/5/5

All (200) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	NAI	O7N-C7N	-2.93	1.17	1.24
3	D	605	NAI	O7N-C7N	-2.81	1.17	1.24
3	D	604	NAI	O7N-C7N	-2.57	1.18	1.24
3	D	603	NAI	O7N-C7N	-2.39	1.18	1.24
4	F	603	GTP	C6-C5	-2.35	1.36	1.41
3	C	603	NAI	O7N-C7N	-2.30	1.18	1.24
3	F	602	NAI	O7N-C7N	-2.23	1.18	1.24
3	E	603	NAI	O7N-C7N	-2.23	1.18	1.24
3	A	603	NAI	O7N-C7N	-2.18	1.19	1.24
3	D	604	NAI	PA-O2A	-2.14	1.45	1.54
3	F	604	NAI	O7N-C7N	-2.13	1.19	1.24
3	B	603	NAI	PA-O2A	-2.10	1.46	1.54
4	D	602	GTP	O4'-C1'	2.00	1.43	1.41
3	F	602	NAI	C5A-N7A	2.00	1.46	1.39
4	F	603	GTP	C2-N1	2.01	1.39	1.35
3	F	604	NAI	PN-O1N	2.03	1.63	1.54
3	D	603	NAI	PN-O1N	2.07	1.63	1.54
3	B	603	NAI	PN-O1N	2.16	1.64	1.54
3	A	603	NAI	C5A-N7A	2.17	1.46	1.39
4	A	602	GTP	PG-O1G	2.21	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	NAI	PN-O1N	2.21	1.64	1.54
3	C	604	NAI	PN-O1N	2.25	1.64	1.54
3	E	603	NAI	PN-O1N	2.26	1.64	1.54
4	C	602	GTP	PG-O1G	2.26	1.58	1.51
4	C	602	GTP	C6-N1	2.26	1.37	1.33
4	D	602	GTP	PG-O1G	2.27	1.58	1.51
3	C	604	NAI	C5A-N7A	2.33	1.47	1.39
3	E	603	NAI	C5A-N7A	2.34	1.47	1.39
3	B	603	NAI	C5A-N7A	2.35	1.47	1.39
3	D	604	NAI	C5A-N7A	2.36	1.47	1.39
4	D	602	GTP	C6-N1	2.38	1.37	1.33
3	C	603	NAI	C6A-N6A	2.38	1.42	1.34
4	B	602	GTP	C6-N1	2.40	1.37	1.33
3	A	603	NAI	PN-O1N	2.42	1.65	1.54
4	E	602	GTP	PG-O1G	2.42	1.59	1.51
4	B	602	GTP	PG-O1G	2.42	1.59	1.51
3	D	605	NAI	C6A-N6A	2.43	1.42	1.34
3	A	604	NAI	PN-O1N	2.44	1.65	1.54
3	F	602	NAI	PN-O1N	2.44	1.65	1.54
3	D	604	NAI	PN-O1N	2.44	1.65	1.54
4	F	603	GTP	PG-O1G	2.45	1.59	1.51
3	C	605	NAI	C6A-N6A	2.46	1.42	1.34
3	C	605	NAI	PN-O1N	2.46	1.65	1.54
4	F	603	GTP	C6-N1	2.49	1.37	1.33
3	A	604	NAI	C6A-N6A	2.52	1.42	1.34
3	D	605	NAI	PN-O1N	2.64	1.66	1.54
4	E	602	GTP	C6-N1	2.68	1.38	1.33
3	C	603	NAI	C5A-C4A	2.68	1.46	1.40
4	A	602	GTP	C6-N1	2.69	1.38	1.33
3	F	602	NAI	C6A-N6A	2.73	1.43	1.34
3	C	605	NAI	C5A-C4A	2.75	1.46	1.40
3	B	603	NAI	C5A-C4A	2.87	1.47	1.40
3	A	604	NAI	C5A-C4A	2.92	1.47	1.40
3	D	604	NAI	C6A-N6A	2.98	1.44	1.34
3	C	605	NAI	C6N-N1N	3.10	1.46	1.37
3	F	604	NAI	PA-O1A	3.11	1.62	1.51
3	B	603	NAI	C6A-N6A	3.12	1.44	1.34
3	E	603	NAI	C6N-N1N	3.14	1.46	1.37
3	C	603	NAI	C6N-N1N	3.15	1.46	1.37
3	C	604	NAI	C6N-N1N	3.29	1.47	1.37
3	A	603	NAI	C6A-N6A	3.32	1.45	1.34
3	F	602	NAI	C5A-C4A	3.33	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	605	NAI	C6N-N1N	3.34	1.47	1.37
3	F	604	NAI	C6N-N1N	3.34	1.47	1.37
3	D	605	NAI	C5A-C4A	3.35	1.48	1.40
3	B	603	NAI	C6N-N1N	3.36	1.47	1.37
3	A	603	NAI	PA-O1A	3.37	1.63	1.51
3	D	603	NAI	C6A-N6A	3.38	1.45	1.34
3	D	604	NAI	C5A-C4A	3.40	1.48	1.40
3	F	604	NAI	C6A-N6A	3.40	1.45	1.34
3	B	603	NAI	PA-O1A	3.41	1.63	1.51
3	C	604	NAI	C6A-N6A	3.41	1.45	1.34
3	D	603	NAI	C6N-N1N	3.42	1.47	1.37
3	D	603	NAI	PA-O1A	3.42	1.63	1.51
3	C	604	NAI	PA-O1A	3.46	1.63	1.51
3	E	603	NAI	C6A-N6A	3.50	1.45	1.34
3	D	603	NAI	O4B-C1B	3.52	1.45	1.41
3	A	603	NAI	C5A-C4A	3.55	1.48	1.40
3	E	603	NAI	PA-O1A	3.59	1.64	1.51
3	A	603	NAI	C6N-N1N	3.65	1.48	1.37
3	D	603	NAI	C5A-C4A	3.66	1.48	1.40
3	C	605	NAI	O4B-C1B	3.69	1.45	1.41
3	F	604	NAI	C5A-C4A	3.73	1.48	1.40
3	D	604	NAI	C6N-N1N	3.74	1.48	1.37
3	C	604	NAI	C5A-C4A	3.80	1.49	1.40
3	B	603	NAI	O4B-C1B	3.83	1.46	1.41
3	D	605	NAI	PA-O1A	3.88	1.65	1.51
3	C	603	NAI	PA-O1A	3.96	1.65	1.51
3	E	603	NAI	C5A-C4A	4.00	1.49	1.40
3	F	602	NAI	PA-O1A	4.05	1.66	1.51
3	D	603	NAI	C7N-N7N	4.06	1.45	1.33
3	A	604	NAI	C6N-N1N	4.09	1.49	1.37
3	C	605	NAI	C7N-N7N	4.12	1.45	1.33
3	C	604	NAI	C7N-N7N	4.14	1.45	1.33
3	B	603	NAI	C7N-N7N	4.14	1.45	1.33
3	A	604	NAI	PA-O1A	4.18	1.66	1.51
3	A	604	NAI	O4B-C1B	4.18	1.46	1.41
3	D	604	NAI	PA-O1A	4.19	1.66	1.51
3	F	602	NAI	C6N-N1N	4.20	1.49	1.37
3	F	602	NAI	C7N-N7N	4.21	1.45	1.33
3	C	603	NAI	O4B-C1B	4.23	1.46	1.41
3	F	604	NAI	C7N-N7N	4.23	1.45	1.33
3	C	605	NAI	PA-O1A	4.24	1.66	1.51
3	D	604	NAI	C7N-N7N	4.31	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	603	GTP	O6-C6	4.35	1.35	1.24
3	A	603	NAI	C7N-N7N	4.36	1.46	1.33
3	E	603	NAI	C7N-N7N	4.40	1.46	1.33
3	A	604	NAI	C7N-N7N	4.42	1.46	1.33
3	F	602	NAI	O4B-C1B	4.44	1.46	1.41
3	E	603	NAI	O4B-C1B	4.47	1.46	1.41
3	C	604	NAI	O4B-C1B	4.48	1.46	1.41
3	D	605	NAI	O4B-C1B	4.54	1.46	1.41
4	B	602	GTP	O6-C6	4.59	1.35	1.24
3	C	603	NAI	C7N-N7N	4.60	1.46	1.33
4	C	602	GTP	O6-C6	4.60	1.35	1.24
4	E	602	GTP	O6-C6	4.67	1.35	1.24
4	D	602	GTP	O6-C6	4.69	1.35	1.24
4	A	602	GTP	O6-C6	4.73	1.36	1.24
3	D	605	NAI	C7N-N7N	4.83	1.47	1.33
3	F	604	NAI	O4B-C1B	4.98	1.47	1.41
3	A	604	NAI	C8A-N7A	5.05	1.44	1.34
3	C	605	NAI	C8A-N7A	5.34	1.44	1.34
3	D	604	NAI	O4B-C1B	5.46	1.48	1.41
3	B	603	NAI	C4A-N3A	5.46	1.43	1.35
3	C	603	NAI	C8A-N7A	5.48	1.45	1.34
3	D	605	NAI	C8A-N7A	5.62	1.45	1.34
3	D	604	NAI	C8A-N7A	5.65	1.45	1.34
3	D	603	NAI	C8A-N7A	5.80	1.45	1.34
3	F	602	NAI	C8A-N7A	5.89	1.45	1.34
3	A	603	NAI	C8A-N7A	6.24	1.46	1.34
3	F	604	NAI	C4A-N3A	6.25	1.44	1.35
3	A	603	NAI	C4A-N3A	6.27	1.44	1.35
3	A	603	NAI	O4B-C1B	6.37	1.49	1.41
4	F	603	GTP	C8-N7	6.43	1.46	1.34
3	C	604	NAI	C4A-N3A	6.46	1.45	1.35
3	C	604	NAI	C8A-N7A	6.53	1.47	1.34
3	F	604	NAI	C8A-N7A	6.53	1.47	1.34
3	E	603	NAI	C8A-N7A	6.68	1.47	1.34
3	C	603	NAI	C2N-C3N	6.76	1.51	1.34
3	E	603	NAI	C4A-N3A	6.78	1.45	1.35
3	B	603	NAI	C8A-N7A	6.82	1.47	1.34
3	D	603	NAI	C4A-N3A	6.84	1.45	1.35
3	A	604	NAI	C2N-C3N	6.85	1.51	1.34
4	B	602	GTP	C8-N7	6.98	1.48	1.34
3	B	603	NAI	C2A-N1A	7.01	1.47	1.33
3	B	603	NAI	C2A-N3A	7.07	1.44	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	602	GTP	C8-N7	7.11	1.48	1.34
3	C	605	NAI	C2N-C3N	7.11	1.52	1.34
4	C	602	GTP	C8-N7	7.11	1.48	1.34
4	A	602	GTP	C8-N7	7.12	1.48	1.34
4	D	602	GTP	C8-N7	7.12	1.48	1.34
3	D	603	NAI	C2N-C3N	7.14	1.52	1.34
3	E	603	NAI	C2N-C3N	7.25	1.52	1.34
3	D	605	NAI	C2N-C3N	7.30	1.52	1.34
3	F	604	NAI	C2N-C3N	7.38	1.52	1.34
3	A	603	NAI	C2N-C3N	7.47	1.53	1.34
3	F	602	NAI	C2N-C3N	7.61	1.53	1.34
3	C	603	NAI	C2A-N1A	7.68	1.48	1.33
3	D	605	NAI	C2A-N1A	7.70	1.48	1.33
3	B	603	NAI	C2N-C3N	7.75	1.53	1.34
3	F	604	NAI	C2A-N1A	7.76	1.48	1.33
3	D	603	NAI	C2A-N1A	7.77	1.48	1.33
3	E	603	NAI	C2A-N1A	7.85	1.48	1.33
3	F	604	NAI	C2A-N3A	7.85	1.46	1.32
3	C	604	NAI	C2A-N3A	7.85	1.46	1.32
3	A	603	NAI	C2A-N1A	7.88	1.48	1.33
3	A	603	NAI	C2A-N3A	7.93	1.46	1.32
3	C	604	NAI	C2N-C3N	7.93	1.54	1.34
3	E	603	NAI	C2A-N3A	7.94	1.46	1.32
3	D	604	NAI	C2A-N1A	7.96	1.49	1.33
3	F	602	NAI	C2A-N1A	7.98	1.49	1.33
3	C	604	NAI	C2A-N1A	8.03	1.49	1.33
3	C	605	NAI	C2A-N1A	8.03	1.49	1.33
3	C	603	NAI	C4A-N3A	8.07	1.47	1.35
3	D	604	NAI	C2N-C3N	8.12	1.54	1.34
3	A	604	NAI	C2A-N1A	8.56	1.50	1.33
3	D	603	NAI	C2A-N3A	8.63	1.47	1.32
3	F	602	NAI	C4A-N3A	8.72	1.48	1.35
3	A	604	NAI	C4A-N3A	8.89	1.48	1.35
3	D	605	NAI	C4A-N3A	9.09	1.49	1.35
3	C	605	NAI	C6N-C5N	9.13	1.51	1.33
3	C	603	NAI	C6N-C5N	9.15	1.51	1.33
3	D	604	NAI	C4A-N3A	9.19	1.49	1.35
3	C	605	NAI	C4A-N3A	9.34	1.49	1.35
3	E	603	NAI	C6N-C5N	9.94	1.52	1.33
3	D	604	NAI	C6N-C5N	9.99	1.52	1.33
3	C	603	NAI	C2A-N3A	10.04	1.49	1.32
3	B	603	NAI	C6N-C5N	10.11	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	604	NAI	C6N-C5N	10.13	1.53	1.33
3	F	602	NAI	C6N-C5N	10.15	1.53	1.33
3	D	605	NAI	C6N-C5N	10.19	1.53	1.33
3	C	604	NAI	C6N-C5N	10.19	1.53	1.33
3	A	603	NAI	C6N-C5N	10.21	1.53	1.33
3	A	604	NAI	C6N-C5N	10.30	1.53	1.33
3	A	604	NAI	C2A-N3A	10.37	1.50	1.32
3	D	603	NAI	C6N-C5N	10.38	1.53	1.33
3	F	602	NAI	C2A-N3A	10.40	1.50	1.32
3	C	605	NAI	C2A-N3A	10.41	1.50	1.32
3	D	604	NAI	C2A-N3A	10.47	1.50	1.32
3	D	605	NAI	C2A-N3A	10.59	1.50	1.32

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	604	NAI	N3A-C2A-N1A	-13.24	118.75	128.89
3	D	605	NAI	N3A-C2A-N1A	-12.80	119.09	128.89
3	A	604	NAI	N3A-C2A-N1A	-12.56	119.28	128.89
3	F	602	NAI	N3A-C2A-N1A	-12.18	119.57	128.89
3	C	603	NAI	N3A-C2A-N1A	-11.63	119.99	128.89
3	C	605	NAI	N3A-C2A-N1A	-9.85	121.35	128.89
3	C	604	NAI	N3A-C2A-N1A	-9.57	121.57	128.89
3	C	603	NAI	PN-O3-PA	-8.85	107.87	132.73
3	E	603	NAI	N3A-C2A-N1A	-8.70	122.23	128.89
3	F	604	NAI	N3A-C2A-N1A	-8.15	122.65	128.89
4	C	602	GTP	C4'-O4'-C1'	-8.10	100.82	109.72
3	A	604	NAI	C2B-C1B-N9A	-7.58	102.71	114.29
3	C	603	NAI	C2B-C1B-N9A	-7.51	102.82	114.29
3	A	603	NAI	N3A-C2A-N1A	-7.45	123.19	128.89
3	B	603	NAI	C1B-N9A-C4A	-7.37	115.82	126.94
3	F	602	NAI	PN-O3-PA	-7.37	112.05	132.73
3	D	603	NAI	N3A-C2A-N1A	-7.15	123.42	128.89
3	A	603	NAI	PN-O3-PA	-6.78	113.69	132.73
3	C	605	NAI	C2B-C1B-N9A	-6.53	104.32	114.29
3	B	603	NAI	N3A-C2A-N1A	-6.53	123.90	128.89
3	D	605	NAI	C2B-C1B-N9A	-6.38	104.54	114.29
3	D	604	NAI	PN-O3-PA	-5.91	116.14	132.73
3	D	603	NAI	PN-O3-PA	-5.85	116.29	132.73
3	A	604	NAI	PN-O3-PA	-5.85	116.30	132.73
3	D	603	NAI	C4B-O4B-C1B	-5.84	103.30	109.72
3	B	603	NAI	PN-O3-PA	-5.61	116.99	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	605	NAI	PN-O3-PA	-5.40	117.57	132.73
3	D	605	NAI	PN-O3-PA	-5.23	118.03	132.73
3	F	604	NAI	PN-O3-PA	-5.07	118.50	132.73
3	F	602	NAI	C2D-C1D-N1N	-5.03	99.77	113.34
4	F	603	GTP	O4'-C4'-C3'	-4.94	95.19	105.15
3	F	602	NAI	C3N-C2N-N1N	-4.83	116.23	123.14
3	D	604	NAI	C1D-N1N-C6N	-4.79	110.09	120.81
3	B	603	NAI	C4A-C5A-N7A	-4.79	105.07	109.48
3	C	605	NAI	C1D-N1N-C6N	-4.73	110.22	120.81
3	C	604	NAI	C4B-O4B-C1B	-4.69	104.57	109.72
4	F	603	GTP	O4'-C1'-N9	-4.54	98.59	108.10
4	F	603	GTP	C2'-C3'-C4'	-4.48	93.41	102.61
3	D	604	NAI	C3N-C2N-N1N	-4.46	116.75	123.14
4	C	602	GTP	O2G-PG-O1G	-4.46	96.23	110.58
3	C	604	NAI	PN-O3-PA	-4.43	120.28	132.73
4	E	602	GTP	O2G-PG-O1G	-4.43	96.32	110.58
3	E	603	NAI	PN-O3-PA	-4.37	120.46	132.73
3	B	603	NAI	C4B-O4B-C1B	-3.96	105.37	109.72
3	C	605	NAI	O4D-C1D-N1N	-3.92	99.80	108.07
3	C	605	NAI	C4B-O4B-C1B	-3.91	105.42	109.72
3	E	603	NAI	C4A-C5A-N7A	-3.90	105.89	109.48
3	F	602	NAI	C4B-O4B-C1B	-3.88	105.45	109.72
3	C	603	NAI	O4D-C1D-N1N	-3.85	99.93	108.07
3	A	604	NAI	C4D-O4D-C1D	-3.84	101.06	109.52
3	C	605	NAI	C3N-C2N-N1N	-3.74	117.78	123.14
3	C	604	NAI	C1B-N9A-C4A	-3.72	121.32	126.94
3	F	604	NAI	C4B-O4B-C1B	-3.62	105.74	109.72
3	A	603	NAI	C4A-C5A-N7A	-3.59	106.18	109.48
4	B	602	GTP	O5'-PA-O1A	-3.58	95.71	109.62
4	F	603	GTP	O2G-PG-O1G	-3.57	99.10	110.58
3	A	604	NAI	C4B-O4B-C1B	-3.55	105.82	109.72
3	A	603	NAI	C4B-O4B-C1B	-3.46	105.92	109.72
3	D	605	NAI	C4B-O4B-C1B	-3.41	105.97	109.72
4	B	602	GTP	O2G-PG-O1G	-3.38	99.71	110.58
3	F	604	NAI	C4A-C5A-N7A	-3.37	106.38	109.48
3	D	604	NAI	C2D-C1D-N1N	-3.37	104.24	113.34
4	D	602	GTP	O5'-PA-O1A	-3.35	96.63	109.62
4	D	602	GTP	O2G-PG-O1G	-3.29	99.98	110.58
3	F	604	NAI	C2D-C1D-N1N	-3.19	104.74	113.34
3	A	603	NAI	C3N-C2N-N1N	-3.16	118.62	123.14
3	E	603	NAI	C3N-C2N-N1N	-3.12	118.67	123.14
3	D	605	NAI	C4D-O4D-C1D	-3.11	102.68	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	602	GTP	N2-C2-N1	-3.08	112.10	117.20
3	D	603	NAI	C3N-C2N-N1N	-3.06	118.76	123.14
3	A	603	NAI	C1B-N9A-C4A	-3.05	122.35	126.94
3	F	602	NAI	C5B-C4B-C3B	-3.01	103.24	115.21
3	E	603	NAI	C1B-N9A-C4A	-3.01	122.39	126.94
3	C	603	NAI	C2D-C1D-N1N	-3.01	105.20	113.34
3	E	603	NAI	C2D-C1D-N1N	-2.97	105.33	113.34
3	D	604	NAI	C4D-O4D-C1D	-2.95	103.02	109.52
3	B	603	NAI	N6A-C6A-N1A	-2.95	112.87	119.20
3	F	602	NAI	C2B-C3B-C4B	-2.95	96.56	102.61
4	A	602	GTP	O2G-PG-O1G	-2.89	101.27	110.58
3	F	602	NAI	C4N-C5N-C6N	-2.89	117.81	122.58
4	C	602	GTP	O5'-PA-O1A	-2.89	98.40	109.62
3	C	604	NAI	C4A-C5A-N7A	-2.86	106.84	109.48
3	D	603	NAI	C2D-C1D-N1N	-2.86	105.63	113.34
3	C	603	NAI	C3N-C2N-N1N	-2.79	119.15	123.14
3	F	604	NAI	C3N-C2N-N1N	-2.78	119.15	123.14
3	B	603	NAI	O7N-C7N-N7N	-2.75	115.93	122.76
3	C	604	NAI	O7N-C7N-N7N	-2.74	115.95	122.76
3	D	605	NAI	C3N-C2N-N1N	-2.71	119.25	123.14
4	E	602	GTP	O5'-PA-O1A	-2.70	99.12	109.62
3	C	603	NAI	C1D-N1N-C6N	-2.70	114.77	120.81
4	B	602	GTP	C1'-N9-C4	-2.69	122.89	126.94
4	F	603	GTP	O5'-PA-O1A	-2.65	99.31	109.62
3	A	604	NAI	C5D-C4D-C3D	-2.64	104.72	115.21
3	D	603	NAI	O7N-C7N-N7N	-2.61	116.27	122.76
4	D	602	GTP	O3'-C3'-C4'	-2.61	103.23	111.05
3	D	604	NAI	C4N-C5N-C6N	-2.59	118.30	122.58
3	D	604	NAI	C2B-C1B-N9A	-2.57	110.36	114.29
3	F	602	NAI	C5D-C4D-C3D	-2.57	105.01	115.21
3	E	603	NAI	C4B-O4B-C1B	-2.55	106.91	109.72
3	F	602	NAI	C1D-N1N-C6N	-2.51	115.20	120.81
4	A	602	GTP	PB-O3B-PG	-2.49	124.33	132.67
3	A	603	NAI	O3D-C3D-C2D	-2.44	103.91	111.83
3	B	603	NAI	C3N-C2N-N1N	-2.43	119.66	123.14
4	B	602	GTP	O4'-C4'-C3'	-2.40	100.30	105.15
3	F	604	NAI	C5D-C4D-C3D	-2.40	105.68	115.21
3	C	603	NAI	C4B-O4B-C1B	-2.39	107.10	109.72
4	A	602	GTP	O5'-PA-O1A	-2.37	100.41	109.62
3	E	603	NAI	C4D-O4D-C1D	-2.35	104.35	109.52
4	D	602	GTP	C5'-C4'-C3'	-2.33	105.97	115.21
3	D	605	NAI	O7N-C7N-N7N	-2.32	117.00	122.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	NAI	O7N-C7N-N7N	-2.31	117.02	122.76
4	C	602	GTP	N2-C2-N1	-2.30	113.40	117.20
3	C	605	NAI	C4N-C5N-C6N	-2.29	118.80	122.58
3	D	603	NAI	C4D-O4D-C1D	-2.28	104.51	109.52
4	F	603	GTP	C5-C6-N1	-2.28	120.48	123.59
3	F	604	NAI	O7N-C7N-N7N	-2.25	117.17	122.76
3	D	605	NAI	C5D-C4D-C3D	-2.24	106.30	115.21
3	C	604	NAI	C1D-N1N-C6N	-2.24	115.81	120.81
3	A	604	NAI	O4D-C1D-N1N	-2.23	103.36	108.07
3	B	603	NAI	O4D-C1D-C2D	-2.22	101.43	106.58
4	B	602	GTP	C6-C5-C4	-2.17	118.31	120.90
4	C	602	GTP	O3'-C3'-C4'	-2.16	104.56	111.05
3	E	603	NAI	O7N-C7N-N7N	-2.16	117.39	122.76
4	F	603	GTP	O2'-C2'-C3'	-2.14	104.86	111.83
3	A	603	NAI	O1N-PN-O5D	-2.13	97.72	108.46
3	D	604	NAI	C5B-C4B-C3B	-2.11	106.82	115.21
3	F	604	NAI	C4D-O4D-C1D	-2.09	104.93	109.52
3	F	604	NAI	C1B-N9A-C4A	-2.06	123.83	126.94
3	D	604	NAI	O7N-C7N-N7N	-2.05	117.67	122.76
3	A	604	NAI	C5B-C4B-C3B	-2.03	107.13	115.21
3	B	603	NAI	O1N-PN-O3	-2.02	95.93	105.09
3	C	603	NAI	C5B-C4B-C3B	-2.02	107.20	115.21
3	A	604	NAI	C1D-N1N-C6N	-2.02	116.30	120.81
4	C	602	GTP	C6-N1-C2	-2.01	113.14	115.94
3	E	603	NAI	C5D-C4D-C3D	-2.01	107.24	115.21
4	D	602	GTP	N3-C2-N1	2.01	130.50	127.44
3	C	604	NAI	C1D-N1N-C2N	2.05	124.47	120.91
3	A	604	NAI	O5D-C5D-C4D	2.05	116.67	109.12
4	B	602	GTP	O2B-PB-O1B	2.07	123.73	112.53
3	C	604	NAI	C5N-C4N-C3N	2.09	118.29	112.52
3	C	604	NAI	C2B-C1B-N9A	2.12	117.53	114.29
3	B	603	NAI	O4B-C1B-N9A	2.13	112.55	108.10
4	C	602	GTP	N3-C2-N1	2.13	130.69	127.44
3	A	603	NAI	O5D-PN-O2N	2.15	117.97	109.62
4	E	602	GTP	O2B-PB-O1B	2.17	124.30	112.53
3	C	605	NAI	O3-PA-O5B	2.19	108.76	102.94
3	F	604	NAI	C2B-C3B-C4B	2.20	107.14	102.61
3	E	603	NAI	O3-PN-O5D	2.25	108.92	102.94
4	F	603	GTP	O2B-PB-O1B	2.28	124.86	112.53
3	A	603	NAI	C2B-C1B-N9A	2.29	117.78	114.29
3	A	603	NAI	C2D-C3D-C4D	2.33	107.41	102.61
3	F	604	NAI	C5N-C4N-C3N	2.35	118.98	112.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	604	NAI	O3-PN-O5D	2.36	109.19	102.94
3	A	603	NAI	C5N-C4N-C3N	2.37	119.05	112.52
3	C	603	NAI	C6N-N1N-C2N	2.38	124.65	118.52
3	A	603	NAI	O4B-C4B-C5B	2.43	118.02	109.32
4	C	602	GTP	O2B-PB-O1B	2.44	125.75	112.53
4	E	602	GTP	O2B-PB-O3B	2.49	116.40	105.09
3	A	604	NAI	N6A-C6A-N1A	2.51	124.60	119.20
3	D	603	NAI	C5N-C4N-C3N	2.56	119.56	112.52
3	E	603	NAI	C2B-C1B-N9A	2.56	118.20	114.29
4	D	602	GTP	C4'-O4'-C1'	2.58	112.55	109.72
4	E	602	GTP	C4'-O4'-C1'	2.66	112.64	109.72
4	F	603	GTP	C2'-C1'-N9	2.67	118.37	114.29
3	D	604	NAI	C5N-C4N-C3N	2.68	119.89	112.52
3	C	605	NAI	C2D-C3D-C4D	2.72	108.21	102.61
3	D	604	NAI	O3-PA-O5B	2.74	110.20	102.94
3	C	605	NAI	N6A-C6A-N1A	2.75	125.11	119.20
4	A	602	GTP	O2B-PB-O1B	2.75	127.45	112.53
3	A	604	NAI	O3-PA-O5B	2.85	110.49	102.94
3	A	603	NAI	O3-PA-O5B	2.86	110.51	102.94
3	F	604	NAI	O3-PA-O5B	2.91	110.64	102.94
3	E	603	NAI	O4D-C1D-N1N	2.92	114.24	108.07
4	A	602	GTP	C4'-O4'-C1'	2.95	112.96	109.72
3	A	604	NAI	C5N-C4N-C3N	2.96	120.67	112.52
3	D	605	NAI	O3-PN-O5D	2.97	110.81	102.94
3	D	604	NAI	C1B-N9A-C4A	2.97	131.43	126.94
3	F	602	NAI	C5N-C4N-C3N	2.99	120.77	112.52
3	C	605	NAI	O3-PN-O5D	3.01	110.92	102.94
3	C	603	NAI	C1B-N9A-C4A	3.05	131.53	126.94
3	D	603	NAI	O4D-C1D-N1N	3.05	114.51	108.07
3	F	602	NAI	C3D-C2D-C1D	3.08	107.59	101.40
3	C	605	NAI	C4A-C5A-N7A	3.09	112.32	109.48
3	F	604	NAI	O4D-C1D-N1N	3.10	114.61	108.07
3	D	604	NAI	C3D-C2D-C1D	3.12	107.68	101.40
4	A	602	GTP	O3G-PG-O2G	3.13	119.29	107.38
3	F	602	NAI	O4B-C1B-N9A	3.14	114.66	108.10
3	C	604	NAI	O3-PN-O5D	3.15	111.29	102.94
3	C	603	NAI	O3-PN-O5D	3.16	111.31	102.94
3	C	605	NAI	C1D-N1N-C2N	3.17	126.42	120.91
3	B	603	NAI	O3-PN-O5D	3.19	111.40	102.94
3	D	604	NAI	O3-PN-O5D	3.30	111.68	102.94
4	C	602	GTP	PA-O3A-PB	3.36	142.17	132.73
3	A	603	NAI	O5B-C5B-C4B	3.38	121.57	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	602	NAI	O3-PN-O5D	3.39	111.93	102.94
3	D	605	NAI	C1B-N9A-C4A	3.47	132.17	126.94
4	F	603	GTP	O3G-PG-O2G	3.58	121.01	107.38
3	C	605	NAI	C1B-N9A-C4A	3.70	132.52	126.94
4	B	602	GTP	O3G-PG-O2G	3.72	121.55	107.38
3	D	605	NAI	C5N-C4N-C3N	3.79	122.96	112.52
3	C	604	NAI	O4D-C1D-N1N	3.82	116.13	108.07
4	C	602	GTP	O4'-C4'-C5'	3.82	122.99	109.32
3	C	605	NAI	C5N-C4N-C3N	3.84	123.10	112.52
4	C	602	GTP	O3G-PG-O2G	3.97	122.50	107.38
4	E	602	GTP	O3G-PG-O2G	4.09	122.97	107.38
3	C	603	NAI	C5N-C4N-C3N	4.12	123.87	112.52
3	F	604	NAI	O3-PN-O5D	4.20	114.08	102.94
4	D	602	GTP	O3G-PG-O2G	4.25	123.56	107.38
3	D	603	NAI	O3-PN-O5D	4.29	114.33	102.94
4	D	602	GTP	PA-O3A-PB	4.36	144.96	132.73
4	D	602	GTP	C2'-C1'-N9	4.40	121.01	114.29
3	A	604	NAI	C1B-N9A-C4A	4.81	134.20	126.94
3	B	603	NAI	C2B-C1B-N9A	4.83	121.66	114.29
3	D	603	NAI	C2B-C1B-N9A	4.93	121.82	114.29
3	D	604	NAI	C1D-N1N-C2N	5.04	129.68	120.91
4	F	603	GTP	PA-O3A-PB	5.06	146.94	132.73
4	A	602	GTP	O3A-PA-O5'	5.90	118.58	102.94
4	C	602	GTP	O3A-PA-O5'	6.18	119.33	102.94
3	F	604	NAI	C2B-C1B-N9A	6.26	123.86	114.29
3	A	603	NAI	O3-PN-O5D	6.76	120.88	102.94
4	F	603	GTP	O3A-PA-O5'	6.79	120.96	102.94
4	E	602	GTP	O3A-PA-O5'	7.21	122.06	102.94
4	B	602	GTP	O3A-PA-O5'	7.32	122.36	102.94
4	D	602	GTP	O3A-PA-O5'	7.56	123.00	102.94

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	605	NAI	C3D
3	D	605	NAI	C4B
3	A	604	NAI	C2D
3	F	604	NAI	C1B
3	D	603	NAI	C1B
3	D	603	NAI	C2B
3	C	604	NAI	C1B
3	C	604	NAI	C2B

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Mol	Chain	Res	Type	Atom
3	C	603	NAI	C2D
4	F	603	GTP	C1'
3	B	603	NAI	C3B
3	E	603	NAI	C1B
3	E	603	NAI	C2B
3	A	603	NAI	C1B
3	A	603	NAI	C2D
3	A	603	NAI	C2B
3	C	605	NAI	C2D
4	C	602	GTP	C1'
4	D	602	GTP	C4'
4	D	602	GTP	C1'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	602	NAI	C2N-C3N-C7N-N7N

There are no ring outliers.

22 monomers are involved in 172 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GLU	5	0
3	A	603	NAI	23	0
3	A	604	NAI	8	0
2	B	601	GLU	8	0
4	B	602	GTP	1	0
3	B	603	NAI	10	0
2	C	601	GLU	9	0
4	C	602	GTP	4	0
3	C	603	NAI	4	0
3	C	604	NAI	15	0
3	C	605	NAI	5	0
2	D	601	GLU	8	0
4	D	602	GTP	2	0
3	D	603	NAI	24	0
3	D	604	NAI	9	0
3	D	605	NAI	11	0
2	E	601	GLU	9	0
3	E	603	NAI	19	0
2	F	601	GLU	7	0
3	F	602	NAI	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	603	GTP	2	0
3	F	604	NAI	16	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	501/501 (100%)	0.20	33 (6%)	22 22	41, 63, 99, 139	0
1	B	501/501 (100%)	0.14	33 (6%)	22 22	37, 61, 98, 140	0
1	C	501/501 (100%)	0.24	43 (8%)	13 13	39, 63, 98, 138	0
1	D	501/501 (100%)	0.28	38 (7%)	17 16	39, 65, 99, 140	0
1	E	501/501 (100%)	0.30	46 (9%)	11 11	38, 68, 103, 138	0
1	F	501/501 (100%)	0.20	46 (9%)	11 11	37, 60, 100, 138	0
All	All	3006/3006 (100%)	0.22	239 (7%)	15 15	37, 63, 101, 140	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	14.4
1	A	1	ALA	11.9
1	E	1	ALA	11.6
1	D	1	ALA	10.4
1	F	1	ALA	10.0
1	C	1	ALA	8.1
1	A	424	HIS	7.8
1	F	424	HIS	7.2
1	D	425	GLY	7.1
1	D	36	GLU	6.3
1	D	3	ARG	6.3
1	D	423	LYS	6.0
1	C	4	GLU	5.8
1	A	501	THR	5.8
1	F	501	THR	5.6
1	B	4	GLU	5.4
1	B	35	ARG	5.4
1	A	2	ASP	5.3
1	D	424	HIS	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	37	THR	5.2
1	C	2	ASP	5.2
1	A	4	GLU	5.2
1	C	36	GLU	5.0
1	E	424	HIS	5.0
1	B	230	ALA	5.0
1	D	4	GLU	4.9
1	D	35	ARG	4.7
1	F	35	ARG	4.7
1	E	345	ALA	4.7
1	B	3	ARG	4.7
1	C	423	LYS	4.7
1	D	2	ASP	4.6
1	F	426	GLY	4.6
1	C	345	ALA	4.6
1	E	35	ARG	4.6
1	A	345	ALA	4.6
1	C	425	GLY	4.6
1	E	323	ILE	4.5
1	E	501	THR	4.4
1	F	2	ASP	4.4
1	C	35	ARG	4.3
1	C	3	ARG	4.2
1	A	423	LYS	4.2
1	D	501	THR	4.2
1	E	36	GLU	4.1
1	D	37	THR	4.1
1	B	33	LYS	4.1
1	E	37	THR	4.0
1	C	40	GLN	4.0
1	F	33	LYS	3.9
1	B	426	GLY	3.9
1	B	2	ASP	3.8
1	F	3	ARG	3.8
1	F	323	ILE	3.8
1	E	302	LEU	3.8
1	E	281	TRP	3.8
1	E	368	ILE	3.8
1	B	323	ILE	3.8
1	A	323	ILE	3.7
1	E	3	ARG	3.7
1	F	368	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	323	ILE	3.7
1	B	40	GLN	3.7
1	F	31	ASP	3.6
1	F	425	GLY	3.6
1	F	36	GLU	3.6
1	A	37	THR	3.5
1	A	3	ARG	3.5
1	B	423	LYS	3.5
1	E	344	ILE	3.5
1	E	298	HIS	3.4
1	D	422	GLY	3.4
1	B	234	SER	3.4
1	D	311	GLU	3.4
1	D	40	GLN	3.4
1	E	243	GLY	3.4
1	E	33	LYS	3.3
1	F	423	LYS	3.3
1	D	30	GLU	3.3
1	F	4	GLU	3.3
1	A	322	LEU	3.3
1	A	40	GLN	3.3
1	A	426	GLY	3.2
1	E	285	GLY	3.2
1	A	36	GLU	3.2
1	D	6	ASP	3.2
1	C	285	GLY	3.2
1	D	33	LYS	3.1
1	C	323	ILE	3.1
1	F	345	ALA	3.1
1	E	31	ASP	3.1
1	E	369	PRO	3.1
1	F	373	LEU	3.1
1	A	33	LYS	3.1
1	D	39	GLU	3.1
1	E	423	LYS	3.1
1	A	31	ASP	3.1
1	B	347	GLY	3.1
1	E	5	ASP	3.1
1	E	371	LEU	3.0
1	C	424	HIS	3.0
1	C	501	THR	3.0
1	D	5	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	348	ALA	3.0
1	E	373	LEU	3.0
1	A	5	ASP	3.0
1	C	33	LYS	3.0
1	B	322	LEU	2.9
1	E	297	GLN	2.9
1	B	37	THR	2.9
1	B	345	ALA	2.9
1	A	368	ILE	2.9
1	C	369	PRO	2.9
1	E	30	GLU	2.9
1	A	344	ILE	2.9
1	A	39	GLU	2.8
1	D	244	ASP	2.8
1	E	4	GLU	2.8
1	F	347	GLY	2.8
1	C	321	ILE	2.8
1	A	30	GLU	2.8
1	D	373	LEU	2.8
1	E	32	LEU	2.8
1	E	308	LYS	2.8
1	A	373	LEU	2.7
1	E	2	ASP	2.7
1	C	281	TRP	2.7
1	A	35	ARG	2.7
1	A	369	PRO	2.7
1	E	309	ILE	2.7
1	F	309	ILE	2.7
1	A	34	THR	2.7
1	C	324	PRO	2.7
1	C	344	ILE	2.7
1	F	325	ALA	2.7
1	D	345	ALA	2.6
1	F	219	VAL	2.6
1	D	31	ASP	2.6
1	F	344	ILE	2.6
1	A	281	TRP	2.6
1	E	234	SER	2.6
1	A	347	GLY	2.6
1	E	40	GLN	2.6
1	B	5	ASP	2.6
1	C	272	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	6	ASP	2.6
1	A	346	GLU	2.6
1	D	297	GLN	2.6
1	B	424	HIS	2.6
1	C	422	GLY	2.5
1	B	344	ILE	2.5
1	B	368	ILE	2.5
1	C	309	ILE	2.5
1	F	374	ASN	2.5
1	C	34	THR	2.5
1	D	38	GLU	2.5
1	E	334	SER	2.5
1	C	308	LYS	2.5
1	C	322	LEU	2.5
1	F	249	VAL	2.5
1	E	230	ALA	2.5
1	C	6	ASP	2.4
1	D	255	VAL	2.4
1	C	325	ALA	2.4
1	E	284	ASP	2.4
1	D	426	GLY	2.4
1	F	422	GLY	2.4
1	C	297	GLN	2.4
1	B	324	PRO	2.4
1	E	311	GLU	2.4
1	C	294	PHE	2.4
1	B	30	GLU	2.4
1	F	8	ASN	2.4
1	F	6	ASP	2.3
1	E	346	GLU	2.3
1	F	324	PRO	2.3
1	C	298	HIS	2.3
1	C	373	LEU	2.3
1	D	322	LEU	2.3
1	F	371	LEU	2.3
1	A	297	GLN	2.3
1	A	425	GLY	2.3
1	F	298	HIS	2.3
1	E	340	LYS	2.3
1	E	322	LEU	2.3
1	F	255	VAL	2.3
1	C	348	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	347	GLY	2.3
1	F	243	GLY	2.3
1	E	39	GLU	2.2
1	F	30	GLU	2.2
1	F	40	GLN	2.2
1	B	348	ALA	2.2
1	B	375	ALA	2.2
1	D	294	PHE	2.2
1	F	322	LEU	2.2
1	A	230	ALA	2.2
1	C	368	ILE	2.2
1	D	243	GLY	2.2
1	B	32	LEU	2.2
1	B	374	ASN	2.2
1	E	313	SER	2.2
1	B	501	THR	2.2
1	E	240	PRO	2.2
1	C	255	VAL	2.2
1	F	367	VAL	2.2
1	E	347	GLY	2.2
1	F	267	GLY	2.2
1	E	321	ILE	2.2
1	F	34	THR	2.2
1	F	369	PRO	2.2
1	D	249	VAL	2.1
1	C	284	ASP	2.1
1	C	37	THR	2.1
1	F	469	MET	2.1
1	D	309	ILE	2.1
1	D	472	ASN	2.1
1	C	333	LYS	2.1
1	B	42	ARG	2.1
1	E	367	VAL	2.1
1	F	308	LYS	2.1
1	B	31	ASP	2.1
1	B	125	ALA	2.1
1	D	256	GLY	2.1
1	F	259	SER	2.1
1	A	374	ASN	2.0
1	B	321	ILE	2.0
1	C	347	GLY	2.0
1	D	298	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	324	PRO	2.0
1	C	31	ASP	2.0
1	B	325	ALA	2.0
1	D	325	ALA	2.0
1	B	367	VAL	2.0
1	C	296	LEU	2.0
1	F	32	LEU	2.0
1	C	219	VAL	2.0
1	F	39	GLU	2.0
1	C	32	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAI	A	604	44/44	0.91	0.18	1.98	42,54,73,83	21
3	NAI	D	605	44/44	0.92	0.18	1.43	45,59,76,81	18
3	NAI	C	605	44/44	0.93	0.17	1.06	41,54,70,82	19
3	NAI	C	603	44/44	0.92	0.16	0.84	44,54,67,78	19
3	NAI	F	602	44/44	0.94	0.16	0.65	47,57,75,81	18
3	NAI	D	604	44/44	0.93	0.15	0.38	42,57,72,80	16
4	GTP	A	602	32/32	0.98	0.15	0.04	58,67,76,81	0
3	NAI	D	603	44/44	0.93	0.19	-0.04	60,69,86,89	0
2	GLU	A	601	10/10	0.96	0.19	-0.09	55,62,68,68	0
3	NAI	B	603	44/44	0.94	0.18	-0.16	47,57,64,72	0
4	GTP	D	602	32/32	0.95	0.15	-0.21	57,76,85,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAI	F	604	44/44	0.94	0.18	-0.22	48,59,65,69	0
4	GTP	C	602	32/32	0.96	0.13	-0.29	62,72,79,84	0
3	NAI	E	603	44/44	0.94	0.15	-0.33	57,72,82,88	0
3	NAI	A	603	44/44	0.93	0.16	-0.43	52,62,69,72	0
4	GTP	F	603	32/32	0.97	0.13	-0.52	50,64,71,76	0
2	GLU	C	601	10/10	0.94	0.17	-0.57	49,57,62,65	0
2	GLU	F	601	10/10	0.97	0.15	-0.64	44,52,63,63	0
3	NAI	C	604	44/44	0.93	0.16	-0.65	49,65,78,82	0
2	GLU	D	601	10/10	0.95	0.16	-0.67	52,60,70,73	0
4	GTP	E	602	32/32	0.98	0.12	-0.69	58,70,81,81	0
4	GTP	B	602	32/32	0.99	0.10	-0.72	50,56,62,67	0
2	GLU	E	601	10/10	0.97	0.15	-0.73	54,61,65,66	0
2	GLU	B	601	10/10	0.96	0.13	-1.37	50,55,58,59	0

6.5 Other polymers

There are no such residues in this entry.