Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:50 PM GMT

PDB ID	:	1H6D
Title	:	OXIDIZED PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE FROM ZYMOMONAS MOBILIS COMPLEXED WITH GLYCEROL
Authors	:	Nurizzo, D.; Baker, E.N.
Deposited on	:	2001-06-12
Resolution	:	2.05 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:

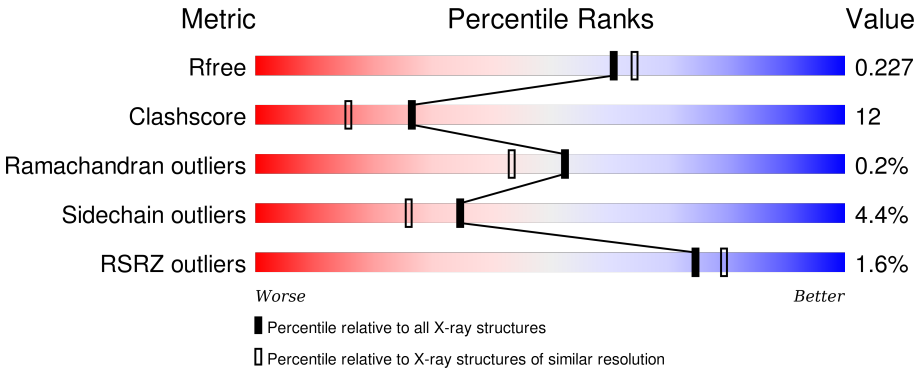
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	433	74% 13% 12%
1	B	433	2% 67% 19% 12%
1	C	433	71% 16% 12%
1	D	433	5% 62% 24% 12%
1	E	433	72% 15% 12%

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Mol	Chain	Length	Quality of chain
1	F	433	3% 59% 26% 12%
1	G	433	% 71% 15% 12%
1	H	433	2% 67% 19% 12%
1	I	433	73% 13% 12%
1	J	433	75% 11% 12%
1	K	433	75% 12% 12%
1	L	433	71% 15% 12%

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
3	GOL	A	600[A]	-	-	-	X
3	GOL	A	600[B]	-	-	-	X
3	GOL	B	600[A]	-	-	-	X
3	GOL	B	600[B]	-	-	-	X
3	GOL	C	600[A]	-	-	X	X
3	GOL	C	600[B]	-	-	-	X
3	GOL	D	600[A]	-	-	-	X
3	GOL	D	600[B]	-	-	X	X
3	GOL	E	600[A]	-	-	X	X
3	GOL	E	600[B]	-	-	-	X
3	GOL	F	600[A]	-	-	-	X
3	GOL	F	600[B]	-	-	-	X
3	GOL	G	600[A]	-	-	-	X
3	GOL	G	600[B]	-	-	-	X
3	GOL	H	600[A]	-	-	-	X
3	GOL	H	600[B]	-	-	-	X
3	GOL	I	600[A]	-	-	-	X
3	GOL	I	600[B]	-	-	-	X
3	GOL	J	600[A]	-	-	-	X
3	GOL	J	600[B]	-	-	-	X
3	GOL	K	600[A]	-	-	-	X
3	GOL	K	600[B]	-	-	-	X
3	GOL	L	600[A]	-	-	X	X
3	GOL	L	600[B]	-	-	-	X

2 Entry composition

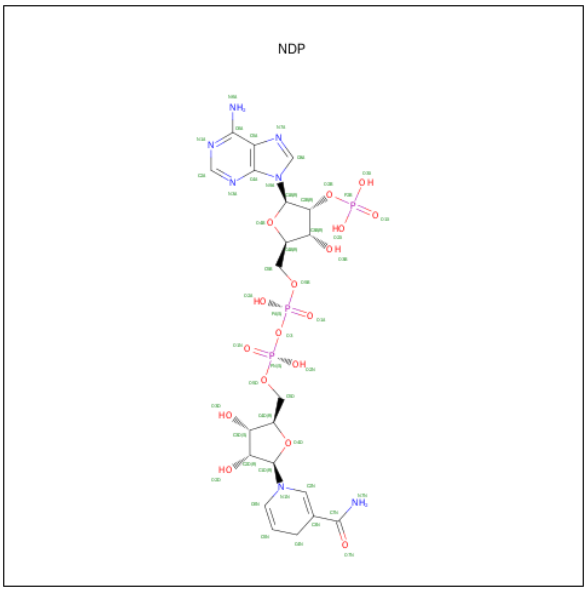
There are 4 unique types of molecules in this entry. The entry contains 40164 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE.

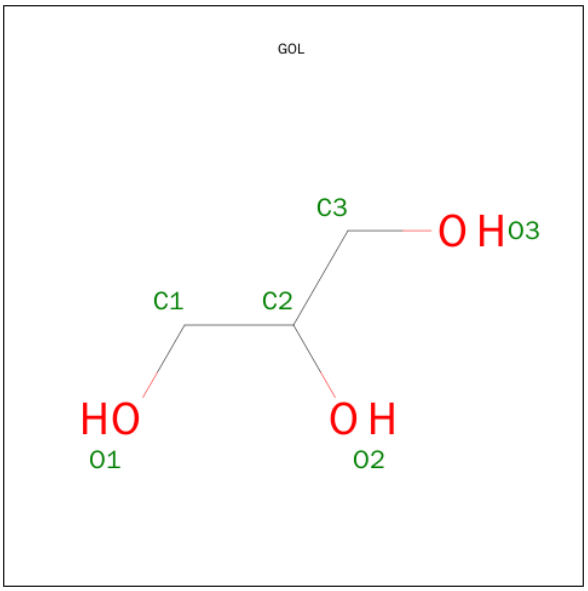
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2970	1862	532	556	20			
1	B	381	Total	C	N	O	S	0	0	0
			2960	1856	530	554	20			
1	C	382	Total	C	N	O	S	0	0	0
			2965	1859	531	555	20			
1	D	382	Total	C	N	O	S	0	0	0
			2965	1859	531	555	20			
1	E	382	Total	C	N	O	S	0	0	0
			2965	1859	531	555	20			
1	F	381	Total	C	N	O	S	0	0	0
			2960	1856	530	554	20			
1	G	381	Total	C	N	O	S	0	0	0
			2960	1856	530	554	20			
1	H	381	Total	C	N	O	S	0	0	0
			2960	1856	530	554	20			
1	I	382	Total	C	N	O	S	0	0	0
			2965	1859	531	555	20			
1	J	381	Total	C	N	O	S	0	0	0
			2960	1856	530	554	20			
1	K	382	Total	C	N	O	S	0	0	0
			2965	1859	531	555	20			
1	L	381	Total	C	N	O	S	0	0	0
			2960	1856	530	554	20			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			7	3	4		
3	B	1	Total	C	O	0	1
			7	3	4		
3	C	1	Total	C	O	0	1
			7	3	4		
3	D	1	Total	C	O	0	1
			7	3	4		
3	E	1	Total	C	O	0	1
			7	3	4		
3	F	1	Total	C	O	0	1
			7	3	4		
3	G	1	Total	C	O	0	1
			7	3	4		
3	H	1	Total	C	O	0	1
			7	3	4		
3	I	1	Total	C	O	0	1
			7	3	4		
3	J	1	Total	C	O	0	1
			7	3	4		
3	K	1	Total	C	O	0	1
			7	3	4		
3	L	1	Total	C	O	0	1
			7	3	4		

- Molecule 4 is water.

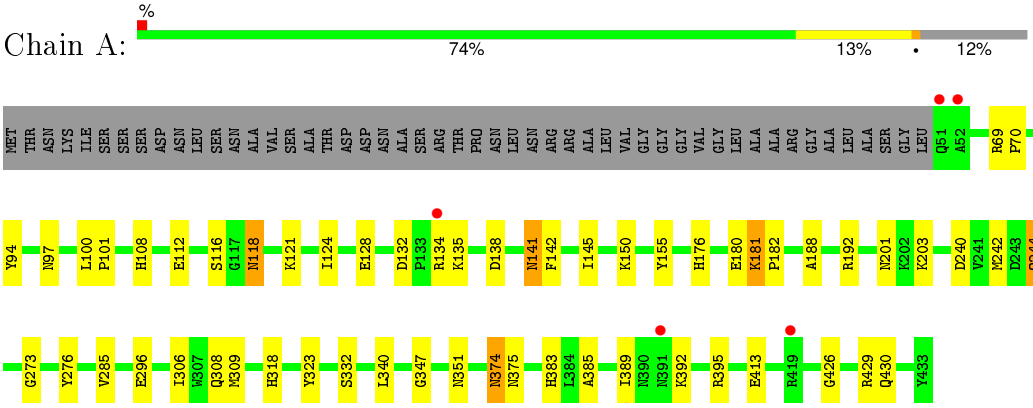
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	390	Total O 390 390	0	0
4	B	295	Total O 295 295	0	0
4	C	320	Total O 320 320	0	0
4	D	213	Total O 213 213	0	0
4	E	341	Total O 341 341	0	0
4	F	219	Total O 219 219	0	0
4	G	371	Total O 371 371	0	0
4	H	289	Total O 289 289	0	0
4	I	391	Total O 391 391	0	0
4	J	377	Total O 377 377	0	0
4	K	386	Total O 386 386	0	0
4	L	357	Total O 357 357	0	0

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.

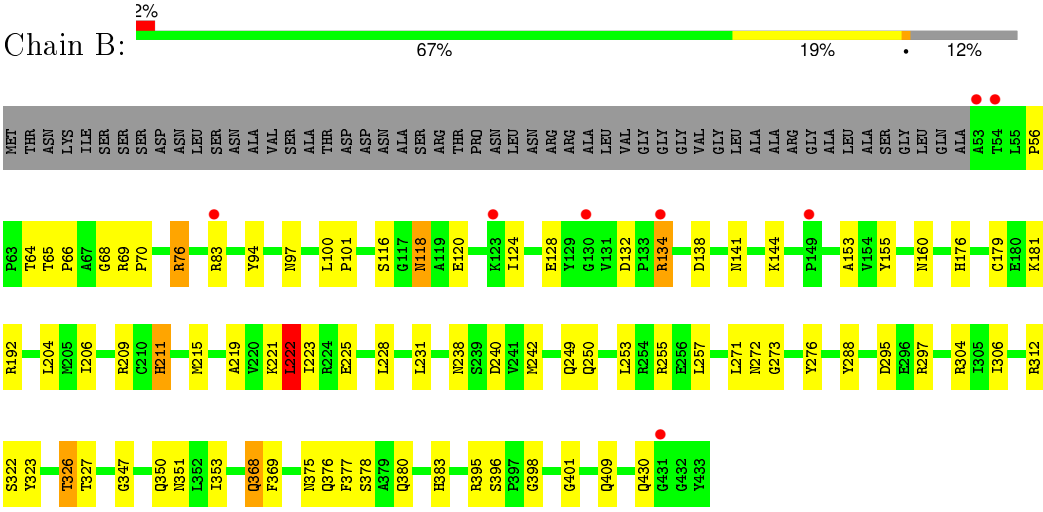
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain A:



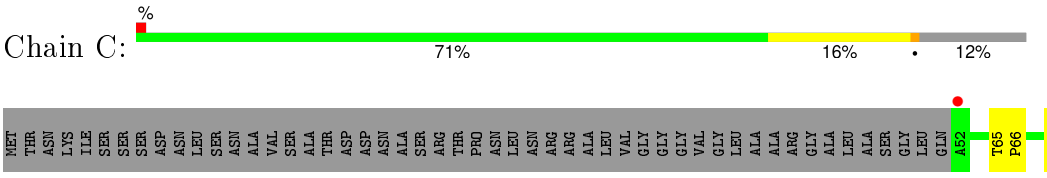
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

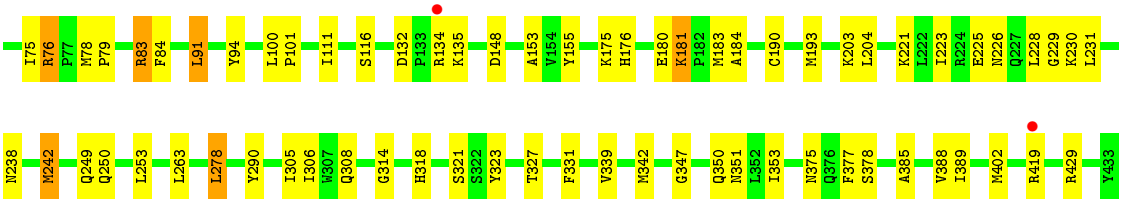
Chain B:



• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

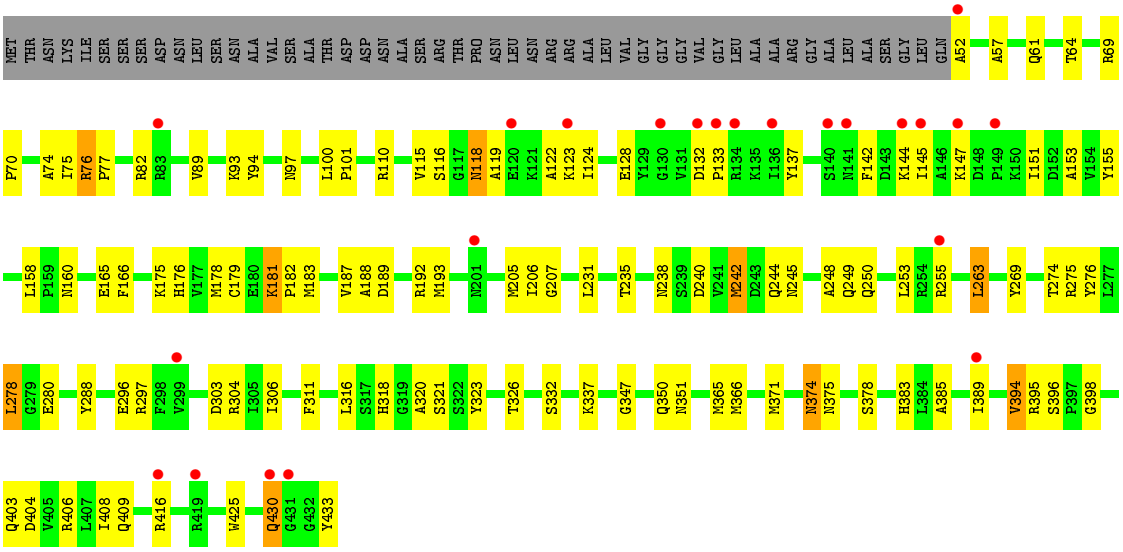
Chain C:





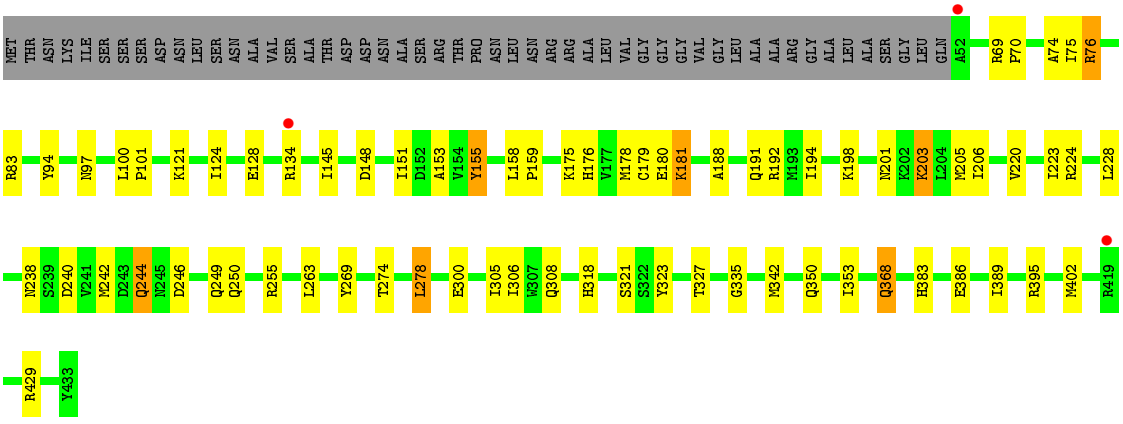
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain D:



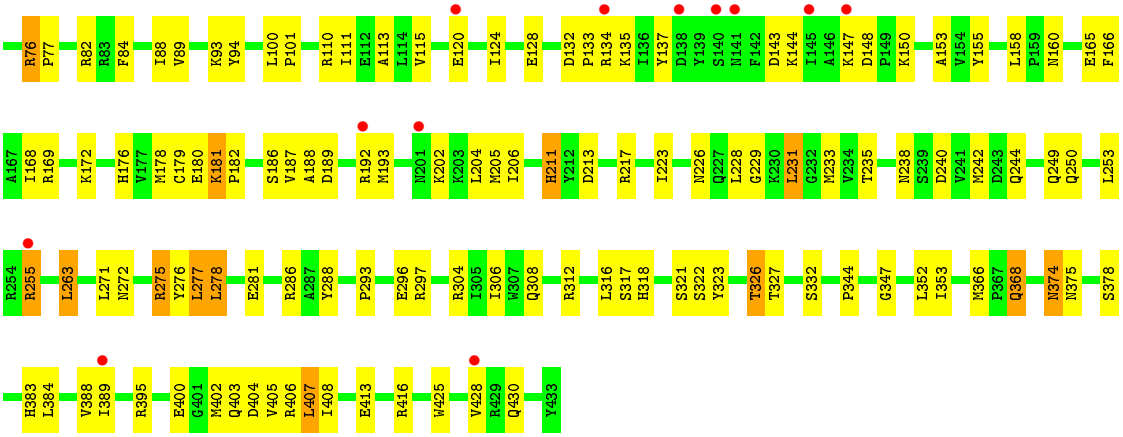
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain E:



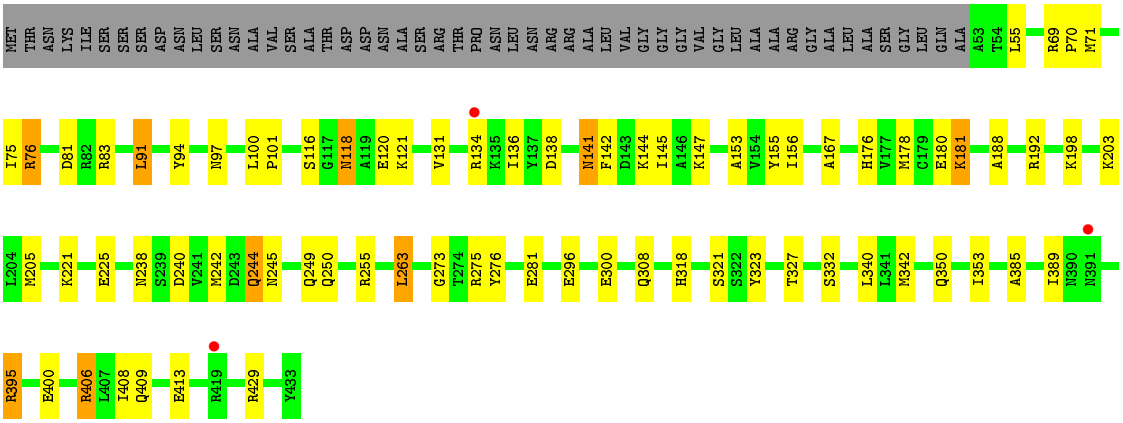
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain F:



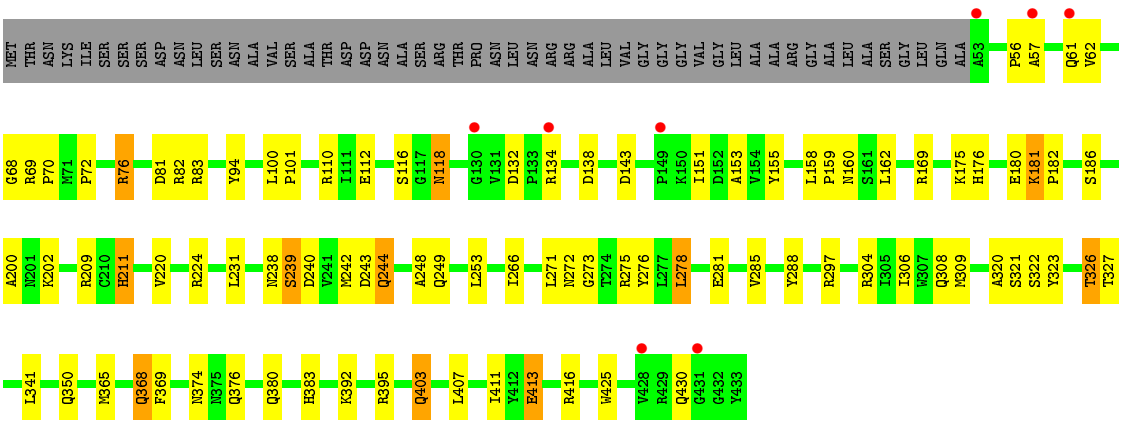
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain G:



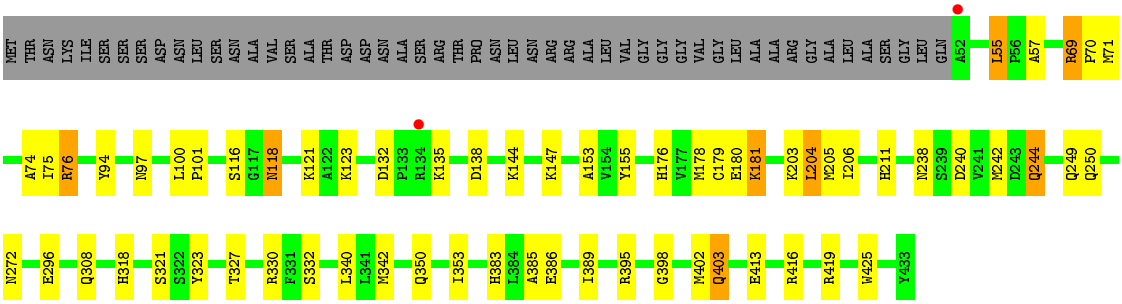
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain H:



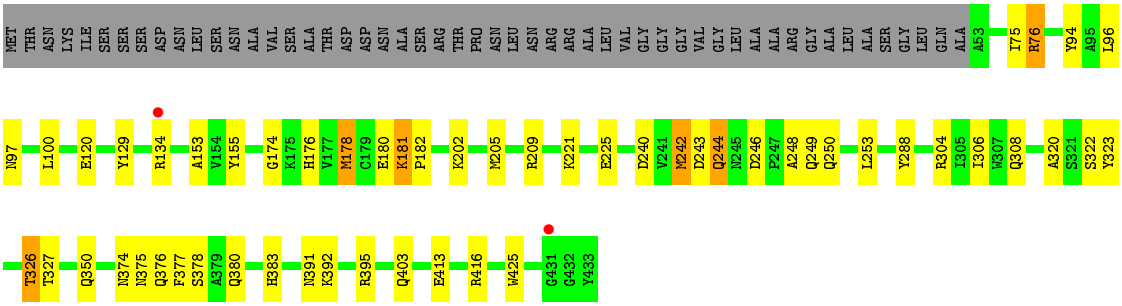
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain I:



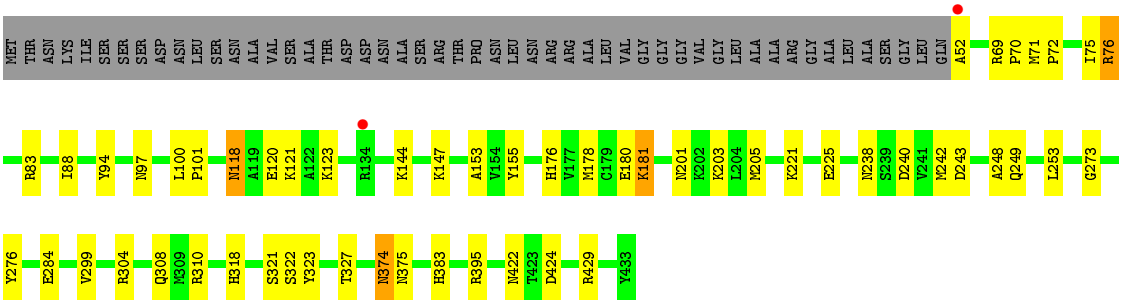
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain J:



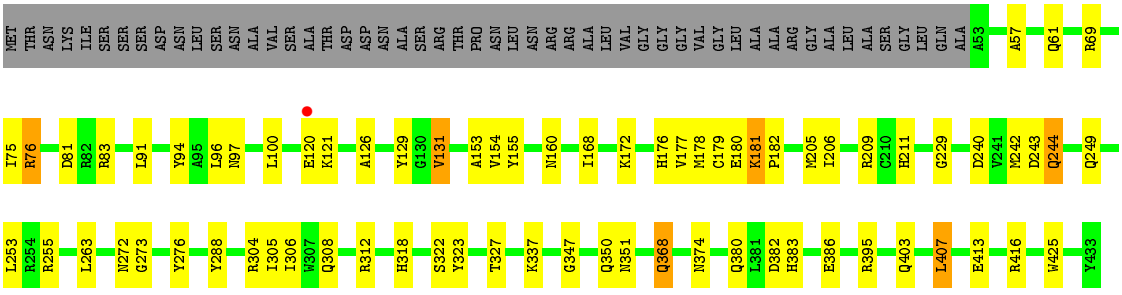
• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain K:



• Molecule 1: PRECURSOR FORM OF GLUCOSE-FRUCTOSE OXIDOREDUCTASE

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.72Å 83.75Å 279.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.05 14.99 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.1 (15.00-2.05) 95.2 (14.99-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.05Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.228 0.197 , 0.227	Depositor DCC
R_{free} test set	1557 reflections (0.49%)	DCC
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 62.3	EDS
Estimated twinning fraction	0.476 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	5 of 317882 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	40164	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.73 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6219e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, NDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.35	0/3034	0.62	0/4107
1	B	0.31	0/3024	0.59	1/4093 (0.0%)
1	C	0.32	0/3029	0.59	0/4100
1	D	0.30	0/3029	0.58	1/4100 (0.0%)
1	E	0.33	0/3029	0.61	0/4100
1	F	0.30	0/3024	0.59	1/4093 (0.0%)
1	G	0.33	0/3024	0.62	0/4093
1	H	0.31	0/3024	0.59	0/4093
1	I	0.34	0/3029	0.61	0/4100
1	J	0.32	0/3024	0.60	0/4093
1	K	0.35	0/3029	0.62	0/4100
1	L	0.33	0/3024	0.62	0/4093
All	All	0.32	0/36323	0.60	3/49165 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	222	LEU	CA-CB-CG	5.87	128.80	115.30
1	F	275	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	275	ARG	NE-CZ-NH2	5.16	122.88	120.30

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	2970	0	2927	57	0
1	B	2960	0	2920	74	0
1	C	2965	0	2925	72	0
1	D	2965	0	2925	102	0
1	E	2965	0	2925	71	0
1	F	2960	0	2920	109	0
1	G	2960	0	2920	70	0
1	H	2960	0	2920	81	0
1	I	2965	0	2925	67	0
1	J	2960	0	2920	64	0
1	K	2965	0	2925	59	0
1	L	2960	0	2920	70	0
2	A	48	0	26	7	0
2	B	48	0	26	5	0
2	C	48	0	26	10	0
2	D	48	0	26	10	0
2	E	48	0	26	10	0
2	F	48	0	26	10	0
2	G	48	0	26	7	0
2	H	48	0	26	8	0
2	I	48	0	26	6	0
2	J	48	0	26	10	0
2	K	48	0	26	9	0
2	L	48	0	26	10	0
3	A	7	0	6	5	0
3	B	7	0	6	4	0
3	C	7	0	6	7	0
3	D	7	0	6	6	0
3	E	7	0	6	8	0
3	F	7	0	6	6	0
3	G	7	0	6	5	0
3	H	7	0	6	5	0
3	I	7	0	6	4	0
3	J	7	0	6	6	0
3	K	7	0	6	5	0
3	L	7	0	6	7	0
4	A	390	0	0	6	0
4	B	295	0	0	3	0
4	C	320	0	0	6	0
4	D	213	0	0	5	0
4	E	341	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	219	0	0	5	0
4	G	371	0	0	7	0
4	H	289	0	0	4	0
4	I	391	0	0	8	0
4	J	377	0	0	4	0
4	K	386	0	0	5	0
4	L	357	0	0	3	0
All	All	40164	0	35456	876	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 12.

All (876) 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:K:500:NDP:H42N	3:K:600[B]:GOL:H31	1.20	1.16
2:G:500:NDP:H42N	3:G:600[B]:GOL:H31	1.27	1.15
2:K:500:NDP:H42N	3:K:600[A]:GOL:H32	1.14	1.13
2:A:500:NDP:H42N	3:A:600[B]:GOL:H31	1.25	1.13
2:B:500:NDP:H42N	3:B:600[A]:GOL:H31	1.15	1.13
1:K:242:MET:HE1	1:K:249:GLN:HB3	1.21	1.12
2:I:500:NDP:H42N	3:I:600[A]:GOL:H32	1.12	1.11
2:H:500:NDP:H42N	3:H:600[B]:GOL:H32	1.12	1.11
2:H:500:NDP:H42N	3:H:600[A]:GOL:H31	1.24	1.10
2:L:500:NDP:H42N	3:L:600[B]:GOL:H32	1.11	1.10
1:H:242:MET:HE1	1:H:249:GLN:HB3	1.22	1.09
2:L:500:NDP:H42N	3:L:600[A]:GOL:H31	1.16	1.09
2:G:500:NDP:H42N	3:G:600[A]:GOL:H32	1.13	1.08
2:B:500:NDP:H42N	3:B:600[B]:GOL:H32	1.15	1.08
2:J:500:NDP:H42N	3:J:600[B]:GOL:H32	1.09	1.08
2:A:500:NDP:H42N	3:A:600[A]:GOL:H32	1.14	1.07
2:I:500:NDP:H42N	3:I:600[B]:GOL:H31	1.15	1.07
2:E:500:NDP:H42N	3:E:600[A]:GOL:H32	1.08	1.07
2:D:500:NDP:H42N	3:D:600[A]:GOL:H31	1.11	1.07
2:F:500:NDP:H42N	3:F:600[A]:GOL:H31	1.07	1.06
2:J:500:NDP:H42N	3:J:600[A]:GOL:H31	1.09	1.06
2:F:500:NDP:H42N	3:F:600[B]:GOL:H32	1.08	1.06
2:C:500:NDP:H42N	3:C:600[A]:GOL:H32	1.08	1.06
2:D:500:NDP:H42N	3:D:600[B]:GOL:H32	1.11	1.06
2:E:500:NDP:C4N	3:E:600[A]:GOL:H32	1.85	1.05
2:E:500:NDP:H42N	3:E:600[B]:GOL:H31	1.05	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:500:NDP:H42N	3:C:600[B]:GOL:H31	1.08	1.05
2:C:500:NDP:C4N	3:C:600[A]:GOL:H32	1.87	1.03
2:L:500:NDP:C4N	3:L:600[A]:GOL:H31	1.89	1.03
1:B:141:ASN:HB2	1:B:144:LYS:HE2	1.40	1.03
2:E:500:NDP:C4N	3:E:600[B]:GOL:H31	1.88	1.02
1:K:242:MET:HE1	1:K:249:GLN:CB	1.89	1.02
2:D:500:NDP:C4N	3:D:600[B]:GOL:H32	1.90	1.01
2:F:500:NDP:C4N	3:F:600[A]:GOL:H31	1.90	1.01
2:J:500:NDP:C4N	3:J:600[A]:GOL:H31	1.91	1.00
2:J:500:NDP:C4N	3:J:600[B]:GOL:H32	1.92	0.99
2:C:500:NDP:C4N	3:C:600[B]:GOL:H31	1.91	0.99
1:L:242:MET:HE1	1:L:249:GLN:HB3	1.45	0.99
1:C:190:CYS:HA	1:C:193:MET:HE3	1.44	0.98
2:F:500:NDP:C4N	3:F:600[B]:GOL:H32	1.92	0.98
2:H:500:NDP:C4N	3:H:600[B]:GOL:H32	1.94	0.97
1:E:145:ILE:HD11	1:E:151:ILE:HG21	1.47	0.97
2:B:500:NDP:C4N	3:B:600[B]:GOL:H32	1.94	0.97
2:K:500:NDP:C4N	3:K:600[B]:GOL:H31	1.93	0.97
1:J:244:GLN:HE21	1:J:244:GLN:H	1.08	0.97
2:H:500:NDP:C4N	3:H:600[A]:GOL:H31	1.94	0.96
2:L:500:NDP:C4N	3:L:600[B]:GOL:H32	1.94	0.96
2:I:500:NDP:C4N	3:I:600[A]:GOL:H32	1.94	0.96
1:B:211:HIS:CE1	1:B:272:ASN:HD21	1.83	0.96
1:E:368:GLN:H	1:E:368:GLN:HE21	1.08	0.95
2:K:500:NDP:C4N	3:K:600[A]:GOL:H32	1.95	0.95
1:I:413:GLU:HA	1:I:416:ARG:HH12	1.29	0.95
1:L:211:HIS:HE1	1:L:272:ASN:HD21	1.06	0.95
2:A:500:NDP:C4N	3:A:600[A]:GOL:H32	1.96	0.94
2:G:500:NDP:C4N	3:G:600[B]:GOL:H31	1.95	0.94
2:A:500:NDP:C4N	3:A:600[B]:GOL:H31	1.96	0.94
2:G:500:NDP:C4N	3:G:600[A]:GOL:H32	1.96	0.94
2:D:500:NDP:C4N	3:D:600[A]:GOL:H31	1.96	0.94
1:I:403:GLN:HE22	1:I:425:TRP:HE1	1.16	0.93
1:A:430:GLN:HE22	1:I:57:ALA:H	1.09	0.93
2:B:500:NDP:C4N	3:B:600[A]:GOL:H31	1.98	0.93
1:B:211:HIS:HE1	1:B:272:ASN:HD21	0.99	0.92
1:C:231:LEU:HD23	1:C:278:LEU:HD12	1.49	0.91
1:I:244:GLN:H	1:I:244:GLN:HE21	0.94	0.91
1:G:244:GLN:HE21	1:G:244:GLN:N	1.69	0.90
1:K:176:HIS:HD2	1:K:203:LYS:H	1.19	0.90
2:I:500:NDP:C4N	3:I:600[B]:GOL:H31	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:242:MET:HE3	1:J:242:MET:HA	1.52	0.90
1:L:211:HIS:CE1	1:L:272:ASN:HD21	1.89	0.90
1:L:368:GLN:HE21	1:L:368:GLN:H	1.12	0.89
1:A:138:ASP:H	1:A:141:ASN:HD21	1.20	0.89
1:G:244:GLN:NE2	1:G:244:GLN:H	1.68	0.89
1:F:263:LEU:HD13	1:F:408:ILE:HG23	1.55	0.89
1:E:244:GLN:HE21	1:E:244:GLN:N	1.71	0.89
1:H:242:MET:HE1	1:H:249:GLN:CB	2.03	0.88
1:I:413:GLU:HA	1:I:416:ARG:NH1	1.87	0.88
1:A:244:GLN:H	1:A:244:GLN:NE2	1.70	0.88
1:A:244:GLN:HE21	1:A:244:GLN:N	1.71	0.88
1:I:176:HIS:HD2	1:I:203:LYS:H	1.20	0.88
1:E:244:GLN:NE2	1:E:244:GLN:H	1.70	0.87
1:L:347:GLY:H	1:L:351:ASN:HD21	1.20	0.86
1:D:263:LEU:HD13	1:D:408:ILE:HG23	1.58	0.85
1:E:176:HIS:HD2	1:E:203:LYS:H	1.24	0.85
1:H:383:HIS:HE1	1:H:395:ARG:H	1.25	0.84
1:B:368:GLN:HE21	1:B:368:GLN:H	1.23	0.84
1:J:383:HIS:HE1	1:J:395:ARG:H	1.26	0.84
1:F:368:GLN:H	1:F:368:GLN:HE21	1.21	0.84
1:L:368:GLN:NE2	1:L:368:GLN:H	1.76	0.83
1:E:383:HIS:HE1	1:E:395:ARG:H	1.27	0.83
1:L:383:HIS:HE1	1:L:395:ARG:H	1.26	0.83
1:J:250:GLN:HE21	1:L:69:ARG:HH22	1.27	0.82
1:L:244:GLN:H	1:L:244:GLN:HE21	1.24	0.82
1:G:406:ARG:HG2	1:G:406:ARG:HH11	1.45	0.82
1:C:190:CYS:HA	1:C:193:MET:CE	2.10	0.81
1:B:69:ARG:HH22	1:D:250:GLN:NE2	1.78	0.81
1:B:69:ARG:HH22	1:D:250:GLN:HE21	1.26	0.81
1:E:145:ILE:HG12	1:E:175:LYS:HE3	1.63	0.80
1:I:55:LEU:HD13	1:K:299:VAL:HB	1.63	0.80
1:C:84:PHE:CE1	1:C:388:VAL:HG11	2.16	0.80
1:B:347:GLY:H	1:B:351:ASN:HD21	1.27	0.80
1:B:211:HIS:HE1	1:B:272:ASN:ND2	1.79	0.79
1:J:403:GLN:HE22	1:J:425:TRP:HE1	1.30	0.79
1:A:176:HIS:HD2	1:A:203:LYS:H	1.29	0.79
1:C:347:GLY:H	1:C:351:ASN:HD21	1.28	0.79
1:E:368:GLN:H	1:E:368:GLN:NE2	1.80	0.79
1:I:383:HIS:HE1	1:I:395:ARG:H	1.29	0.79
1:I:244:GLN:H	1:I:244:GLN:NE2	1.77	0.79
1:D:347:GLY:H	1:D:351:ASN:HD21	1.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:403:GLN:HE22	1:H:425:TRP:HE1	1.31	0.78
1:F:250:GLN:NE2	1:H:69:ARG:HH22	1.82	0.78
1:B:250:GLN:HE21	1:D:69:ARG:HH22	1.32	0.78
1:H:383:HIS:CE1	1:H:395:ARG:H	2.01	0.78
1:D:383:HIS:HE1	1:D:395:ARG:H	1.29	0.77
1:C:308:GLN:NE2	1:D:288:TYR:HB3	1.99	0.77
1:B:368:GLN:NE2	1:B:368:GLN:H	1.83	0.77
1:F:250:GLN:HE21	1:H:69:ARG:HH22	1.32	0.77
1:B:97:ASN:ND2	1:D:75:ILE:H	1.83	0.76
1:K:383:HIS:HE1	1:K:395:ARG:H	1.32	0.76
1:E:383:HIS:CE1	1:E:395:ARG:H	2.03	0.76
1:H:242:MET:CE	1:H:249:GLN:HB3	2.08	0.76
1:K:308:GLN:NE2	1:L:288:TYR:HB3	2.00	0.76
1:A:244:GLN:H	1:A:244:GLN:HE21	0.86	0.76
1:F:368:GLN:H	1:F:368:GLN:NE2	1.84	0.75
1:B:383:HIS:HE1	1:B:395:ARG:H	1.34	0.75
1:K:52:ALA:HA	4:K:2002:HOH:O	1.86	0.75
1:G:242:MET:CE	1:G:249:GLN:HB3	2.17	0.74
1:C:176:HIS:HD2	1:C:203:LYS:H	1.33	0.74
1:L:211:HIS:HE1	1:L:272:ASN:ND2	1.84	0.74
1:L:242:MET:HE1	1:L:249:GLN:CB	2.16	0.74
1:E:308:GLN:NE2	1:F:288:TYR:HB3	2.03	0.74
1:L:242:MET:HE3	1:L:242:MET:HA	1.69	0.74
1:B:206:ILE:HD11	1:B:398:GLY:HA2	1.70	0.74
1:C:308:GLN:HE22	1:D:288:TYR:HB3	1.52	0.74
1:I:121:LYS:HG3	1:K:71:MET:SD	2.27	0.74
1:C:318:HIS:HB3	1:D:306:ILE:HD13	1.70	0.73
1:A:308:GLN:NE2	1:B:288:TYR:HB3	2.02	0.73
1:I:383:HIS:CE1	1:I:395:ARG:H	2.07	0.73
1:H:244:GLN:H	1:H:244:GLN:HE21	1.36	0.73
1:L:242:MET:CE	1:L:249:GLN:HB3	2.19	0.73
1:J:242:MET:HE1	1:J:249:GLN:HB3	1.70	0.73
1:C:183:MET:HG2	1:C:193:MET:HE1	1.70	0.72
1:D:403:GLN:HE22	1:D:425:TRP:HE1	1.38	0.72
1:F:403:GLN:HA	1:F:403:GLN:HE21	1.53	0.72
1:K:383:HIS:CE1	1:K:395:ARG:H	2.07	0.72
1:J:75:ILE:H	1:L:97:ASN:HD21	1.38	0.72
1:A:347:GLY:H	1:A:351:ASN:HD21	1.36	0.72
1:J:97:ASN:HD21	1:L:75:ILE:H	1.38	0.71
1:G:263:LEU:HD13	1:G:408:ILE:HG23	1.71	0.71
1:B:206:ILE:HD13	1:B:401:GLY:HA3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:383:HIS:CE1	1:L:395:ARG:H	2.09	0.71
1:J:242:MET:HE1	1:J:249:GLN:CG	2.20	0.71
1:J:250:GLN:NE2	1:L:69:ARG:HH22	1.89	0.71
1:B:250:GLN:NE2	1:D:69:ARG:HH22	1.88	0.71
1:J:244:GLN:NE2	1:J:244:GLN:H	1.88	0.70
1:D:153:ALA:HB2	1:D:176:HIS:HB2	1.72	0.70
1:L:244:GLN:H	1:L:244:GLN:NE2	1.89	0.70
1:J:383:HIS:CE1	1:J:395:ARG:H	2.09	0.70
1:J:97:ASN:ND2	1:L:75:ILE:H	1.87	0.70
1:G:91:LEU:HD22	1:G:116:SER:HB2	1.74	0.70
1:H:211:HIS:HE1	1:H:272:ASN:OD1	1.75	0.70
1:K:242:MET:CE	1:K:249:GLN:HB3	2.12	0.69
1:D:383:HIS:CE1	1:D:395:ARG:H	2.09	0.69
1:J:75:ILE:H	1:L:97:ASN:ND2	1.89	0.69
1:F:413:GLU:HG3	1:F:416:ARG:NH2	2.07	0.69
1:E:250:GLN:HE21	1:G:69:ARG:HH22	1.40	0.69
1:L:403:GLN:HE22	1:L:425:TRP:HE1	1.41	0.69
1:E:244:GLN:HE21	1:E:244:GLN:H	0.85	0.69
1:A:383:HIS:HE1	1:A:395:ARG:H	1.41	0.69
1:K:318:HIS:ND1	1:L:318:HIS:HD2	1.91	0.69
1:B:383:HIS:CE1	1:B:395:ARG:H	2.10	0.68
1:B:97:ASN:HD21	1:D:75:ILE:H	1.40	0.68
1:D:77:PRO:HD2	1:D:371:MET:HE2	1.74	0.68
1:F:402:MET:O	1:F:405:VAL:HG22	1.94	0.68
1:I:250:GLN:HE21	1:K:69:ARG:HH22	1.39	0.68
1:B:118:ASN:C	1:B:118:ASN:HD22	1.98	0.67
1:C:221:LYS:O	1:C:225:GLU:HG3	1.95	0.67
1:F:375:ASN:HD21	1:F:378:SER:H	1.39	0.67
1:F:383:HIS:CE1	1:F:395:ARG:H	2.12	0.67
1:G:138:ASP:H	1:G:141:ASN:HD21	1.40	0.67
1:I:97:ASN:ND2	1:K:75:ILE:H	1.92	0.67
1:I:71:MET:SD	1:K:121:LYS:HG3	2.36	0.66
1:K:308:GLN:HE22	1:L:288:TYR:HB3	1.61	0.66
1:G:69:ARG:HB3	1:G:70:PRO:HD2	1.78	0.66
1:G:275:ARG:HD2	1:G:281:GLU:OE1	1.95	0.66
1:B:375:ASN:ND2	1:B:378:SER:H	1.93	0.66
1:A:383:HIS:CE1	1:A:395:ARG:H	2.13	0.66
1:L:413:GLU:HG3	1:L:416:ARG:HH12	1.60	0.66
1:G:176:HIS:HD2	1:G:203:LYS:H	1.44	0.66
1:F:403:GLN:HE22	1:F:425:TRP:HE1	1.43	0.65
1:F:375:ASN:ND2	1:F:378:SER:H	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:HH22	1:C:250:GLN:HE21	1.44	0.65
1:F:124:ILE:O	1:F:128:GLU:HG3	1.96	0.65
1:D:375:ASN:HD21	1:D:378:SER:H	1.43	0.65
1:A:97:ASN:ND2	1:C:75:ILE:H	1.95	0.65
1:E:75:ILE:H	1:G:97:ASN:ND2	1.95	0.65
1:E:83:ARG:HD2	1:E:389:ILE:HD11	1.77	0.64
1:E:121:LYS:HG3	1:G:71:MET:SD	2.38	0.64
1:I:244:GLN:HE21	1:I:244:GLN:N	1.80	0.64
1:I:242:MET:SD	1:I:249:GLN:HB3	2.38	0.64
1:B:295:ASP:OD1	1:B:297:ARG:HD3	1.96	0.64
1:C:83:ARG:CB	1:C:83:ARG:HH11	2.10	0.64
1:I:403:GLN:HA	1:I:403:GLN:HE21	1.62	0.64
1:E:194:ILE:HD12	1:E:402:MET:HE1	1.78	0.64
1:D:430:GLN:N	1:D:430:GLN:HE21	1.95	0.64
1:B:219:ALA:O	1:B:222:LEU:HD13	1.97	0.64
1:K:118:ASN:C	1:K:118:ASN:HD22	2.01	0.64
1:B:375:ASN:HD21	1:B:378:SER:H	1.44	0.64
1:I:69:ARG:HD3	4:K:2379:HOH:O	1.97	0.64
1:J:242:MET:CE	1:J:249:GLN:HB3	2.28	0.64
1:D:124:ILE:O	1:D:128:GLU:HG3	1.98	0.64
1:K:221:LYS:O	1:K:225:GLU:HG3	1.98	0.64
1:G:406:ARG:NH1	1:G:406:ARG:HG2	2.13	0.63
1:F:383:HIS:HE1	1:F:395:ARG:H	1.45	0.63
1:K:123:LYS:NZ	1:K:123:LYS:HB2	2.13	0.63
1:K:242:MET:HE1	1:K:249:GLN:CG	2.27	0.63
1:C:83:ARG:HE	1:C:389:ILE:HD13	1.62	0.63
1:D:119:ALA:O	1:D:123:LYS:HG3	1.99	0.63
1:L:126:ALA:HB1	1:L:131:VAL:HG22	1.81	0.63
1:I:123:LYS:HB2	1:I:123:LYS:NZ	2.13	0.63
1:E:308:GLN:HE22	1:F:288:TYR:HB3	1.62	0.63
1:D:394:VAL:HG13	1:D:396:SER:H	1.64	0.63
1:A:176:HIS:CD2	1:A:203:LYS:H	2.14	0.63
1:K:178:MET:HE3	1:K:205:MET:HB3	1.80	0.63
1:B:124:ILE:O	1:B:128:GLU:HG3	1.98	0.63
1:A:121:LYS:HG3	1:C:71:MET:SD	2.38	0.63
1:H:244:GLN:H	1:H:244:GLN:NE2	1.96	0.62
1:D:77:PRO:HD2	1:D:371:MET:CE	2.29	0.62
1:G:141:ASN:C	1:G:141:ASN:HD22	2.02	0.62
1:H:143:ASP:OD1	1:H:169:ARG:HD2	1.99	0.62
1:E:83:ARG:HD2	1:E:389:ILE:CD1	2.30	0.62
1:E:194:ILE:HD12	1:E:402:MET:CE	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:ILE:H	1:K:97:ASN:ND2	1.96	0.62
1:A:308:GLN:HE22	1:B:288:TYR:HB3	1.63	0.62
1:E:181:LYS:O	1:E:181:LYS:HD3	1.99	0.62
1:G:118:ASN:HD22	1:G:118:ASN:C	2.03	0.62
1:J:242:MET:HE1	1:J:249:GLN:CB	2.29	0.62
1:C:181:LYS:HD3	1:C:181:LYS:O	1.98	0.62
1:J:76:ARG:HG3	1:L:97:ASN:HD22	1.65	0.62
1:C:91:LEU:HD22	1:C:116:SER:HB2	1.81	0.62
1:A:430:GLN:NE2	1:I:57:ALA:H	1.89	0.61
1:A:138:ASP:N	1:A:141:ASN:HD21	1.97	0.61
1:F:84:PHE:CE1	1:F:388:VAL:HG21	2.36	0.61
1:E:242:MET:SD	1:E:249:GLN:HB3	2.41	0.61
1:F:88:ILE:HD12	1:F:88:ILE:N	2.16	0.61
1:H:403:GLN:HA	1:H:403:GLN:HE21	1.66	0.61
1:E:97:ASN:ND2	1:G:75:ILE:H	1.99	0.61
1:F:148:ASP:OD1	1:F:150:LYS:HB2	2.00	0.61
1:I:118:ASN:C	1:I:118:ASN:HD22	2.05	0.60
1:D:375:ASN:ND2	1:D:378:SER:H	1.98	0.60
1:C:83:ARG:NE	1:C:389:ILE:HD13	2.15	0.60
1:J:96:LEU:HD23	1:J:100:LEU:HD22	1.82	0.60
1:A:181:LYS:O	1:A:181:LYS:HD3	2.00	0.60
1:D:403:GLN:HA	1:D:403:GLN:HE21	1.66	0.60
1:J:180:GLU:OE1	2:J:500:NDP:H2N	2.02	0.60
1:L:403:GLN:HA	1:L:403:GLN:HE21	1.66	0.60
1:C:223:ILE:HG12	1:C:228:LEU:HD22	1.82	0.60
1:L:178:MET:HE3	1:L:205:MET:CG	2.31	0.60
1:H:118:ASN:HD22	1:H:118:ASN:C	2.05	0.60
1:K:242:MET:SD	1:K:253:LEU:HD21	2.42	0.60
1:G:245:ASN:ND2	4:G:2207:HOH:O	2.35	0.59
1:F:296:GLU:OE2	1:H:56:PRO:HG3	2.01	0.59
1:G:100:LEU:HB2	1:G:101:PRO:HD3	1.84	0.59
1:K:181:LYS:HD3	1:K:181:LYS:O	2.02	0.59
1:J:242:MET:HE1	1:J:249:GLN:NE2	2.17	0.59
1:I:385:ALA:O	1:I:389:ILE:HG22	2.03	0.59
1:E:145:ILE:CD1	1:E:151:ILE:HG21	2.29	0.59
1:C:100:LEU:HB2	1:C:101:PRO:HD3	1.85	0.59
1:F:132:ASP:HB3	1:F:135:LYS:HG3	1.85	0.59
1:A:132:ASP:HB3	1:A:135:LYS:HD3	1.85	0.59
1:D:116:SER:HB2	2:D:500:NDP:O2X	2.01	0.59
1:I:97:ASN:HD21	1:K:75:ILE:H	1.49	0.59
1:I:181:LYS:HD3	1:I:181:LYS:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:MET:SD	1:C:253:LEU:HD21	2.43	0.58
1:L:347:GLY:N	1:L:351:ASN:HD21	1.95	0.58
1:F:100:LEU:HB2	1:F:101:PRO:HD3	1.85	0.58
1:F:168:ILE:HG13	1:F:169:ARG:N	2.18	0.58
1:B:242:MET:SD	1:B:249:GLN:HB3	2.42	0.58
1:A:347:GLY:N	1:A:351:ASN:HD21	2.01	0.58
4:A:2272:HOH:O	1:K:120:GLU:HG2	2.03	0.58
1:D:242:MET:CE	1:D:249:GLN:HB3	2.34	0.58
1:J:326:THR:HG22	1:J:327:THR:H	1.67	0.58
1:I:100:LEU:HB2	1:I:101:PRO:HD3	1.86	0.58
1:L:242:MET:HE1	1:L:249:GLN:CG	2.32	0.58
1:E:145:ILE:HD11	1:E:151:ILE:CG2	2.29	0.58
1:F:160:ASN:OD1	1:F:182:PRO:HD2	2.03	0.58
1:G:221:LYS:O	1:G:225:GLU:HG3	2.04	0.58
1:I:403:GLN:NE2	1:I:425:TRP:HE1	1.96	0.58
1:H:413:GLU:HG2	1:H:416:ARG:HH21	1.69	0.58
1:A:118:ASN:HD22	1:A:118:ASN:C	2.07	0.58
1:D:253:LEU:HD22	1:D:297:ARG:O	2.04	0.58
1:J:242:MET:HE3	1:J:242:MET:CA	2.30	0.57
1:E:250:GLN:NE2	1:G:69:ARG:HH22	2.02	0.57
1:D:100:LEU:HB2	1:D:101:PRO:HD3	1.86	0.57
1:I:211:HIS:HE1	1:I:272:ASN:OD1	1.87	0.57
1:E:180:GLU:OE1	2:E:500:NDP:H2N	2.05	0.57
1:E:318:HIS:HD2	1:F:318:HIS:ND1	2.02	0.57
1:A:100:LEU:HB2	1:A:101:PRO:HD3	1.87	0.57
1:D:205:MET:HG3	1:D:394:VAL:HG11	1.85	0.57
1:F:344:PRO:CG	1:H:368:GLN:HG2	2.34	0.57
1:B:221:LYS:O	1:B:225:GLU:HG3	2.05	0.57
1:F:275:ARG:NH2	1:F:400:GLU:OE2	2.38	0.57
1:A:374:ASN:HD22	1:A:375:ASN:H	1.53	0.57
1:K:242:MET:HE2	1:K:243:ASP:N	2.19	0.57
1:E:69:ARG:HH22	1:G:250:GLN:HE21	1.53	0.57
1:J:221:LYS:O	1:J:225:GLU:HG3	2.03	0.57
1:D:151:ILE:HB	1:D:175:LYS:HE3	1.87	0.57
1:I:97:ASN:HD22	1:K:76:ARG:HG3	1.69	0.56
1:H:239:SER:HB3	1:H:322:SER:HB3	1.87	0.56
1:H:407:LEU:O	1:H:411:ILE:HG12	2.05	0.56
1:D:118:ASN:HD22	1:D:118:ASN:C	2.08	0.56
1:I:69:ARG:HD2	2:K:500:NDP:C2A	2.35	0.56
1:C:83:ARG:HB2	1:C:83:ARG:HH11	1.69	0.56
1:D:231:LEU:HD13	1:D:278:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:275:ARG:HD2	1:H:281:GLU:OE1	2.05	0.56
1:E:134:ARG:HG3	1:E:134:ARG:HH11	1.70	0.56
1:J:97:ASN:HD22	1:L:76:ARG:HG3	1.70	0.56
1:D:183:MET:HE3	1:D:206:ILE:HD11	1.87	0.56
1:L:57:ALA:O	1:L:61:GLN:HG3	2.06	0.56
1:D:245:ASN:HD22	1:D:245:ASN:N	2.02	0.56
1:A:413:GLU:HG3	4:A:2352:HOH:O	2.04	0.56
1:D:242:MET:HE1	1:D:249:GLN:HB3	1.87	0.56
1:A:138:ASP:H	1:A:141:ASN:ND2	1.95	0.56
1:H:62:VAL:HG22	1:H:69:ARG:NH1	2.21	0.56
1:H:392:LYS:HE2	4:H:2246:HOH:O	2.05	0.56
1:K:176:HIS:CD2	1:K:203:LYS:H	2.10	0.55
1:D:57:ALA:O	1:D:61:GLN:HG3	2.05	0.55
2:H:500:NDP:C3N	3:H:600[A]:GOL:H31	2.36	0.55
1:F:144:LYS:HD3	1:F:147:LYS:NZ	2.21	0.55
1:J:242:MET:HE2	1:J:243:ASP:N	2.20	0.55
1:C:242:MET:CE	1:C:249:GLN:NE2	2.69	0.55
1:L:229:GLY:HA3	1:L:337:LYS:HG3	1.88	0.55
1:J:209:ARG:HA	1:J:380:GLN:HE21	1.71	0.55
1:I:342:MET:HG2	1:I:353:ILE:HG22	1.88	0.55
1:G:178:MET:HE3	1:G:205:MET:CG	2.36	0.55
1:A:273:GLY:HA2	1:A:276:TYR:CE2	2.42	0.55
1:F:180:GLU:OE1	2:F:500:NDP:H2N	2.07	0.55
1:F:189:ASP:O	1:F:193:MET:HG3	2.05	0.55
1:G:244:GLN:HE21	1:G:244:GLN:H	0.84	0.55
1:E:76:ARG:HG3	1:G:97:ASN:HD22	1.72	0.55
1:K:242:MET:CE	1:K:243:ASP:N	2.70	0.55
1:I:144:LYS:HD2	1:I:147:LYS:HZ2	1.71	0.55
1:I:180:GLU:OE1	2:I:500:NDP:H2N	2.06	0.55
1:D:178:MET:HE3	1:D:205:MET:HB3	1.88	0.55
1:F:168:ILE:HG13	1:F:169:ARG:H	1.72	0.55
1:H:413:GLU:HG2	1:H:416:ARG:NH2	2.20	0.55
1:J:413:GLU:HA	1:J:416:ARG:NH1	2.22	0.55
1:C:347:GLY:N	1:C:351:ASN:HD21	2.00	0.55
1:B:219:ALA:HA	1:B:222:LEU:CD1	2.37	0.55
1:L:178:MET:HE3	1:L:205:MET:HG2	1.89	0.55
1:K:100:LEU:HB2	1:K:101:PRO:HD3	1.89	0.55
1:C:69:ARG:HB3	1:C:70:PRO:HD2	1.89	0.54
1:J:134:ARG:HH11	1:J:134:ARG:HG3	1.71	0.54
1:H:180:GLU:OE1	2:H:500:NDP:H2N	2.07	0.54
1:A:97:ASN:HD22	1:C:76:ARG:HG3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:HIS:HE1	1:F:272:ASN:OD1	1.90	0.54
1:J:120:GLU:CD	1:J:120:GLU:H	2.10	0.54
1:I:386:GLU:HA	1:I:389:ILE:CG2	2.37	0.54
2:G:500:NDP:C3N	3:G:600[B]:GOL:H31	2.36	0.54
1:H:248:ALA:HA	2:H:500:NDP:O1A	2.07	0.54
1:B:100:LEU:HB2	1:B:101:PRO:HD3	1.89	0.54
1:B:206:ILE:CD1	1:B:398:GLY:HA2	2.38	0.54
1:C:242:MET:HE2	1:C:249:GLN:HE21	1.72	0.54
1:A:180:GLU:OE1	2:A:500:NDP:H2N	2.08	0.54
1:F:76:ARG:HG2	1:F:77:PRO:HD2	1.89	0.54
1:L:180:GLU:OE1	2:L:500:NDP:H2N	2.08	0.54
1:B:206:ILE:HD13	1:B:401:GLY:CA	2.37	0.54
1:B:297:ARG:HD2	4:B:2183:HOH:O	2.08	0.54
1:B:223:ILE:HG12	1:B:228:LEU:HD22	1.90	0.54
1:I:144:LYS:HD2	1:I:147:LYS:NZ	2.23	0.54
1:A:250:GLN:HE21	1:C:69:ARG:HH22	1.56	0.54
1:G:81:ASP:OD1	1:G:83:ARG:HG2	2.08	0.54
1:J:375:ASN:ND2	1:J:378:SER:H	2.05	0.54
1:A:242:MET:SD	1:A:249:GLN:HB3	2.48	0.54
1:B:153:ALA:HB2	1:B:176:HIS:HB2	1.90	0.54
1:A:69:ARG:HB3	1:A:70:PRO:HD2	1.89	0.54
1:F:388:VAL:HG23	1:F:389:ILE:N	2.23	0.54
1:G:332:SER:HA	1:G:340:LEU:O	2.08	0.54
1:H:242:MET:CE	1:H:243:ASP:N	2.71	0.53
1:L:368:GLN:HE21	1:L:368:GLN:N	1.94	0.53
1:G:255:ARG:HD3	1:G:300:GLU:O	2.09	0.53
1:E:124:ILE:O	1:E:128:GLU:HG3	2.08	0.53
1:G:180:GLU:OE1	2:G:500:NDP:H2N	2.09	0.53
1:L:244:GLN:N	1:L:244:GLN:HE21	2.01	0.53
1:B:69:ARG:HB3	1:B:70:PRO:HD2	1.90	0.53
1:G:429:ARG:NH2	4:G:2356:HOH:O	2.40	0.53
1:H:100:LEU:HB2	1:H:101:PRO:HD3	1.90	0.53
1:K:71:MET:HE3	1:K:72:PRO:HD2	1.91	0.53
1:F:276:TYR:CE1	1:F:277:LEU:HD13	2.43	0.53
1:G:181:LYS:HD3	1:G:181:LYS:O	2.07	0.53
1:B:65:THR:HB	1:B:66:PRO:HD2	1.91	0.53
1:H:239:SER:HA	1:H:266:ILE:HD12	1.90	0.53
1:H:285:VAL:HG21	1:H:411:ILE:HD13	1.90	0.53
1:E:100:LEU:HB2	1:E:101:PRO:HD3	1.91	0.53
1:H:62:VAL:HG22	1:H:69:ARG:HH12	1.74	0.53
1:D:242:MET:SD	1:D:253:LEU:HD21	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:LYS:NZ	1:D:337:LYS:HB3	2.24	0.53
1:L:153:ALA:HB2	1:L:176:HIS:HB2	1.89	0.53
1:G:308:GLN:NE2	1:H:288:TYR:HB3	2.24	0.53
1:F:255:ARG:O	1:F:255:ARG:HD2	2.09	0.53
1:F:403:GLN:HA	1:F:403:GLN:NE2	2.21	0.53
1:A:395:ARG:HG3	1:A:395:ARG:HH11	1.74	0.53
1:L:96:LEU:HD23	1:L:100:LEU:HD22	1.90	0.53
1:E:300:GLU:HG3	1:G:55:LEU:HD21	1.90	0.53
1:D:306:ILE:HG12	1:D:320:ALA:HB2	1.92	0.52
1:J:375:ASN:HD21	1:J:378:SER:H	1.56	0.52
1:H:76:ARG:HG2	1:H:76:ARG:HH11	1.73	0.52
1:K:180:GLU:OE1	2:K:500:NDP:H2N	2.09	0.52
1:B:375:ASN:HD22	1:B:377:PHE:H	1.58	0.52
1:D:144:LYS:O	1:D:147:LYS:HG2	2.09	0.52
1:A:97:ASN:HD21	1:C:75:ILE:H	1.56	0.52
1:E:191:GLN:N	1:E:402:MET:HE2	2.24	0.52
1:F:352:LEU:C	1:F:352:LEU:HD23	2.30	0.52
1:F:178:MET:HE3	1:F:205:MET:CG	2.40	0.52
1:H:326:THR:HG22	1:H:327:THR:H	1.74	0.52
1:D:189:ASP:O	1:D:193:MET:HG3	2.08	0.52
1:F:275:ARG:HH22	1:F:400:GLU:CD	2.13	0.52
1:F:352:LEU:HD23	1:F:353:ILE:N	2.25	0.52
1:G:273:GLY:HA2	1:G:276:TYR:CE2	2.45	0.52
1:F:244:GLN:HG3	1:F:297:ARG:HG2	1.91	0.52
1:F:404:ASP:O	1:F:408:ILE:HG13	2.10	0.52
1:D:274:THR:O	1:D:278:LEU:HB2	2.10	0.52
1:J:391:ASN:HB2	4:J:2326:HOH:O	2.08	0.52
1:L:91:LEU:HB2	1:L:121:LYS:HE3	1.92	0.52
1:L:181:LYS:HD3	1:L:181:LYS:O	2.10	0.52
1:F:244:GLN:CG	1:F:297:ARG:HG2	2.40	0.52
1:D:181:LYS:O	1:D:181:LYS:HD3	2.10	0.52
1:H:209:ARG:HH11	1:H:376:GLN:HE22	1.58	0.52
1:E:158:LEU:HB3	1:E:159:PRO:HD2	1.92	0.52
1:A:141:ASN:C	1:A:141:ASN:HD22	2.12	0.52
1:J:403:GLN:HA	1:J:403:GLN:HE21	1.75	0.52
1:B:56:PRO:HG3	1:D:296:GLU:CD	2.29	0.52
1:J:178:MET:HE3	1:J:205:MET:CG	2.39	0.52
1:F:165:GLU:HG3	1:F:166:PHE:CD1	2.45	0.51
1:A:332:SER:HA	1:A:340:LEU:O	2.11	0.51
1:B:57:ALA:O	1:B:61:GLN:HG3	2.10	0.51
1:H:181:LYS:HD3	1:H:181:LYS:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:285:VAL:HG12	1:H:309:MET:HG2	1.92	0.51
1:D:280:GLU:HG3	1:D:311:PHE:CD2	2.45	0.51
1:F:312:ARG:HD2	4:F:2211:HOH:O	2.10	0.51
1:B:116:SER:O	1:B:138:ASP:HA	2.10	0.51
1:L:383:HIS:HD2	4:L:2304:HOH:O	1.94	0.51
1:F:366:MET:O	1:H:350:GLN:HG3	2.10	0.51
4:F:2071:HOH:O	1:H:365:MET:HE2	2.09	0.51
1:I:296:GLU:HG2	4:I:2263:HOH:O	2.10	0.51
1:K:273:GLY:HA2	1:K:276:TYR:CE2	2.46	0.51
1:D:347:GLY:N	1:D:351:ASN:HD21	2.05	0.51
1:E:263:LEU:HB2	1:E:305:ILE:HG21	1.91	0.51
1:L:242:MET:HE2	1:L:243:ASP:N	2.26	0.51
1:F:293:PRO:HG3	4:F:2135:HOH:O	2.11	0.51
1:K:94:TYR:CD1	2:K:500:NDP:H41N	2.45	0.51
1:G:178:MET:HE3	1:G:205:MET:HG2	1.93	0.51
1:C:419:ARG:HD3	4:C:2298:HOH:O	2.10	0.51
1:A:81:ASP:OD2	1:A:108:HIS:HD2	1.94	0.51
1:I:250:GLN:NE2	1:K:69:ARG:HH22	2.07	0.51
1:G:131:VAL:HG12	4:G:2087:HOH:O	2.10	0.51
1:C:153:ALA:HB2	1:C:176:HIS:HB2	1.93	0.50
1:E:386:GLU:HG2	4:E:2075:HOH:O	2.09	0.50
1:C:134:ARG:HG3	1:C:134:ARG:HH11	1.76	0.50
1:H:153:ALA:HB2	1:H:176:HIS:HB2	1.93	0.50
1:J:244:GLN:HE21	1:J:244:GLN:N	1.92	0.50
1:G:242:MET:HE3	1:G:249:GLN:HB3	1.93	0.50
1:G:116:SER:O	1:G:138:ASP:HA	2.11	0.50
1:H:239:SER:HA	1:H:266:ILE:CD1	2.42	0.50
2:L:500:NDP:C3N	3:L:600[A]:GOL:H31	2.42	0.50
1:H:242:MET:HE3	1:H:243:ASP:H	1.75	0.50
1:J:383:HIS:HD2	4:J:2164:HOH:O	1.94	0.50
1:B:347:GLY:N	1:B:351:ASN:HD21	2.02	0.50
1:C:132:ASP:OD1	1:C:134:ARG:NH1	2.42	0.50
1:K:242:MET:HE3	1:K:242:MET:HA	1.93	0.50
1:C:180:GLU:OE1	2:C:500:NDP:H2N	2.12	0.50
1:F:186:SER:HB3	1:F:189:ASP:OD2	2.10	0.50
1:K:422:ASN:ND2	1:K:424:ASP:H	2.10	0.50
2:K:500:NDP:C3N	3:K:600[B]:GOL:H31	2.41	0.50
1:I:75:ILE:H	1:K:97:ASN:HD21	1.59	0.50
1:H:238:ASN:O	1:H:321:SER:HA	2.11	0.50
1:C:314:GLY:O	1:D:304:ARG:NH2	2.41	0.50
1:L:242:MET:SD	1:L:253:LEU:HD21	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:500:NDP:C3N	3:A:600[B]:GOL:H31	2.40	0.50
1:J:242:MET:CE	1:J:242:MET:HA	2.35	0.50
1:B:97:ASN:HD22	1:D:76:ARG:HG3	1.76	0.50
1:A:392:LYS:HA	1:A:392:LYS:HE2	1.94	0.50
1:L:94:TYR:CD1	2:L:500:NDP:H41N	2.47	0.50
1:H:383:HIS:HE1	1:H:395:ARG:N	2.04	0.50
1:G:176:HIS:CD2	1:G:203:LYS:H	2.27	0.50
1:F:374:ASN:HD22	1:F:375:ASN:H	1.58	0.49
1:D:406:ARG:HD2	4:D:2194:HOH:O	2.11	0.49
1:I:118:ASN:ND2	1:I:121:LYS:H	2.10	0.49
1:F:403:GLN:O	1:F:407:LEU:HD22	2.12	0.49
1:J:153:ALA:HB2	1:J:176:HIS:HB2	1.92	0.49
1:G:395:ARG:O	1:G:395:ARG:HG3	2.10	0.49
1:H:242:MET:HE2	1:H:243:ASP:N	2.27	0.49
1:I:383:HIS:HD2	4:I:2167:HOH:O	1.95	0.49
1:E:75:ILE:H	1:G:97:ASN:HD21	1.58	0.49
1:H:81:ASP:OD1	1:H:83:ARG:HG2	2.12	0.49
1:B:94:TYR:CD1	2:B:500:NDP:H41N	2.48	0.49
1:E:383:HIS:HE1	1:E:395:ARG:N	2.05	0.49
1:B:369:PHE:CE1	1:D:347:GLY:HA2	2.48	0.49
1:F:413:GLU:HG3	1:F:416:ARG:HH21	1.76	0.49
1:F:233:MET:HE3	1:F:316:LEU:O	2.12	0.49
1:C:342:MET:HG2	1:C:353:ILE:HG22	1.95	0.49
1:K:144:LYS:HG2	1:K:147:LYS:HE2	1.94	0.49
1:G:153:ALA:HB2	1:G:176:HIS:HB2	1.93	0.49
1:G:118:ASN:ND2	1:G:121:LYS:H	2.10	0.49
1:E:134:ARG:HG3	1:E:134:ARG:NH1	2.28	0.49
1:D:179:CYS:O	1:D:206:ILE:HA	2.12	0.49
1:J:375:ASN:HD22	1:J:377:PHE:H	1.59	0.49
1:F:296:GLU:CD	1:H:56:PRO:HG3	2.33	0.49
1:C:242:MET:CE	1:C:242:MET:HA	2.43	0.49
1:C:135:LYS:HD2	4:C:2085:HOH:O	2.12	0.49
1:H:350:GLN:HB3	4:H:2208:HOH:O	2.12	0.49
1:F:238:ASN:O	1:F:321:SER:HA	2.13	0.49
2:E:500:NDP:C5N	3:E:600[A]:GOL:H32	2.41	0.49
1:K:178:MET:HE3	1:K:205:MET:CB	2.41	0.49
1:C:78:MET:HG3	1:C:79:PRO:HD2	1.94	0.49
1:C:429:ARG:NH1	4:C:2308:HOH:O	2.46	0.49
1:G:198:LYS:HD2	4:G:2150:HOH:O	2.13	0.49
1:D:77:PRO:CD	1:D:371:MET:HE2	2.43	0.49
1:I:76:ARG:HG3	1:K:97:ASN:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:LYS:HD3	1:F:181:LYS:O	2.13	0.49
1:B:326:THR:HG22	1:B:327:THR:H	1.78	0.49
1:D:89:VAL:HG12	1:D:158:LEU:HD21	1.95	0.49
1:H:110:ARG:HE	1:H:112:GLU:HG2	1.77	0.49
1:E:350:GLN:HB3	4:E:2268:HOH:O	2.12	0.49
1:D:183:MET:HE3	1:D:398:GLY:HA2	1.95	0.48
1:H:82:ARG:HB3	1:H:110:ARG:HB3	1.95	0.48
1:B:160:ASN:ND2	1:B:182:PRO:HD2	2.27	0.48
1:F:178:MET:HE3	1:F:205:MET:HB3	1.95	0.48
1:F:231:LEU:HD23	1:F:278:LEU:HD12	1.95	0.48
1:D:350:GLN:HB3	4:D:2153:HOH:O	2.14	0.48
1:H:69:ARG:HB3	1:H:70:PRO:HD2	1.96	0.48
1:E:97:ASN:HD21	1:G:75:ILE:H	1.60	0.48
1:D:238:ASN:O	1:D:321:SER:HA	2.12	0.48
1:B:68:GLY:HA2	2:D:500:NDP:O1X	2.14	0.48
1:F:176:HIS:CE1	1:F:202:LYS:HD2	2.48	0.48
1:C:230:LYS:HE2	4:C:2160:HOH:O	2.13	0.48
1:F:253:LEU:HD22	1:F:297:ARG:O	2.13	0.48
1:F:213:ASP:O	1:F:217:ARG:HG2	2.13	0.48
1:B:304:ARG:HG2	1:B:322:SER:HB2	1.95	0.48
1:C:242:MET:HE1	1:C:249:GLN:NE2	2.27	0.48
2:E:500:NDP:C5N	3:E:600[B]:GOL:H31	2.42	0.48
1:E:269:TYR:HE2	3:E:600[A]:GOL:HO3	1.62	0.48
1:E:368:GLN:N	1:E:368:GLN:HE21	1.92	0.48
1:F:187:VAL:HG12	4:F:2204:HOH:O	2.13	0.48
1:F:388:VAL:HG23	1:F:389:ILE:H	1.79	0.48
1:A:112:GLU:HG3	1:A:150:LYS:O	2.14	0.48
2:L:500:NDP:C5N	3:L:600[A]:GOL:H31	2.44	0.48
1:J:242:MET:CE	1:J:249:GLN:HE21	2.27	0.48
1:J:94:TYR:CD1	2:J:500:NDP:H41N	2.48	0.48
1:D:404:ASP:O	1:D:408:ILE:HG13	2.14	0.48
1:K:383:HIS:HD2	4:K:2158:HOH:O	1.96	0.48
1:J:350:GLN:HB3	4:J:2287:HOH:O	2.13	0.48
1:K:374:ASN:HD22	1:K:375:ASN:H	1.62	0.48
1:I:318:HIS:HB3	1:J:306:ILE:HD13	1.96	0.48
1:E:223:ILE:HG12	1:E:228:LEU:HD22	1.95	0.48
1:K:429:ARG:NH1	4:K:2367:HOH:O	2.46	0.48
1:J:181:LYS:O	1:J:181:LYS:HD3	2.14	0.47
1:H:94:TYR:CD1	2:H:500:NDP:H41N	2.49	0.47
1:F:187:VAL:HG21	1:F:406:ARG:HD3	1.95	0.47
4:E:2238:HOH:O	1:F:308:GLN:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:ASN:HD21	1:F:229:GLY:HA2	1.79	0.47
1:G:142:PHE:O	1:G:145:ILE:HG23	2.15	0.47
1:J:100:LEU:HB3	1:J:129:TYR:CZ	2.49	0.47
1:D:280:GLU:HG3	1:D:311:PHE:HD2	1.79	0.47
1:C:375:ASN:HD21	1:C:378:SER:H	1.61	0.47
1:C:375:ASN:ND2	1:C:378:SER:H	2.11	0.47
1:G:138:ASP:H	1:G:141:ASN:ND2	2.11	0.47
1:H:306:ILE:HG12	1:H:320:ALA:HB2	1.97	0.47
1:J:304:ARG:HG2	1:J:322:SER:HB2	1.95	0.47
1:E:188:ALA:O	1:E:192:ARG:HG3	2.14	0.47
1:L:350:GLN:HB3	4:L:2266:HOH:O	2.13	0.47
1:C:238:ASN:O	1:C:321:SER:HA	2.14	0.47
1:B:350:GLN:HG3	1:D:366:MET:O	2.14	0.47
1:F:223:ILE:HG12	1:F:228:LEU:HD22	1.97	0.47
1:E:220:VAL:O	1:E:224:ARG:HG2	2.15	0.47
1:I:94:TYR:CD1	2:I:500:NDP:H41N	2.49	0.47
1:H:209:ARG:HA	1:H:380:GLN:HE21	1.80	0.47
1:F:89:VAL:HG12	1:F:158:LEU:HD21	1.97	0.47
1:F:242:MET:SD	1:F:249:GLN:HB3	2.54	0.47
1:E:97:ASN:HD22	1:G:76:ARG:HG3	1.80	0.46
1:B:56:PRO:HD3	1:D:296:GLU:O	2.15	0.46
1:B:238:ASN:O	1:B:321:SER:HA	2.15	0.46
1:L:312:ARG:HD2	4:L:2342:HOH:O	2.14	0.46
1:B:209:ARG:HA	1:B:380:GLN:HE21	1.79	0.46
1:G:144:LYS:HG2	1:G:147:LYS:HE2	1.98	0.46
1:E:145:ILE:HG13	1:E:151:ILE:CD1	2.45	0.46
1:K:318:HIS:HB3	1:L:306:ILE:HD13	1.98	0.46
1:I:123:LYS:HB2	1:I:123:LYS:HZ3	1.80	0.46
1:C:306:ILE:HD13	1:D:318:HIS:HB3	1.97	0.46
1:D:165:GLU:HG3	1:D:166:PHE:CD1	2.50	0.46
1:C:347:GLY:H	1:C:351:ASN:ND2	2.06	0.46
1:I:386:GLU:HA	1:I:389:ILE:HG22	1.96	0.46
1:D:151:ILE:O	1:D:175:LYS:HE3	2.15	0.46
1:I:330:ARG:HG3	4:I:2283:HOH:O	2.16	0.46
1:H:116:SER:O	1:H:138:ASP:HA	2.15	0.46
1:D:248:ALA:HA	2:D:500:NDP:O1A	2.15	0.46
1:F:168:ILE:O	1:F:172:LYS:HG2	2.15	0.46
1:D:181:LYS:HA	1:D:182:PRO:C	2.36	0.46
1:G:134:ARG:HH11	1:G:134:ARG:HG3	1.80	0.46
1:E:178:MET:HE3	1:E:205:MET:HG2	1.98	0.46
1:J:242:MET:HE1	1:J:249:GLN:HE21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:430:GLN:HG2	4:H:2093:HOH:O	2.16	0.46
1:I:153:ALA:HB2	1:I:176:HIS:HB2	1.98	0.46
1:D:242:MET:CE	1:D:249:GLN:NE2	2.79	0.46
1:B:132:ASP:OD1	1:B:134:ARG:HG3	2.16	0.46
1:I:132:ASP:HB3	1:I:135:LYS:HG3	1.97	0.46
1:I:332:SER:HA	1:I:340:LEU:O	2.15	0.46
1:C:242:MET:HA	1:C:242:MET:HE2	1.98	0.46
1:G:134:ARG:NH1	1:G:134:ARG:HG3	2.30	0.46
2:J:500:NDP:C5N	3:J:600[A]:GOL:H31	2.45	0.46
1:H:383:HIS:HD2	4:H:2088:HOH:O	1.98	0.46
1:K:422:ASN:HD21	1:K:424:ASP:HB3	1.81	0.46
1:D:187:VAL:HG11	1:D:406:ARG:HD3	1.98	0.46
1:C:184:ALA:HB2	1:C:193:MET:CE	2.46	0.46
1:E:176:HIS:CD2	1:E:203:LYS:H	2.16	0.46
1:C:339:VAL:HG23	1:D:326:THR:HG23	1.98	0.46
1:A:76:ARG:HH11	1:A:76:ARG:HG2	1.81	0.46
1:D:69:ARG:HB3	1:D:70:PRO:HD2	1.98	0.46
1:D:115:VAL:HA	1:D:137:TYR:O	2.16	0.46
2:D:500:NDP:C5N	3:D:600[B]:GOL:H32	2.44	0.45
1:F:181:LYS:HA	1:F:182:PRO:C	2.36	0.45
1:F:179:CYS:O	1:F:206:ILE:HA	2.16	0.45
1:I:402:MET:HE1	4:I:2164:HOH:O	2.16	0.45
1:K:284:GLU:CD	1:K:310:ARG:HH21	2.18	0.45
1:C:350:GLN:HB3	4:C:2244:HOH:O	2.15	0.45
1:D:116:SER:OG	1:D:122:ALA:HB2	2.15	0.45
1:C:388:VAL:HG13	1:C:389:ILE:N	2.30	0.45
1:J:178:MET:HE3	1:J:205:MET:SD	2.57	0.45
1:G:342:MET:HG2	1:G:353:ILE:HG22	1.98	0.45
1:A:306:ILE:HD13	1:B:318:HIS:HB3	1.98	0.45
1:I:350:GLN:HB3	4:I:2304:HOH:O	2.16	0.45
1:G:94:TYR:CD1	2:G:500:NDP:H41N	2.51	0.45
1:G:242:MET:HE3	1:G:249:GLN:CB	2.46	0.45
1:F:275:ARG:HD2	1:F:281:GLU:OE1	2.15	0.45
1:G:136:ILE:HG13	4:G:2087:HOH:O	2.15	0.45
1:L:160:ASN:ND2	1:L:182:PRO:HD2	2.32	0.45
1:H:242:MET:HE3	1:H:243:ASP:N	2.32	0.45
1:I:416:ARG:HH11	1:I:416:ARG:HB3	1.81	0.45
1:J:242:MET:HE2	1:J:243:ASP:H	1.81	0.45
1:C:100:LEU:HD22	1:C:111:ILE:HD13	1.98	0.45
1:F:326:THR:HG22	1:F:327:THR:H	1.80	0.45
1:G:385:ALA:O	1:G:389:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:500:NDP:C5N	3:J:600[B]:GOL:H32	2.46	0.45
1:I:308:GLN:OE1	1:J:288:TYR:HB3	2.17	0.45
1:I:383:HIS:HE1	1:I:395:ARG:N	2.07	0.45
1:A:383:HIS:HD2	4:A:2164:HOH:O	2.00	0.45
1:K:123:LYS:HB2	1:K:123:LYS:HZ2	1.80	0.45
1:A:285:VAL:HG12	1:A:309:MET:HG2	1.99	0.45
1:I:238:ASN:O	1:I:321:SER:HA	2.16	0.45
2:F:500:NDP:C5N	3:F:600[A]:GOL:H31	2.46	0.45
1:C:94:TYR:CD1	2:C:500:NDP:H41N	2.52	0.45
1:D:142:PHE:O	1:D:145:ILE:HG23	2.17	0.45
1:E:274:THR:O	1:E:278:LEU:HB2	2.17	0.45
1:C:83:ARG:NH1	1:C:83:ARG:HB2	2.31	0.45
1:E:69:ARG:HB3	1:E:70:PRO:HD2	1.98	0.45
1:D:245:ASN:ND2	1:D:245:ASN:N	2.65	0.45
1:F:76:ARG:HD3	1:F:77:PRO:O	2.17	0.45
1:C:375:ASN:HD22	1:C:377:PHE:H	1.64	0.45
1:B:350:GLN:HB3	4:B:2219:HOH:O	2.16	0.45
1:I:69:ARG:HB3	1:I:70:PRO:HD2	1.99	0.44
1:C:184:ALA:HB2	1:C:193:MET:HE1	1.99	0.44
2:C:500:NDP:C5N	3:C:600[A]:GOL:H32	2.46	0.44
1:J:242:MET:SD	1:J:253:LEU:HD21	2.58	0.44
1:F:132:ASP:HB3	1:F:135:LYS:CG	2.47	0.44
1:D:160:ASN:ND2	1:D:182:PRO:HD2	2.33	0.44
1:D:403:GLN:NE2	1:D:403:GLN:HA	2.31	0.44
1:F:144:LYS:HD3	1:F:147:LYS:HZ1	1.83	0.44
1:I:144:LYS:HE2	4:I:2117:HOH:O	2.17	0.44
1:K:238:ASN:O	1:K:321:SER:HA	2.17	0.44
1:F:304:ARG:HG2	1:F:322:SER:HB2	2.00	0.44
1:F:120:GLU:HA	4:F:2038:HOH:O	2.17	0.44
1:C:134:ARG:HG3	1:C:134:ARG:NH1	2.33	0.44
1:F:153:ALA:HB2	1:F:176:HIS:HB2	1.98	0.44
1:E:178:MET:HE3	1:E:205:MET:CG	2.48	0.44
1:D:132:ASP:O	1:D:132:ASP:OD1	2.35	0.44
1:J:242:MET:HE1	1:J:249:GLN:HG3	1.98	0.44
1:F:406:ARG:HB3	1:F:425:TRP:CZ2	2.53	0.44
1:E:306:ILE:HD13	1:F:318:HIS:HB3	2.00	0.44
1:F:326:THR:HG22	1:F:327:THR:N	2.32	0.44
1:H:231:LEU:HD13	1:H:278:LEU:HD12	2.00	0.44
1:F:57:ALA:O	1:F:61:GLN:HG3	2.17	0.44
1:F:235:THR:HB	1:F:332:SER:HB3	1.99	0.44
1:B:253:LEU:HD22	1:B:297:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HD22	1:B:223:ILE:N	2.32	0.44
1:G:76:ARG:HH11	1:G:76:ARG:HG2	1.83	0.44
1:D:416:ARG:HD2	4:D:2197:HOH:O	2.18	0.44
1:B:188:ALA:O	1:B:192:ARG:HG3	2.18	0.44
1:L:120:GLU:HG3	1:L:121:LYS:N	2.32	0.44
1:A:318:HIS:HB3	1:B:306:ILE:HD13	2.00	0.44
1:C:402:MET:HE1	4:C:2127:HOH:O	2.17	0.44
1:G:296:GLU:HG2	4:G:2241:HOH:O	2.18	0.44
1:G:413:GLU:HG3	4:G:2337:HOH:O	2.18	0.44
1:K:248:ALA:HA	2:K:500:NDP:O1A	2.18	0.43
1:J:242:MET:HE1	1:J:249:GLN:CD	2.38	0.43
1:G:308:GLN:HE22	1:H:288:TYR:HB3	1.83	0.43
1:F:134:ARG:HH11	1:F:134:ARG:HG3	1.83	0.43
1:B:211:HIS:CE1	1:B:272:ASN:ND2	2.66	0.43
1:E:198:LYS:HD2	4:E:2152:HOH:O	2.18	0.43
1:L:81:ASP:OD1	1:L:83:ARG:HG2	2.18	0.43
1:J:326:THR:HG22	1:J:327:THR:N	2.32	0.43
1:L:242:MET:HE1	1:L:249:GLN:OE1	2.19	0.43
1:J:242:MET:CE	1:J:242:MET:CA	2.95	0.43
1:E:153:ALA:HB2	1:E:176:HIS:HB2	2.00	0.43
1:B:179:CYS:O	1:B:206:ILE:HA	2.17	0.43
1:K:88:ILE:HG13	1:K:100:LEU:HD21	2.00	0.43
1:D:115:VAL:HG22	1:D:137:TYR:HB2	2.00	0.43
1:D:52:ALA:HA	4:D:2001:HOH:O	2.17	0.43
1:A:142:PHE:O	1:A:145:ILE:HG23	2.17	0.43
1:L:403:GLN:HA	1:L:403:GLN:NE2	2.34	0.43
1:A:94:TYR:CD1	2:A:500:NDP:H41N	2.53	0.43
1:D:94:TYR:CD1	2:D:500:NDP:H41N	2.53	0.43
1:F:233:MET:CE	1:F:317:SER:HA	2.49	0.43
1:E:318:HIS:HB3	1:F:306:ILE:HD13	2.00	0.43
1:B:97:ASN:HD21	1:D:74:ALA:HA	1.84	0.43
1:I:74:ALA:HA	1:K:97:ASN:HD21	1.83	0.43
1:A:245:ASN:ND2	4:A:2224:HOH:O	2.47	0.43
1:B:312:ARG:HD2	4:B:2279:HOH:O	2.17	0.43
1:K:69:ARG:HB3	1:K:70:PRO:HD2	2.01	0.43
1:F:88:ILE:CD1	1:F:88:ILE:N	2.80	0.43
1:E:228:LEU:O	1:E:335:GLY:HA3	2.19	0.43
1:F:188:ALA:O	1:F:192:ARG:HG3	2.19	0.43
1:H:57:ALA:HB1	1:H:61:GLN:NE2	2.34	0.43
2:L:500:NDP:C5N	3:L:600[B]:GOL:H32	2.47	0.43
1:F:94:TYR:CD1	2:F:500:NDP:H41N	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ARG:NH2	1:D:250:GLN:NE2	2.57	0.43
1:D:371:MET:HE3	4:D:2180:HOH:O	2.17	0.43
1:D:303:ASP:OD2	1:D:304:ARG:HD2	2.19	0.43
1:G:156:ILE:HD11	1:G:167:ALA:HA	2.01	0.43
1:H:220:VAL:O	1:H:224:ARG:HG2	2.19	0.43
1:H:244:GLN:HE21	1:H:244:GLN:N	2.10	0.43
1:L:407:LEU:HA	1:L:407:LEU:HD12	1.90	0.43
1:C:242:MET:SD	1:C:249:GLN:HB3	2.59	0.43
1:J:209:ARG:HH11	1:J:376:GLN:NE2	2.17	0.43
1:L:100:LEU:HB3	1:L:129:TYR:CZ	2.54	0.43
1:C:331:PHE:HB2	1:C:342:MET:HB2	2.01	0.43
1:C:148:ASP:O	1:C:175:LYS:NZ	2.52	0.43
1:L:209:ARG:HA	1:L:380:GLN:HE21	1.83	0.43
1:B:215:MET:CE	1:B:353:ILE:HG12	2.49	0.43
1:F:82:ARG:HB3	1:F:110:ARG:HB3	2.01	0.43
1:E:94:TYR:CD1	2:E:500:NDP:H41N	2.54	0.42
1:F:113:ALA:HB1	1:F:135:LYS:O	2.19	0.42
1:F:165:GLU:HG3	1:F:166:PHE:HD1	1.83	0.42
1:H:110:ARG:HH21	1:H:112:GLU:HG3	1.84	0.42
1:G:318:HIS:HB3	1:H:306:ILE:HD13	2.01	0.42
1:B:209:ARG:HH11	1:B:376:GLN:HE22	1.67	0.42
1:F:428:VAL:HG13	1:F:428:VAL:O	2.18	0.42
1:G:242:MET:CE	1:G:249:GLN:CB	2.95	0.42
1:D:178:MET:HE3	1:D:205:MET:CB	2.48	0.42
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.83	0.42
1:G:275:ARG:NH2	1:G:400:GLU:OE2	2.47	0.42
1:E:74:ALA:HA	1:G:97:ASN:HD21	1.84	0.42
1:G:188:ALA:O	1:G:192:ARG:HG3	2.19	0.42
1:I:179:CYS:O	1:I:206:ILE:HA	2.20	0.42
1:A:426:GLY:HA3	1:I:70:PRO:HG3	2.01	0.42
1:J:306:ILE:HG12	1:J:320:ALA:HB2	2.02	0.42
1:H:200:ALA:O	1:H:202:LYS:HG2	2.20	0.42
2:F:500:NDP:C5N	3:F:600[B]:GOL:H32	2.48	0.42
2:F:500:NDP:O1X	1:H:68:GLY:HA2	2.20	0.42
1:A:118:ASN:ND2	1:A:121:LYS:H	2.18	0.42
1:F:76:ARG:NH1	1:F:76:ARG:HG3	2.34	0.42
1:J:174:GLY:O	1:J:202:LYS:HE2	2.19	0.42
1:L:351:ASN:HD22	1:L:351:ASN:HA	1.65	0.42
1:C:65:THR:HB	1:C:66:PRO:HD2	2.02	0.42
1:D:269:TYR:HE2	3:D:600[B]:GOL:HO3	1.67	0.42
1:K:153:ALA:HB2	1:K:176:HIS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:HH22	1:C:250:GLN:NE2	2.13	0.42
1:D:374:ASN:HD22	1:D:375:ASN:H	1.66	0.42
1:J:96:LEU:CD2	1:J:100:LEU:HD22	2.49	0.42
1:B:76:ARG:HG2	1:B:76:ARG:HH11	1.84	0.42
1:I:178:MET:CE	1:I:205:MET:HG2	2.50	0.42
1:B:62:VAL:HG22	1:B:69:ARG:NH1	2.35	0.42
1:D:430:GLN:HE21	1:D:430:GLN:H	1.65	0.42
1:A:181:LYS:HA	1:A:182:PRO:C	2.40	0.42
1:F:233:MET:HE3	1:F:316:LEU:C	2.40	0.42
1:G:242:MET:HE1	1:G:249:GLN:HB3	1.98	0.42
1:H:118:ASN:C	1:H:118:ASN:ND2	2.73	0.42
1:F:100:LEU:HD22	1:F:111:ILE:HD13	2.00	0.42
4:A:2054:HOH:O	1:C:78:MET:HG2	2.18	0.42
1:F:308:GLN:HA	1:F:317:SER:O	2.18	0.42
1:L:304:ARG:HG2	1:L:322:SER:HB2	2.00	0.42
1:E:238:ASN:O	1:E:321:SER:HA	2.20	0.42
1:G:238:ASN:O	1:G:321:SER:HA	2.20	0.42
2:C:500:NDP:C5N	3:C:600[B]:GOL:H31	2.49	0.41
1:H:211:HIS:CE1	1:H:272:ASN:OD1	2.64	0.41
1:D:178:MET:HE3	1:D:205:MET:CG	2.51	0.41
1:C:226:ASN:HD21	1:C:229:GLY:HA2	1.85	0.41
1:E:342:MET:HG2	1:E:353:ILE:HG22	2.02	0.41
1:F:69:ARG:HB3	1:F:70:PRO:HD2	2.02	0.41
1:I:204:LEU:HD13	1:I:398:GLY:HA3	2.01	0.41
1:I:116:SER:O	1:I:138:ASP:HA	2.20	0.41
1:K:383:HIS:HE1	1:K:395:ARG:N	2.08	0.41
1:I:144:LYS:CD	1:I:147:LYS:NZ	2.83	0.41
1:H:326:THR:HG22	1:H:327:THR:N	2.35	0.41
1:H:151:ILE:O	1:H:175:LYS:HD2	2.20	0.41
1:G:350:GLN:HB3	1:G:350:GLN:HE21	1.65	0.41
1:L:179:CYS:O	1:L:206:ILE:HA	2.21	0.41
1:C:263:LEU:HB2	1:C:305:ILE:HG21	2.02	0.41
1:A:124:ILE:O	1:A:128:GLU:HG3	2.20	0.41
1:H:273:GLY:HA2	1:H:276:TYR:CE2	2.55	0.41
1:K:308:GLN:HG3	4:K:2264:HOH:O	2.20	0.41
1:K:178:MET:CE	1:K:205:MET:HG2	2.50	0.41
1:F:286:ARG:HH11	1:F:286:ARG:HG3	1.84	0.41
1:D:385:ALA:O	1:D:389:ILE:HG23	2.20	0.41
1:I:416:ARG:HB3	1:I:416:ARG:NH1	2.36	0.41
1:B:118:ASN:C	1:B:118:ASN:ND2	2.68	0.41
1:C:76:ARG:HG2	1:C:76:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:178:MET:HE3	1:L:205:MET:HB3	2.02	0.41
1:H:304:ARG:HG2	1:H:322:SER:HB2	2.03	0.41
1:I:135:LYS:HD3	4:I:2104:HOH:O	2.20	0.41
1:D:82:ARG:HB3	1:D:110:ARG:HB3	2.03	0.41
1:A:188:ALA:O	1:A:192:ARG:HG3	2.20	0.41
1:D:276:TYR:HB2	1:D:433:TYR:HB3	2.03	0.41
1:J:248:ALA:HA	2:J:500:NDP:O1A	2.20	0.41
1:J:246:ASP:HB3	1:J:249:GLN:HG2	2.03	0.41
1:C:71:MET:HE3	1:C:72:PRO:HD2	2.03	0.41
1:H:285:VAL:CG2	1:H:411:ILE:HD13	2.51	0.41
1:I:419:ARG:NE	4:I:2359:HOH:O	2.53	0.41
1:D:409:GLN:HA	1:D:409:GLN:NE2	2.36	0.41
2:E:500:NDP:C3N	3:E:600[A]:GOL:H32	2.46	0.41
1:B:211:HIS:HD2	1:B:396:SER:OG	2.03	0.41
1:L:407:LEU:HD13	1:L:425:TRP:CZ2	2.56	0.41
1:B:219:ALA:HA	1:B:222:LEU:HD11	2.02	0.41
1:E:318:HIS:CD2	1:F:318:HIS:ND1	2.86	0.41
1:A:296:GLU:HG2	4:A:2259:HOH:O	2.20	0.41
1:A:116:SER:O	1:A:138:ASP:HA	2.21	0.41
1:A:347:GLY:H	1:A:351:ASN:ND2	2.11	0.41
1:L:126:ALA:CB	1:L:131:VAL:HG22	2.51	0.41
1:E:246:ASP:HB3	1:E:249:GLN:HG2	2.03	0.41
1:F:132:ASP:HA	1:F:133:PRO:HD3	1.92	0.41
1:E:306:ILE:HD11	1:F:233:MET:HE1	2.03	0.41
1:F:344:PRO:HG2	1:H:368:GLN:HG2	2.03	0.41
1:J:209:ARG:HH11	1:J:376:GLN:HE22	1.69	0.41
1:F:278:LEU:HD12	1:F:278:LEU:HA	1.95	0.41
1:C:290:TYR:HB3	1:D:316:LEU:HD11	2.03	0.41
1:F:115:VAL:HG22	1:F:137:TYR:HB2	2.03	0.41
1:B:273:GLY:HA2	1:B:276:TYR:CE2	2.55	0.41
1:L:263:LEU:HB2	1:L:305:ILE:HG21	2.03	0.41
1:E:429:ARG:NH1	4:E:2326:HOH:O	2.52	0.41
1:B:257:LEU:HD21	1:D:64:THR:HA	2.03	0.41
1:D:93:LYS:O	1:D:97:ASN:HB2	2.20	0.41
1:K:304:ARG:HG2	1:K:322:SER:HB2	2.03	0.41
1:K:242:MET:HE1	1:K:249:GLN:HG3	2.00	0.41
1:G:141:ASN:ND2	1:G:141:ASN:C	2.72	0.41
1:L:382:ASP:O	1:L:386:GLU:HG3	2.21	0.41
1:E:179:CYS:O	1:E:206:ILE:HA	2.21	0.41
1:L:168:ILE:HG22	1:L:172:LYS:HE2	2.02	0.41
1:H:132:ASP:OD1	1:H:134:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:GLN:HG2	1:D:245:ASN:ND2	2.36	0.40
1:J:181:LYS:HA	1:J:182:PRO:C	2.40	0.40
1:D:132:ASP:HA	1:D:133:PRO:HD3	1.94	0.40
1:L:154:VAL:HG22	1:L:177:VAL:HG22	2.02	0.40
2:C:500:NDP:C3N	3:C:600[A]:GOL:H32	2.47	0.40
1:E:145:ILE:HG13	1:E:151:ILE:HD12	2.03	0.40
1:L:178:MET:HE3	1:L:205:MET:CB	2.51	0.40
1:E:155:TYR:HA	1:E:178:MET:O	2.22	0.40
1:A:385:ALA:O	1:A:389:ILE:HG13	2.21	0.40
1:L:273:GLY:HA2	1:L:276:TYR:CE2	2.57	0.40
1:H:253:LEU:HD22	1:H:297:ARG:O	2.21	0.40
1:L:181:LYS:C	1:L:181:LYS:HE2	2.41	0.40
1:J:392:LYS:HE2	4:J:2325:HOH:O	2.21	0.40
1:D:235:THR:HB	1:D:332:SER:HB3	2.04	0.40
1:D:188:ALA:O	1:D:192:ARG:HG3	2.22	0.40
1:F:93:LYS:HA	1:H:72:PRO:HB2	2.04	0.40
1:E:148:ASP:O	1:E:175:LYS:NZ	2.53	0.40
1:C:385:ALA:O	1:C:388:VAL:HG12	2.22	0.40
1:B:120:GLU:O	1:B:124:ILE:HG13	2.21	0.40
1:D:118:ASN:ND2	1:D:118:ASN:C	2.74	0.40
1:H:181:LYS:HA	1:H:182:PRO:C	2.42	0.40
1:H:160:ASN:OD1	1:H:182:PRO:HD2	2.21	0.40
1:H:158:LEU:HB3	1:H:159:PRO:HD2	2.03	0.40
1:F:347:GLY:HA2	1:H:369:PHE:CE1	2.57	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	381/433 (88%)	370 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	379/433 (88%)	366 (97%)	13 (3%)	0	100	100
1	C	380/433 (88%)	366 (96%)	13 (3%)	1 (0%)	46	36
1	D	380/433 (88%)	364 (96%)	15 (4%)	1 (0%)	46	36
1	E	380/433 (88%)	368 (97%)	11 (3%)	1 (0%)	46	36
1	F	379/433 (88%)	364 (96%)	15 (4%)	0	100	100
1	G	379/433 (88%)	367 (97%)	11 (3%)	1 (0%)	46	36
1	H	379/433 (88%)	365 (96%)	14 (4%)	0	100	100
1	I	380/433 (88%)	369 (97%)	10 (3%)	1 (0%)	46	36
1	J	379/433 (88%)	367 (97%)	12 (3%)	0	100	100
1	K	380/433 (88%)	367 (97%)	12 (3%)	1 (0%)	46	36
1	L	379/433 (88%)	366 (97%)	12 (3%)	1 (0%)	46	36
All	All	4555/5196 (88%)	4399 (97%)	149 (3%)	7 (0%)	52	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	THR
1	E	327	THR
1	G	327	THR
1	I	327	THR
1	K	327	THR
1	L	327	THR
1	D	207	GLY

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	308/345 (89%)	297 (96%)	11 (4%)	42	34
1	B	308/345 (89%)	289 (94%)	19 (6%)	23	13
1	C	308/345 (89%)	299 (97%)	9 (3%)	50	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	308/345 (89%)	294 (96%)	14 (4%)	34	25
1	E	308/345 (89%)	297 (96%)	11 (4%)	42	34
1	F	308/345 (89%)	288 (94%)	20 (6%)	21	11
1	G	308/345 (89%)	294 (96%)	14 (4%)	34	25
1	H	308/345 (89%)	288 (94%)	20 (6%)	21	11
1	I	308/345 (89%)	297 (96%)	11 (4%)	42	34
1	J	308/345 (89%)	297 (96%)	11 (4%)	42	34
1	K	308/345 (89%)	299 (97%)	9 (3%)	50	42
1	L	308/345 (89%)	296 (96%)	12 (4%)	39	30
All	All	3696/4140 (89%)	3535 (96%)	161 (4%)	35	26

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	118	ASN
1	A	141	ASN
1	A	155	TYR
1	A	181	LYS
1	A	201	ASN
1	A	240	ASP
1	A	244	GLN
1	A	323	TYR
1	A	374	ASN
1	A	429	ARG
1	B	64	THR
1	B	76	ARG
1	B	83	ARG
1	B	118	ASN
1	B	134	ARG
1	B	155	TYR
1	B	181	LYS
1	B	204	LEU
1	B	211	HIS
1	B	222	LEU
1	B	231	LEU
1	B	240	ASP
1	B	255	ARG
1	B	271	LEU

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Mol	Chain	Res	Type
1	B	323	TYR
1	B	326	THR
1	B	368	GLN
1	B	409	GLN
1	B	430	GLN
1	C	76	ARG
1	C	83	ARG
1	C	91	LEU
1	C	155	TYR
1	C	181	LYS
1	C	204	LEU
1	C	242	MET
1	C	278	LEU
1	C	323	TYR
1	D	76	ARG
1	D	118	ASN
1	D	155	TYR
1	D	181	LYS
1	D	240	ASP
1	D	242	MET
1	D	255	ARG
1	D	263	LEU
1	D	278	LEU
1	D	323	TYR
1	D	365	MET
1	D	374	ASN
1	D	394	VAL
1	D	430	GLN
1	E	76	ARG
1	E	155	TYR
1	E	181	LYS
1	E	201	ASN
1	E	203	LYS
1	E	240	ASP
1	E	244	GLN
1	E	255	ARG
1	E	278	LEU
1	E	323	TYR
1	E	368	GLN
1	F	76	ARG
1	F	143	ASP
1	F	155	TYR

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Mol	Chain	Res	Type
1	F	181	LYS
1	F	204	LEU
1	F	211	HIS
1	F	231	LEU
1	F	240	ASP
1	F	255	ARG
1	F	263	LEU
1	F	271	LEU
1	F	277	LEU
1	F	278	LEU
1	F	323	TYR
1	F	326	THR
1	F	368	GLN
1	F	374	ASN
1	F	384	LEU
1	F	407	LEU
1	F	430	GLN
1	G	76	ARG
1	G	91	LEU
1	G	118	ASN
1	G	120	GLU
1	G	141	ASN
1	G	155	TYR
1	G	181	LYS
1	G	240	ASP
1	G	244	GLN
1	G	263	LEU
1	G	323	TYR
1	G	395	ARG
1	G	406	ARG
1	G	409	GLN
1	H	76	ARG
1	H	118	ASN
1	H	155	TYR
1	H	162	LEU
1	H	181	LYS
1	H	186	SER
1	H	211	HIS
1	H	239	SER
1	H	240	ASP
1	H	244	GLN
1	H	271	LEU

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Mol	Chain	Res	Type
1	H	278	LEU
1	H	308	GLN
1	H	323	TYR
1	H	326	THR
1	H	341	LEU
1	H	368	GLN
1	H	374	ASN
1	H	403	GLN
1	H	413	GLU
1	I	55	LEU
1	I	69	ARG
1	I	76	ARG
1	I	118	ASN
1	I	155	TYR
1	I	181	LYS
1	I	204	LEU
1	I	240	ASP
1	I	244	GLN
1	I	323	TYR
1	I	403	GLN
1	J	76	ARG
1	J	155	TYR
1	J	178	MET
1	J	181	LYS
1	J	240	ASP
1	J	242	MET
1	J	244	GLN
1	J	308	GLN
1	J	323	TYR
1	J	326	THR
1	J	374	ASN
1	K	76	ARG
1	K	83	ARG
1	K	118	ASN
1	K	155	TYR
1	K	181	LYS
1	K	201	ASN
1	K	240	ASP
1	K	323	TYR
1	K	374	ASN
1	L	76	ARG
1	L	131	VAL

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Mol	Chain	Res	Type
1	L	155	TYR
1	L	181	LYS
1	L	240	ASP
1	L	244	GLN
1	L	255	ARG
1	L	308	GLN
1	L	323	TYR
1	L	368	GLN
1	L	374	ASN
1	L	407	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (212) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	97	ASN
1	A	108	HIS
1	A	118	ASN
1	A	141	ASN
1	A	176	HIS
1	A	201	ASN
1	A	244	GLN
1	A	250	GLN
1	A	308	GLN
1	A	334	GLN
1	A	351	ASN
1	A	360	HIS
1	A	374	ASN
1	A	380	GLN
1	A	383	HIS
1	A	430	GLN
1	B	61	GLN
1	B	97	ASN
1	B	98	GLN
1	B	118	ASN
1	B	160	ASN
1	B	211	HIS
1	B	226	ASN
1	B	227	GLN
1	B	250	GLN
1	B	272	ASN
1	B	351	ASN

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Mol	Chain	Res	Type
1	B	356	GLN
1	B	360	HIS
1	B	368	GLN
1	B	375	ASN
1	B	376	GLN
1	B	380	GLN
1	B	383	HIS
1	B	390	ASN
1	B	430	GLN
1	C	108	HIS
1	C	160	ASN
1	C	176	HIS
1	C	226	ASN
1	C	227	GLN
1	C	238	ASN
1	C	249	GLN
1	C	250	GLN
1	C	308	GLN
1	C	334	GLN
1	C	351	ASN
1	C	356	GLN
1	C	362	ASN
1	C	375	ASN
1	C	390	ASN
1	C	391	ASN
1	C	409	GLN
1	D	118	ASN
1	D	160	ASN
1	D	201	ASN
1	D	216	ASN
1	D	245	ASN
1	D	249	GLN
1	D	250	GLN
1	D	272	ASN
1	D	350	GLN
1	D	351	ASN
1	D	360	HIS
1	D	362	ASN
1	D	374	ASN
1	D	375	ASN
1	D	383	HIS
1	D	390	ASN

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Mol	Chain	Res	Type
1	D	403	GLN
1	D	409	GLN
1	D	430	GLN
1	E	61	GLN
1	E	97	ASN
1	E	160	ASN
1	E	176	HIS
1	E	201	ASN
1	E	216	ASN
1	E	226	ASN
1	E	244	GLN
1	E	245	ASN
1	E	250	GLN
1	E	308	GLN
1	E	318	HIS
1	E	334	GLN
1	E	360	HIS
1	E	363	GLN
1	E	368	GLN
1	E	383	HIS
1	F	98	GLN
1	F	108	HIS
1	F	201	ASN
1	F	211	HIS
1	F	226	ASN
1	F	227	GLN
1	F	249	GLN
1	F	250	GLN
1	F	308	GLN
1	F	356	GLN
1	F	360	HIS
1	F	362	ASN
1	F	368	GLN
1	F	374	ASN
1	F	375	ASN
1	F	376	GLN
1	F	383	HIS
1	F	403	GLN
1	F	422	ASN
1	G	97	ASN
1	G	118	ASN
1	G	141	ASN

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Mol	Chain	Res	Type
1	G	176	HIS
1	G	216	ASN
1	G	226	ASN
1	G	227	GLN
1	G	244	GLN
1	G	250	GLN
1	G	308	GLN
1	G	334	GLN
1	G	360	HIS
1	G	380	GLN
1	G	390	ASN
1	H	61	GLN
1	H	98	GLN
1	H	118	ASN
1	H	201	ASN
1	H	211	HIS
1	H	226	ASN
1	H	244	GLN
1	H	294	ASN
1	H	308	GLN
1	H	360	HIS
1	H	374	ASN
1	H	376	GLN
1	H	380	GLN
1	H	383	HIS
1	H	403	GLN
1	H	430	GLN
1	I	97	ASN
1	I	118	ASN
1	I	176	HIS
1	I	211	HIS
1	I	227	GLN
1	I	244	GLN
1	I	245	ASN
1	I	250	GLN
1	I	294	ASN
1	I	334	GLN
1	I	356	GLN
1	I	360	HIS
1	I	363	GLN
1	I	383	HIS
1	I	390	ASN

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Mol	Chain	Res	Type
1	I	403	GLN
1	J	97	ASN
1	J	160	ASN
1	J	201	ASN
1	J	216	ASN
1	J	226	ASN
1	J	227	GLN
1	J	238	ASN
1	J	244	GLN
1	J	249	GLN
1	J	250	GLN
1	J	272	ASN
1	J	308	GLN
1	J	350	GLN
1	J	356	GLN
1	J	360	HIS
1	J	374	ASN
1	J	375	ASN
1	J	376	GLN
1	J	380	GLN
1	J	383	HIS
1	J	403	GLN
1	K	61	GLN
1	K	97	ASN
1	K	118	ASN
1	K	176	HIS
1	K	191	GLN
1	K	201	ASN
1	K	216	ASN
1	K	226	ASN
1	K	250	GLN
1	K	308	GLN
1	K	334	GLN
1	K	360	HIS
1	K	362	ASN
1	K	374	ASN
1	K	383	HIS
1	K	390	ASN
1	K	409	GLN
1	K	422	ASN
1	L	97	ASN
1	L	160	ASN

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Mol	Chain	Res	Type
1	L	211	HIS
1	L	226	ASN
1	L	244	GLN
1	L	272	ASN
1	L	308	GLN
1	L	318	HIS
1	L	351	ASN
1	L	360	HIS
1	L	363	GLN
1	L	368	GLN
1	L	374	ASN
1	L	376	GLN
1	L	380	GLN
1	L	383	HIS
1	L	403	GLN
1	L	422	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

36 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	NDP	A	500	-	42,52,52	1.66	8 (19%)	55,80,80	2.08	10 (18%)
3	GOL	A	600[A]	-	5,5,5	1.05	0	5,5,5	0.52	0
3	GOL	A	600[B]	-	5,5,5	1.04	0	5,5,5	0.52	0
2	NDP	B	500	-	42,52,52	1.61	7 (16%)	55,80,80	2.03	9 (16%)
3	GOL	B	600[A]	-	5,5,5	1.04	0	5,5,5	0.52	0
3	GOL	B	600[B]	-	5,5,5	1.03	0	5,5,5	0.52	0
2	NDP	C	500	-	42,52,52	1.58	8 (19%)	55,80,80	2.04	10 (18%)
3	GOL	C	600[A]	-	5,5,5	1.04	0	5,5,5	0.53	0
3	GOL	C	600[B]	-	5,5,5	1.04	0	5,5,5	0.53	0
2	NDP	D	500	-	42,52,52	1.63	10 (23%)	55,80,80	1.99	11 (20%)
3	GOL	D	600[A]	-	5,5,5	1.03	0	5,5,5	0.53	0
3	GOL	D	600[B]	-	5,5,5	1.02	0	5,5,5	0.53	0
2	NDP	E	500	-	42,52,52	1.59	9 (21%)	55,80,80	2.05	10 (18%)
3	GOL	E	600[A]	-	5,5,5	1.01	0	5,5,5	0.53	0
3	GOL	E	600[B]	-	5,5,5	1.01	0	5,5,5	0.53	0
2	NDP	F	500	-	42,52,52	1.63	10 (23%)	55,80,80	1.99	11 (20%)
3	GOL	F	600[A]	-	5,5,5	1.02	0	5,5,5	0.53	0
3	GOL	F	600[B]	-	5,5,5	1.01	0	5,5,5	0.53	0
2	NDP	G	500	-	42,52,52	1.65	8 (19%)	55,80,80	2.06	9 (16%)
3	GOL	G	600[A]	-	5,5,5	1.02	0	5,5,5	0.53	0
3	GOL	G	600[B]	-	5,5,5	1.01	0	5,5,5	0.53	0
2	NDP	H	500	-	42,52,52	1.60	8 (19%)	55,80,80	2.03	9 (16%)
3	GOL	H	600[A]	-	5,5,5	1.00	0	5,5,5	0.53	0
3	GOL	H	600[B]	-	5,5,5	1.00	0	5,5,5	0.53	0
2	NDP	I	500	-	42,52,52	1.63	9 (21%)	55,80,80	2.07	9 (16%)
3	GOL	I	600[A]	-	5,5,5	0.99	0	5,5,5	0.52	0
3	GOL	I	600[B]	-	5,5,5	0.99	0	5,5,5	0.52	0
2	NDP	J	500	-	42,52,52	1.63	7 (16%)	55,80,80	2.05	10 (18%)
3	GOL	J	600[A]	-	5,5,5	0.98	0	5,5,5	0.52	0
3	GOL	J	600[B]	-	5,5,5	0.97	0	5,5,5	0.52	0
2	NDP	K	500	-	42,52,52	1.66	9 (21%)	55,80,80	2.08	10 (18%)
3	GOL	K	600[A]	-	5,5,5	0.97	0	5,5,5	0.52	0
3	GOL	K	600[B]	-	5,5,5	0.96	0	5,5,5	0.52	0
2	NDP	L	500	-	42,52,52	1.61	7 (16%)	55,80,80	2.05	10 (18%)
3	GOL	L	600[A]	-	5,5,5	0.97	0	5,5,5	0.52	0
3	GOL	L	600[B]	-	5,5,5	0.96	0	5,5,5	0.52	0

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	NDP	A	500	-	-	0/30/77/77	0/5/5/5
3	GOL	A	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	A	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	B	500	-	-	0/30/77/77	0/5/5/5
3	GOL	B	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	B	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	C	500	-	-	0/30/77/77	0/5/5/5
3	GOL	C	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	C	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	D	500	-	-	0/30/77/77	0/5/5/5
3	GOL	D	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	D	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	E	500	-	-	0/30/77/77	0/5/5/5
3	GOL	E	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	E	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	F	500	-	-	0/30/77/77	0/5/5/5
3	GOL	F	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	F	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	G	500	-	-	0/30/77/77	0/5/5/5
3	GOL	G	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	G	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	H	500	-	-	0/30/77/77	0/5/5/5
3	GOL	H	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	H	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	I	500	-	-	0/30/77/77	0/5/5/5
3	GOL	I	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	I	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	J	500	-	-	0/30/77/77	0/5/5/5
3	GOL	J	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	J	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	K	500	-	-	0/30/77/77	0/5/5/5
3	GOL	K	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	K	600[B]	-	-	0/4/4/4	0/0/0/0
2	NDP	L	500	-	-	0/30/77/77	0/5/5/5
3	GOL	L	600[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	L	600[B]	-	-	0/4/4/4	0/0/0/0

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	500	NDP	P2B-O2X	-4.94	1.37	1.54
2	A	500	NDP	P2B-O2X	-4.90	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	NDP	P2B-O2X	-4.88	1.37	1.54
2	K	500	NDP	P2B-O2X	-4.86	1.37	1.54
2	G	500	NDP	P2B-O2X	-4.81	1.37	1.54
2	J	500	NDP	P2B-O2X	-4.80	1.37	1.54
2	E	500	NDP	P2B-O2X	-4.75	1.37	1.54
2	L	500	NDP	P2B-O2X	-4.75	1.37	1.54
2	F	500	NDP	P2B-O2X	-4.70	1.37	1.54
2	C	500	NDP	P2B-O2X	-4.68	1.37	1.54
2	H	500	NDP	P2B-O2X	-4.59	1.38	1.54
2	B	500	NDP	P2B-O2X	-4.53	1.38	1.54
2	I	500	NDP	C4N-C5N	-2.20	1.44	1.49
2	D	500	NDP	C4N-C5N	-2.17	1.44	1.49
2	K	500	NDP	C4N-C5N	-2.17	1.44	1.49
2	K	500	NDP	C5A-N7A	-2.11	1.32	1.39
2	E	500	NDP	C4N-C5N	-2.09	1.44	1.49
2	C	500	NDP	C4N-C5N	-2.07	1.44	1.49
2	F	500	NDP	C4N-C5N	-2.07	1.44	1.49
2	G	500	NDP	C5A-N7A	-2.07	1.32	1.39
2	A	500	NDP	C5A-N7A	-2.07	1.32	1.39
2	A	500	NDP	C4N-C5N	-2.07	1.44	1.49
2	E	500	NDP	C5A-N7A	-2.06	1.32	1.39
2	J	500	NDP	C4N-C5N	-2.04	1.44	1.49
2	I	500	NDP	C5A-N7A	-2.04	1.32	1.39
2	G	500	NDP	C4N-C5N	-2.03	1.44	1.49
2	L	500	NDP	C4N-C5N	-2.03	1.44	1.49
2	B	500	NDP	P2B-O1X	2.00	1.57	1.51
2	I	500	NDP	O4D-C1D	2.00	1.47	1.42
2	E	500	NDP	P2B-O1X	2.01	1.57	1.51
2	C	500	NDP	P2B-O2B	2.01	1.66	1.60
2	F	500	NDP	O4D-C1D	2.01	1.47	1.42
2	G	500	NDP	P2B-O1X	2.02	1.57	1.51
2	E	500	NDP	C4A-N3A	2.02	1.38	1.35
2	H	500	NDP	P2B-O2B	2.03	1.66	1.60
2	D	500	NDP	O4D-C1D	2.03	1.47	1.42
2	C	500	NDP	P2B-O1X	2.04	1.57	1.51
2	K	500	NDP	C4A-N3A	2.04	1.38	1.35
2	D	500	NDP	P2B-O1X	2.06	1.57	1.51
2	K	500	NDP	P2B-O1X	2.09	1.58	1.51
2	F	500	NDP	P2B-O1X	2.10	1.58	1.51
2	L	500	NDP	P2B-O1X	2.10	1.58	1.51
2	I	500	NDP	P2B-O1X	2.13	1.58	1.51
2	F	500	NDP	C4A-N3A	2.15	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NDP	P2B-O1X	2.15	1.58	1.51
2	J	500	NDP	P2B-O1X	2.15	1.58	1.51
2	H	500	NDP	P2B-O1X	2.16	1.58	1.51
2	H	500	NDP	C4A-N3A	2.22	1.38	1.35
2	D	500	NDP	C4A-N3A	2.24	1.38	1.35
2	L	500	NDP	C6N-N1N	2.28	1.44	1.37
2	D	500	NDP	P2B-O2B	2.32	1.67	1.60
2	E	500	NDP	C6N-N1N	2.33	1.44	1.37
2	I	500	NDP	C6N-N1N	2.35	1.44	1.37
2	G	500	NDP	C6N-N1N	2.36	1.44	1.37
2	J	500	NDP	C6N-N1N	2.36	1.44	1.37
2	K	500	NDP	C6N-N1N	2.37	1.44	1.37
2	F	500	NDP	C6N-N1N	2.39	1.44	1.37
2	A	500	NDP	C6N-N1N	2.39	1.44	1.37
2	C	500	NDP	C6N-N1N	2.42	1.44	1.37
2	B	500	NDP	C4A-N3A	2.43	1.39	1.35
2	D	500	NDP	C6N-N1N	2.44	1.44	1.37
2	H	500	NDP	C6N-N1N	2.46	1.44	1.37
2	F	500	NDP	P2B-O2B	2.49	1.67	1.60
2	B	500	NDP	C6N-N1N	2.52	1.44	1.37
2	L	500	NDP	C2N-C3N	2.59	1.41	1.34
2	H	500	NDP	C2N-C3N	2.66	1.41	1.34
2	B	500	NDP	C2N-C3N	2.67	1.41	1.34
2	J	500	NDP	C2N-C3N	2.77	1.41	1.34
2	D	500	NDP	O4B-C1B	2.81	1.44	1.41
2	G	500	NDP	C2N-C3N	2.82	1.41	1.34
2	K	500	NDP	C2N-C3N	2.83	1.41	1.34
2	E	500	NDP	C2N-C3N	2.84	1.41	1.34
2	C	500	NDP	C2N-C3N	2.85	1.41	1.34
2	F	500	NDP	C2N-C3N	2.85	1.41	1.34
2	A	500	NDP	C2N-C3N	2.87	1.41	1.34
2	D	500	NDP	C2N-C3N	2.91	1.41	1.34
2	I	500	NDP	C2N-C3N	2.92	1.41	1.34
2	H	500	NDP	O4B-C1B	2.93	1.44	1.41
2	C	500	NDP	O4B-C1B	2.94	1.44	1.41
2	J	500	NDP	O4B-C1B	3.02	1.45	1.41
2	F	500	NDP	O4B-C1B	3.10	1.45	1.41
2	B	500	NDP	O4B-C1B	3.19	1.45	1.41
2	I	500	NDP	O4B-C1B	3.27	1.45	1.41
2	E	500	NDP	O4B-C1B	3.32	1.45	1.41
2	G	500	NDP	O4B-C1B	3.34	1.45	1.41
2	L	500	NDP	O4B-C1B	3.38	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NDP	O4B-C1B	3.83	1.46	1.41
2	K	500	NDP	O4B-C1B	3.98	1.46	1.41
2	E	500	NDP	C6N-C5N	4.18	1.41	1.33
2	A	500	NDP	C6N-C5N	4.21	1.41	1.33
2	C	500	NDP	C6N-C5N	4.23	1.41	1.33
2	B	500	NDP	C6N-C5N	4.26	1.41	1.33
2	D	500	NDP	C6N-C5N	4.26	1.41	1.33
2	F	500	NDP	C6N-C5N	4.29	1.41	1.33
2	J	500	NDP	C6N-C5N	4.32	1.41	1.33
2	H	500	NDP	C6N-C5N	4.32	1.41	1.33
2	G	500	NDP	C6N-C5N	4.36	1.41	1.33
2	L	500	NDP	C6N-C5N	4.39	1.41	1.33
2	K	500	NDP	C6N-C5N	4.40	1.41	1.33
2	I	500	NDP	C6N-C5N	4.40	1.41	1.33

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	500	NDP	N3A-C2A-N1A	-10.53	120.83	128.89
2	E	500	NDP	N3A-C2A-N1A	-10.46	120.89	128.89
2	H	500	NDP	N3A-C2A-N1A	-10.44	120.90	128.89
2	G	500	NDP	N3A-C2A-N1A	-10.42	120.92	128.89
2	A	500	NDP	N3A-C2A-N1A	-10.40	120.93	128.89
2	C	500	NDP	N3A-C2A-N1A	-10.36	120.96	128.89
2	F	500	NDP	N3A-C2A-N1A	-10.35	120.97	128.89
2	B	500	NDP	N3A-C2A-N1A	-10.33	120.98	128.89
2	K	500	NDP	N3A-C2A-N1A	-10.32	120.99	128.89
2	D	500	NDP	N3A-C2A-N1A	-10.29	121.02	128.89
2	J	500	NDP	N3A-C2A-N1A	-10.25	121.05	128.89
2	L	500	NDP	N3A-C2A-N1A	-10.17	121.11	128.89
2	D	500	NDP	C3N-C2N-N1N	-3.44	118.21	123.14
2	A	500	NDP	C3N-C2N-N1N	-3.33	118.37	123.14
2	K	500	NDP	C3N-C2N-N1N	-3.31	118.40	123.14
2	E	500	NDP	C3N-C2N-N1N	-3.30	118.42	123.14
2	F	500	NDP	C3N-C2N-N1N	-3.30	118.42	123.14
2	I	500	NDP	C3N-C2N-N1N	-3.25	118.48	123.14
2	C	500	NDP	C3N-C2N-N1N	-3.25	118.48	123.14
2	B	500	NDP	C3N-C2N-N1N	-3.22	118.53	123.14
2	G	500	NDP	C3N-C2N-N1N	-3.13	118.66	123.14
2	H	500	NDP	C3N-C2N-N1N	-3.13	118.66	123.14
2	J	500	NDP	C3N-C2N-N1N	-3.07	118.74	123.14
2	L	500	NDP	C3N-C2N-N1N	-3.07	118.75	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	NDP	C4N-C5N-C6N	-3.01	117.61	122.58
2	K	500	NDP	C4N-C5N-C6N	-2.99	117.66	122.58
2	D	500	NDP	C4N-C5N-C6N	-2.98	117.66	122.58
2	C	500	NDP	C4N-C5N-C6N	-2.98	117.67	122.58
2	A	500	NDP	C4N-C5N-C6N	-2.98	117.67	122.58
2	F	500	NDP	C4N-C5N-C6N	-2.97	117.67	122.58
2	L	500	NDP	C4N-C5N-C6N	-2.97	117.68	122.58
2	H	500	NDP	C4N-C5N-C6N	-2.97	117.69	122.58
2	G	500	NDP	C4N-C5N-C6N	-2.91	117.78	122.58
2	J	500	NDP	C4N-C5N-C6N	-2.89	117.82	122.58
2	E	500	NDP	C4N-C5N-C6N	-2.88	117.83	122.58
2	I	500	NDP	C4N-C5N-C6N	-2.88	117.84	122.58
2	L	500	NDP	C1D-N1N-C2N	-2.65	116.30	120.91
2	B	500	NDP	C1D-N1N-C2N	-2.62	116.34	120.91
2	K	500	NDP	C1D-N1N-C2N	-2.55	116.47	120.91
2	H	500	NDP	C1D-N1N-C2N	-2.54	116.48	120.91
2	I	500	NDP	C1D-N1N-C2N	-2.49	116.56	120.91
2	J	500	NDP	C1D-N1N-C2N	-2.46	116.62	120.91
2	G	500	NDP	C1D-N1N-C2N	-2.44	116.66	120.91
2	F	500	NDP	C1D-N1N-C2N	-2.38	116.76	120.91
2	C	500	NDP	C1D-N1N-C2N	-2.37	116.77	120.91
2	A	500	NDP	C1D-N1N-C2N	-2.36	116.79	120.91
2	E	500	NDP	C1D-N1N-C2N	-2.36	116.80	120.91
2	D	500	NDP	C1D-N1N-C2N	-2.28	116.93	120.91
2	A	500	NDP	O5B-C5B-C4B	-2.00	101.73	109.12
2	E	500	NDP	O2X-P2B-O1X	2.02	117.09	110.58
2	G	500	NDP	O2X-P2B-O1X	2.02	117.10	110.58
2	F	500	NDP	O2X-P2B-O1X	2.04	117.14	110.58
2	C	500	NDP	O2X-P2B-O1X	2.04	117.15	110.58
2	F	500	NDP	C3B-C2B-C1B	2.05	106.69	102.73
2	D	500	NDP	C3B-C2B-C1B	2.05	106.70	102.73
2	D	500	NDP	O2X-P2B-O1X	2.06	117.20	110.58
2	B	500	NDP	O2X-P2B-O1X	2.07	117.23	110.58
2	L	500	NDP	O2X-P2B-O1X	2.08	117.26	110.58
2	J	500	NDP	O2X-P2B-O1X	2.08	117.26	110.58
2	K	500	NDP	O2X-P2B-O1X	2.08	117.28	110.58
2	A	500	NDP	O2X-P2B-O1X	2.08	117.29	110.58
2	I	500	NDP	O2X-P2B-O1X	2.09	117.30	110.58
2	H	500	NDP	O2X-P2B-O1X	2.09	117.32	110.58
2	E	500	NDP	P2B-O2B-C2B	2.10	126.59	121.56
2	F	500	NDP	P2B-O2B-C2B	2.11	126.61	121.56
2	D	500	NDP	P2B-O2B-C2B	2.18	126.78	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	500	NDP	P2B-O2B-C2B	2.20	126.84	121.56
2	B	500	NDP	C4A-C5A-N7A	2.21	111.51	109.48
2	C	500	NDP	P2B-O2B-C2B	2.21	126.86	121.56
2	H	500	NDP	C4A-C5A-N7A	2.23	111.53	109.48
2	F	500	NDP	C4A-C5A-N7A	2.26	111.56	109.48
2	D	500	NDP	C4A-C5A-N7A	2.27	111.56	109.48
2	L	500	NDP	P2B-O2B-C2B	2.28	127.04	121.56
2	J	500	NDP	P2B-O2B-C2B	2.33	127.14	121.56
2	D	500	NDP	O4B-C1B-N9A	2.33	112.99	108.10
2	J	500	NDP	C4A-C5A-N7A	2.33	111.63	109.48
2	L	500	NDP	C4A-C5A-N7A	2.34	111.63	109.48
2	F	500	NDP	O4B-C1B-N9A	2.36	113.05	108.10
2	G	500	NDP	C4A-C5A-N7A	2.37	111.66	109.48
2	C	500	NDP	C4A-C5A-N7A	2.38	111.67	109.48
2	A	500	NDP	C4A-C5A-N7A	2.40	111.69	109.48
2	I	500	NDP	C4A-C5A-N7A	2.44	111.72	109.48
2	E	500	NDP	C4A-C5A-N7A	2.48	111.76	109.48
2	K	500	NDP	C4A-C5A-N7A	2.50	111.78	109.48
2	H	500	NDP	O4B-C1B-N9A	2.93	114.23	108.10
2	B	500	NDP	O4B-C1B-N9A	3.06	114.50	108.10
2	C	500	NDP	O4B-C1B-N9A	3.14	114.68	108.10
2	G	500	NDP	C5N-C4N-C3N	3.27	121.54	112.52
2	I	500	NDP	C5N-C4N-C3N	3.31	121.65	112.52
2	H	500	NDP	C5N-C4N-C3N	3.33	121.69	112.52
2	J	500	NDP	C5N-C4N-C3N	3.34	121.72	112.52
2	K	500	NDP	C5N-C4N-C3N	3.35	121.75	112.52
2	L	500	NDP	C5N-C4N-C3N	3.35	121.75	112.52
2	E	500	NDP	C5N-C4N-C3N	3.36	121.77	112.52
2	B	500	NDP	C5N-C4N-C3N	3.37	121.81	112.52
2	A	500	NDP	C5N-C4N-C3N	3.39	121.87	112.52
2	C	500	NDP	C5N-C4N-C3N	3.40	121.87	112.52
2	F	500	NDP	C5N-C4N-C3N	3.40	121.89	112.52
2	E	500	NDP	O4B-C1B-N9A	3.45	115.31	108.10
2	D	500	NDP	C5N-C4N-C3N	3.46	122.06	112.52
2	I	500	NDP	O4B-C1B-N9A	3.51	115.44	108.10
2	J	500	NDP	O4B-C1B-N9A	3.57	115.57	108.10
2	L	500	NDP	O4B-C1B-N9A	3.58	115.59	108.10
2	K	500	NDP	O4B-C1B-N9A	3.77	116.00	108.10
2	G	500	NDP	O4B-C1B-N9A	4.00	116.47	108.10
2	A	500	NDP	O4B-C1B-N9A	4.07	116.62	108.10
2	F	500	NDP	O3-PA-O5B	4.21	114.09	102.94
2	D	500	NDP	O3-PA-O5B	4.35	114.49	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	500	NDP	O3-PA-O5B	5.05	116.34	102.94
2	B	500	NDP	O3-PA-O5B	5.19	116.71	102.94
2	E	500	NDP	O3-PA-O5B	5.27	116.92	102.94
2	C	500	NDP	O3-PA-O5B	5.28	116.93	102.94
2	I	500	NDP	O3-PA-O5B	5.37	117.17	102.94
2	G	500	NDP	O3-PA-O5B	5.44	117.36	102.94
2	A	500	NDP	O3-PA-O5B	5.48	117.48	102.94
2	J	500	NDP	O3-PA-O5B	5.48	117.48	102.94
2	L	500	NDP	O3-PA-O5B	5.56	117.68	102.94
2	K	500	NDP	O3-PA-O5B	5.66	117.95	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

36 monomers are involved in 104 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NDP	7	0
3	A	600[A]	GOL	2	0
3	A	600[B]	GOL	3	0
2	B	500	NDP	5	0
3	B	600[A]	GOL	2	0
3	B	600[B]	GOL	2	0
2	C	500	NDP	10	0
3	C	600[A]	GOL	4	0
3	C	600[B]	GOL	3	0
2	D	500	NDP	10	0
3	D	600[A]	GOL	2	0
3	D	600[B]	GOL	4	0
2	E	500	NDP	10	0
3	E	600[A]	GOL	5	0
3	E	600[B]	GOL	3	0
2	F	500	NDP	10	0
3	F	600[A]	GOL	3	0
3	F	600[B]	GOL	3	0
2	G	500	NDP	7	0
3	G	600[A]	GOL	2	0
3	G	600[B]	GOL	3	0
2	H	500	NDP	8	0
3	H	600[A]	GOL	3	0
3	H	600[B]	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	500	NDP	6	0
3	I	600[A]	GOL	2	0
3	I	600[B]	GOL	2	0
2	J	500	NDP	10	0
3	J	600[A]	GOL	3	0
3	J	600[B]	GOL	3	0
2	K	500	NDP	9	0
3	K	600[A]	GOL	2	0
3	K	600[B]	GOL	3	0
2	L	500	NDP	10	0
3	L	600[A]	GOL	4	0
3	L	600[B]	GOL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	383/433 (88%)	-0.47	5 (1%) 79 83	12, 18, 30, 48	0
1	B	381/433 (87%)	-0.21	9 (2%) 62 68	13, 23, 38, 45	0
1	C	382/433 (88%)	-0.36	3 (0%) 87 90	14, 21, 32, 45	0
1	D	382/433 (88%)	0.11	23 (6%) 25 28	16, 31, 44, 53	0
1	E	382/433 (88%)	-0.34	3 (0%) 87 90	14, 22, 32, 44	0
1	F	381/433 (87%)	0.09	12 (3%) 52 60	16, 30, 46, 52	0
1	G	381/433 (87%)	-0.47	3 (0%) 87 90	12, 18, 30, 40	0
1	H	381/433 (87%)	-0.17	8 (2%) 67 72	14, 23, 39, 46	0
1	I	382/433 (88%)	-0.54	2 (0%) 91 93	10, 16, 28, 39	0
1	J	381/433 (87%)	-0.44	2 (0%) 91 93	11, 19, 30, 42	0
1	K	382/433 (88%)	-0.54	2 (0%) 91 93	10, 16, 27, 39	0
1	L	381/433 (87%)	-0.43	1 (0%) 94 95	11, 19, 29, 40	0
All	All	4579/5196 (88%)	-0.31	73 (1%) 74 79	10, 21, 38, 53	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	52	ALA	7.0
1	C	52	ALA	6.0
1	K	52	ALA	5.7
1	E	52	ALA	5.4
1	I	52	ALA	5.0
1	A	51	GLN	4.8
1	F	147	LYS	4.6
1	D	147	LYS	4.0
1	A	52	ALA	3.9
1	E	134	ARG	3.6
1	F	201	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	134	ARG	3.4
1	D	201	ASN	3.2
1	D	299	VAL	3.0
1	C	134	ARG	3.0
1	F	145	ILE	3.0
1	F	138	ASP	3.0
1	D	389	ILE	2.9
1	B	134	ARG	2.9
1	F	134	ARG	2.9
1	H	134	ARG	2.9
1	D	149	PRO	2.8
1	B	53	ALA	2.8
1	G	134	ARG	2.8
1	G	419	ARG	2.8
1	G	391	ASN	2.8
1	H	431	GLY	2.7
1	B	123	LYS	2.7
1	H	149	PRO	2.6
1	K	134	ARG	2.6
1	J	134	ARG	2.6
1	H	428	VAL	2.5
1	D	140	SER	2.5
1	D	416	ARG	2.5
1	E	419	ARG	2.5
1	D	419	ARG	2.5
1	D	144	LYS	2.4
1	H	53	ALA	2.4
1	D	255	ARG	2.4
1	A	391	ASN	2.4
1	D	141	ASN	2.4
1	F	255	ARG	2.4
1	F	120	GLU	2.3
1	I	134	ARG	2.3
1	F	389	ILE	2.3
1	H	57	ALA	2.3
1	F	140	SER	2.3
1	D	120	GLU	2.3
1	D	130	GLY	2.3
1	F	192	ARG	2.2
1	J	431	GLY	2.2
1	A	134	ARG	2.2
1	B	431	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	130	GLY	2.2
1	F	141	ASN	2.2
1	D	136	ILE	2.2
1	C	419	ARG	2.2
1	B	130	GLY	2.2
1	B	57	ALA	2.2
1	B	149	PRO	2.2
1	A	419	ARG	2.1
1	D	83	ARG	2.1
1	D	123	LYS	2.1
1	D	133	PRO	2.1
1	F	428	VAL	2.1
1	D	431	GLY	2.1
1	H	61	GLN	2.1
1	B	54	THR	2.1
1	L	120	GLU	2.1
1	B	83	ARG	2.0
1	D	430	GLN	2.0
1	D	132	ASP	2.0
1	D	145	ILE	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	GOL	I	600[B]	6/6	0.63	0.31	20.04	30,30,32,33	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	I	600[A]	6/6	0.63	0.31	20.04	29,30,32,33	1
3	GOL	L	600[B]	6/6	0.41	0.40	16.46	31,34,35,35	1
3	GOL	L	600[A]	6/6	0.41	0.40	16.46	32,34,35,35	1
3	GOL	K	600[B]	6/6	0.56	0.32	15.29	31,31,32,33	1
3	GOL	K	600[A]	6/6	0.56	0.32	15.29	29,31,32,33	1
3	GOL	E	600[B]	6/6	0.46	0.34	14.46	32,34,34,35	1
3	GOL	E	600[A]	6/6	0.46	0.34	14.46	33,34,34,35	1
3	GOL	C	600[B]	6/6	0.56	0.31	13.91	31,33,33,33	1
3	GOL	C	600[A]	6/6	0.56	0.31	13.91	32,33,33,33	1
3	GOL	J	600[A]	6/6	0.41	0.34	13.90	30,30,31,31	1
3	GOL	H	600[B]	6/6	0.45	0.33	12.60	36,37,38,38	1
3	GOL	H	600[A]	6/6	0.45	0.33	12.60	36,37,38,38	1
3	GOL	G	600[B]	6/6	0.48	0.28	11.85	28,29,30,31	1
3	GOL	G	600[A]	6/6	0.48	0.28	11.85	25,28,29,31	1
3	GOL	A	600[B]	6/6	0.59	0.28	11.61	21,23,25,25	1
3	GOL	A	600[A]	6/6	0.59	0.28	11.61	18,22,23,25	1
3	GOL	J	600[B]	6/6	0.41	0.34	11.22	27,30,31,31	1
3	GOL	B	600[B]	6/6	0.50	0.33	10.06	31,33,35,35	1
3	GOL	B	600[A]	6/6	0.50	0.33	9.60	33,34,35,35	1
3	GOL	F	600[A]	6/6	0.37	0.29	8.27	42,43,43,43	1
3	GOL	F	600[B]	6/6	0.37	0.29	8.27	42,43,43,43	1
3	GOL	D	600[B]	6/6	0.47	0.30	7.29	43,44,44,44	1
3	GOL	D	600[A]	6/6	0.47	0.30	7.29	42,44,44,44	1
2	NDP	C	500	48/48	0.96	0.10	0.46	15,19,24,26	0
2	NDP	A	500	48/48	0.96	0.10	0.42	12,15,17,17	0
2	NDP	K	500	48/48	0.97	0.09	0.33	10,16,18,18	0
2	NDP	L	500	48/48	0.97	0.09	0.17	13,19,21,22	0
2	NDP	I	500	48/48	0.97	0.09	0.15	10,15,18,18	0
2	NDP	G	500	48/48	0.97	0.09	0.15	13,16,18,19	0
2	NDP	F	500	48/48	0.91	0.13	0.14	28,33,42,43	0
2	NDP	J	500	48/48	0.96	0.09	0.13	15,19,22,22	0
2	NDP	E	500	48/48	0.96	0.10	0.13	15,20,22,23	0
2	NDP	B	500	48/48	0.96	0.10	-0.12	18,23,26,26	0
2	NDP	D	500	48/48	0.93	0.12	-0.27	25,34,43,43	0
2	NDP	H	500	48/48	0.96	0.09	-0.27	19,22,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.