Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:22 PM GMT

PDB ID	:	1T9K
Title	:	X-ray crystal structure of aIF-2B alpha subunit-related translation initiation factor [Thermotoga maritima]
Authors	:	Osipiuk, J.; Skarina, T.; Savchenko, A.; Edwards, A.; Cymborowski, M.; Minor, W.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2004-05-17
Resolution	:	2.60 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:

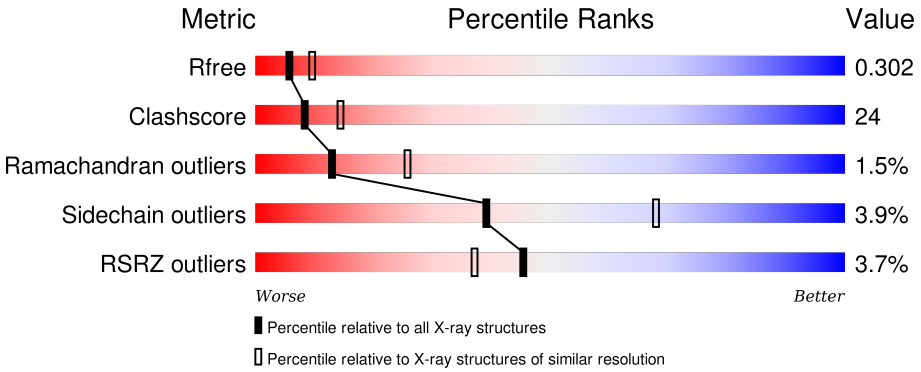
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	347	% 61% 35%
1	B	347	% 59% 36%
1	C	347	6% 52% 42%
1	D	347	6% 55% 39% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10854 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 Probable methylthioribose-1-phosphate isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	Se	0	0	0
			2650	1684	458	497	3	8			
1	B	340	Total	C	N	O	S	Se	0	0	0
			2650	1684	458	497	3	8			
1	C	342	Total	C	N	O	S	Se	0	0	0
			2667	1695	461	499	3	9			
1	D	342	Total	C	N	O	S	Se	0	0	0
			2667	1695	461	499	3	9			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q9X013
A	0	HIS	-	CLONING ARTIFACT	UNP Q9X013
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
A	8	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
A	45	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
A	77	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
A	101	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
A	125	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
A	203	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
A	216	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
A	221	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
A	344	GLY	-	CLONING ARTIFACT	UNP Q9X013
A	345	SER	-	CLONING ARTIFACT	UNP Q9X013
B	-1	GLY	-	CLONING ARTIFACT	UNP Q9X013
B	0	HIS	-	CLONING ARTIFACT	UNP Q9X013
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
B	8	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
B	45	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
B	77	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
B	101	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
B	125	MSE	MET	MODIFIED RESIDUE	UNP Q9X013

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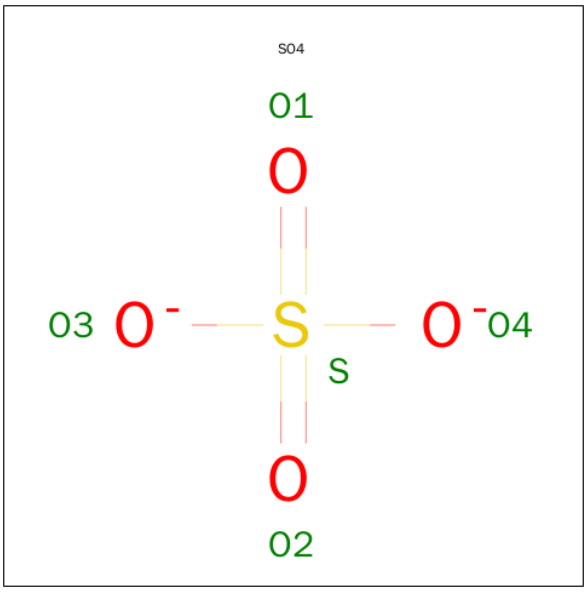
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
B	216	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
B	221	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
B	344	GLY	-	CLONING ARTIFACT	UNP Q9X013
B	345	SER	-	CLONING ARTIFACT	UNP Q9X013
C	-1	GLY	-	CLONING ARTIFACT	UNP Q9X013
C	0	HIS	-	CLONING ARTIFACT	UNP Q9X013
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
C	8	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
C	45	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
C	77	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
C	101	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
C	125	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
C	203	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
C	216	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
C	221	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
C	344	GLY	-	CLONING ARTIFACT	UNP Q9X013
C	345	SER	-	CLONING ARTIFACT	UNP Q9X013
D	-1	GLY	-	CLONING ARTIFACT	UNP Q9X013
D	0	HIS	-	CLONING ARTIFACT	UNP Q9X013
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
D	8	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
D	45	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
D	77	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
D	101	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
D	125	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
D	203	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
D	216	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
D	221	MSE	MET	MODIFIED RESIDUE	UNP Q9X013
D	344	GLY	-	CLONING ARTIFACT	UNP Q9X013
D	345	SER	-	CLONING ARTIFACT	UNP Q9X013

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	50	Total O 50 50	0	0
4	B	50	Total O 50 50	0	0
4	C	49	Total O 49 49	0	0

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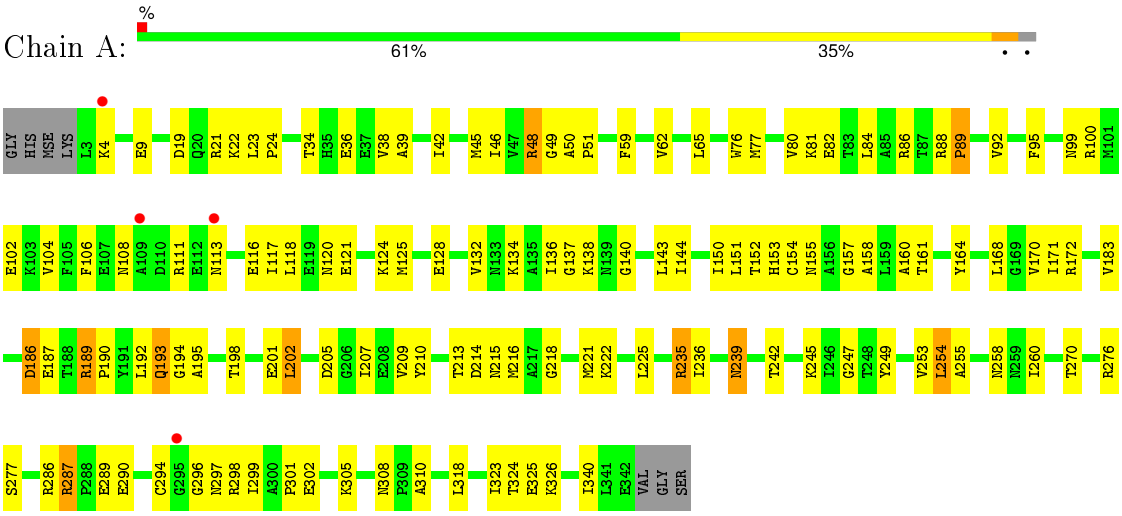
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	49	Total O 49 49	0	0

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.

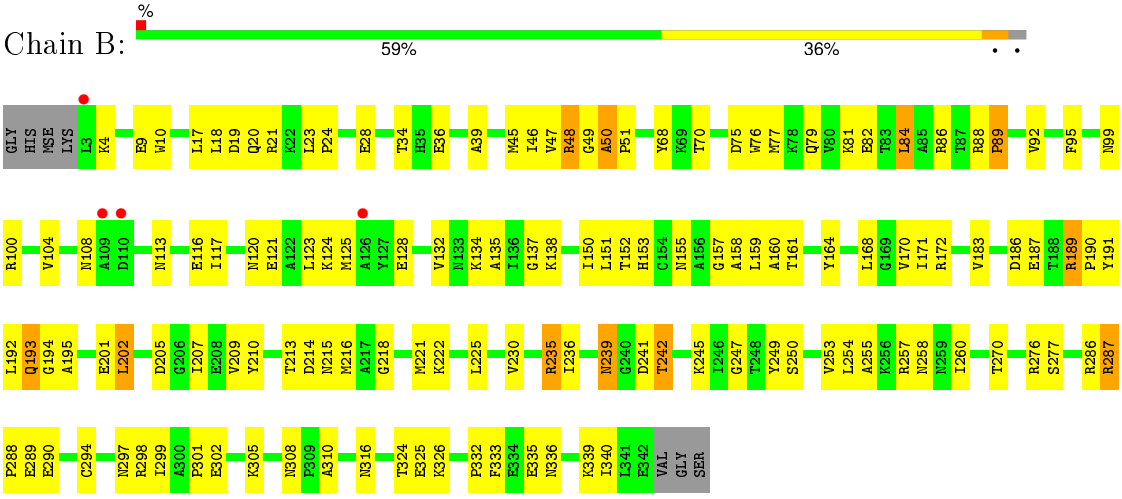
- Molecule 1: Probable methylthioribose-1-phosphate isomerase

Chain A:



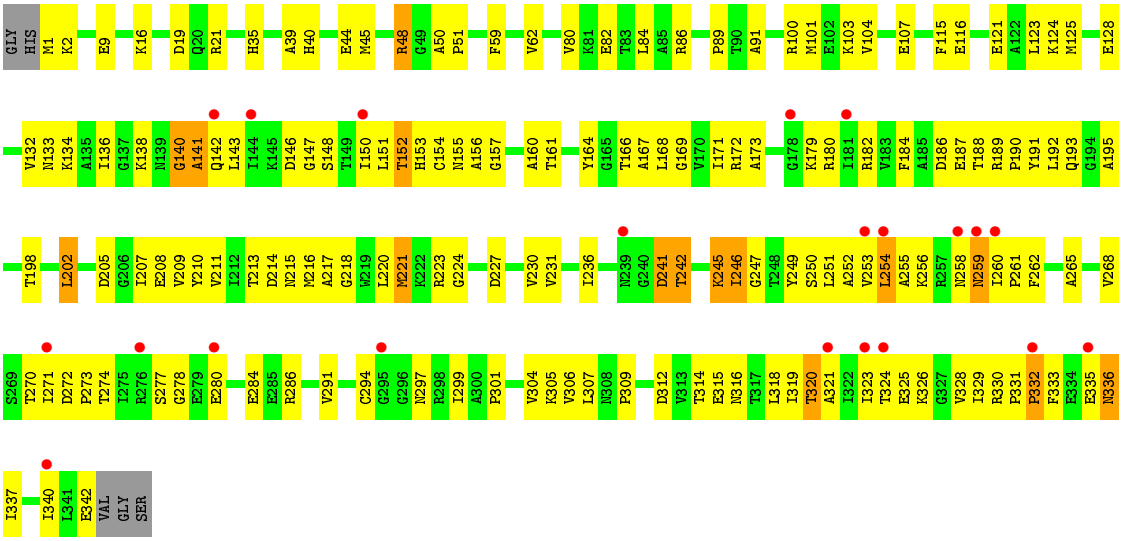
- Molecule 1: Probable methylthioribose-1-phosphate isomerase

Chain B:



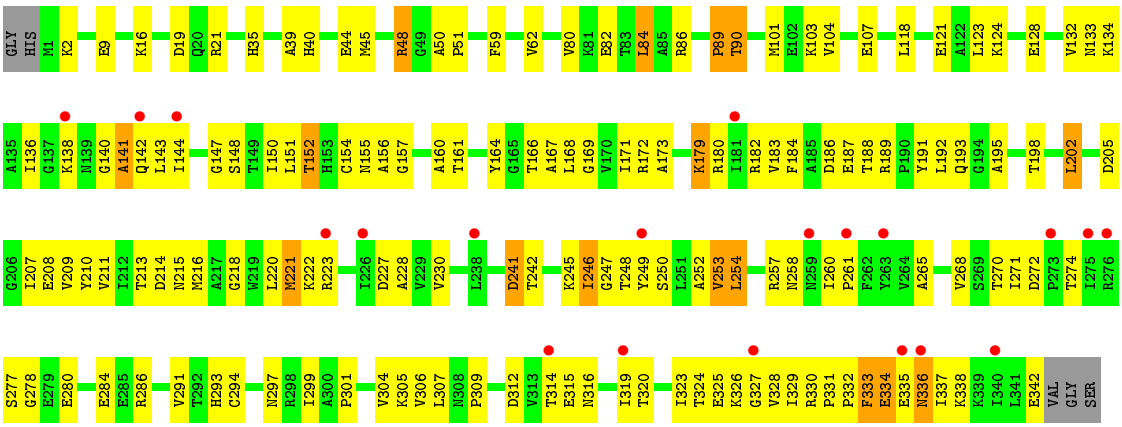
- Molecule 1: Probable methylthioribose-1-phosphate isomerase

Chain C:



- Molecule 1: Probable methylthioribose-1-phosphate isomerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.89Å 103.89Å 259.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.33 – 2.60 34.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (34.33-2.60) 98.6 (34.32-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.33 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.298 0.245 , 0.302	Depositor DCC
R_{free} test set	2468 reflections (4.92%)	DCC
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 18.1	EDS
Estimated twinning fraction	0.488 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 96655 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10854	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: SO4, CL

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	0.30	0/2687	0.58	0/3626
1	B	0.30	0/2687	0.57	0/3626
1	C	0.31	0/2704	0.57	0/3647
1	D	0.31	0/2704	0.57	0/3647
All	All	0.30	0/10782	0.57	0/14546

There are no bond length outliers.

There are no bond angle outliers.

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	2650	0	2701	126	0
1	B	2650	0	2701	129	0
1	C	2667	0	2725	154	0
1	D	2667	0	2725	157	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	50	0	0	1	0
4	B	50	0	0	0	0
4	C	49	0	0	1	0
4	D	49	0	0	0	0
All	All	10854	0	10852	520	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 24.

All (520) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLN:HE21	1:B:193:GLN:H	1.06	1.03
1:D:324:THR:HG22	1:D:326:LYS:H	1.19	1.02
1:D:258:ASN:HB2	1:D:260:ILE:HD11	1.38	1.02
1:C:258:ASN:HB2	1:C:260:ILE:HD11	1.42	1.01
1:C:324:THR:HG22	1:C:326:LYS:H	1.26	0.99
1:D:104:VAL:HG21	1:D:121:GLU:HG3	1.44	0.98
1:C:104:VAL:HG21	1:C:121:GLU:HG3	1.46	0.97
1:A:104:VAL:HG21	1:A:121:GLU:HG3	1.44	0.97
1:B:34:THR:HG22	1:B:36:GLU:H	1.31	0.96
1:A:193:GLN:NE2	1:A:193:GLN:H	1.64	0.95
1:B:324:THR:HG22	1:B:326:LYS:H	1.27	0.94
1:D:268:VAL:O	1:D:271:ILE:HG22	1.68	0.93
1:B:104:VAL:HG21	1:B:121:GLU:HG3	1.49	0.92
1:A:202:LEU:HB3	1:A:209:VAL:HG21	1.52	0.90
1:A:157:GLY:HA3	1:A:168:LEU:HD12	1.52	0.90
1:C:221:MSE:HE2	1:C:254:LEU:HD12	1.52	0.89
1:A:193:GLN:HE21	1:A:193:GLN:H	0.91	0.89
1:C:268:VAL:O	1:C:271:ILE:HG22	1.74	0.88
1:A:193:GLN:HE21	1:A:193:GLN:N	1.72	0.87
1:B:202:LEU:HB3	1:B:209:VAL:HG21	1.53	0.87
1:D:48:ARG:HH12	1:D:155:ASN:HD22	1.22	0.87
1:A:4:LYS:HG2	1:A:9:GLU:HG3	1.54	0.87
1:D:221:MSE:HE3	1:D:254:LEU:O	1.74	0.87
1:D:19:ASP:OD1	1:D:21:ARG:HG2	1.75	0.86
1:C:48:ARG:HH12	1:C:155:ASN:HD22	1.19	0.85
1:C:132:VAL:HG13	1:C:325:GLU:HB3	1.58	0.85
1:C:331:PRO:HA	1:C:333:PHE:N	1.92	0.85
1:A:34:THR:HG22	1:A:36:GLU:H	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:PRO:HA	1:C:333:PHE:H	1.40	0.84
1:B:50:ALA:HB3	1:B:51:PRO:HD3	1.59	0.83
1:C:19:ASP:OD1	1:C:21:ARG:HG2	1.78	0.83
1:B:239:ASN:HB2	1:B:276:ARG:O	1.77	0.83
1:D:132:VAL:HG13	1:D:325:GLU:HB3	1.60	0.82
1:A:239:ASN:HB2	1:A:276:ARG:O	1.81	0.81
1:A:324:THR:HG22	1:A:326:LYS:H	1.45	0.81
1:C:316:ASN:HB2	1:C:333:PHE:HD1	1.46	0.80
1:C:82:GLU:OE2	1:C:86:ARG:HD3	1.82	0.79
1:B:157:GLY:HA3	1:B:168:LEU:HD12	1.63	0.79
1:A:50:ALA:HB3	1:A:51:PRO:HD3	1.65	0.79
1:D:331:PRO:HA	1:D:333:PHE:N	1.97	0.79
1:B:193:GLN:HE21	1:B:193:GLN:N	1.82	0.78
1:C:193:GLN:HE22	1:C:245:LYS:HE2	1.48	0.78
1:A:207:ILE:O	1:A:209:VAL:HG23	1.84	0.78
1:C:265:ALA:HB2	1:C:323:ILE:HD12	1.64	0.77
1:D:221:MSE:HG2	1:D:258:ASN:HD22	1.49	0.77
1:C:50:ALA:HB3	1:C:51:PRO:HD3	1.67	0.76
1:D:202:LEU:HD23	1:D:209:VAL:HG11	1.66	0.76
1:B:171:ILE:HD13	1:B:183:VAL:HG21	1.69	0.75
1:D:50:ALA:HB3	1:D:51:PRO:HD3	1.68	0.75
1:B:287:ARG:HG2	1:B:290:GLU:HG3	1.69	0.74
1:A:294:CYS:HG	1:B:294:CYS:HG	1.34	0.74
1:B:152:THR:HG22	1:B:153:HIS:H	1.52	0.74
1:D:9:GLU:HB3	1:D:16:LYS:HB2	1.71	0.72
1:A:189:ARG:HG2	1:A:190:PRO:HA	1.71	0.72
1:A:287:ARG:HG2	1:A:290:GLU:HG3	1.71	0.72
1:B:207:ILE:O	1:B:209:VAL:HG23	1.90	0.71
1:A:171:ILE:HD13	1:A:183:VAL:HG21	1.72	0.71
1:B:189:ARG:HG2	1:B:190:PRO:HA	1.72	0.70
1:B:19:ASP:OD1	1:B:21:ARG:HG3	1.92	0.70
1:C:316:ASN:HB2	1:C:333:PHE:CD1	2.26	0.70
1:B:245:LYS:HE3	1:B:245:LYS:HA	1.73	0.70
1:D:277:SER:HB3	1:D:280:GLU:HG3	1.73	0.70
1:C:297:ASN:ND2	1:D:297:ASN:ND2	2.39	0.69
1:D:82:GLU:OE2	1:D:86:ARG:HD3	1.92	0.69
1:B:324:THR:HG22	1:B:326:LYS:N	2.05	0.68
1:B:51:PRO:HB2	1:B:161:THR:HG22	1.73	0.68
1:D:183:VAL:HB	1:D:209:VAL:HG12	1.76	0.68
1:A:19:ASP:OD1	1:A:21:ARG:HG3	1.93	0.68
1:C:128:GLU:O	1:C:132:VAL:HG23	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MSE:HE2	1:A:286:ARG:NE	2.09	0.67
1:C:254:LEU:HD23	1:D:254:LEU:HD23	1.74	0.67
1:D:316:ASN:HB2	1:D:333:PHE:HD1	1.58	0.67
1:A:298:ARG:HH21	1:A:302:GLU:HA	1.59	0.67
1:C:100:ARG:HD3	1:C:125:MSE:HE2	1.77	0.67
1:D:265:ALA:HB2	1:D:323:ILE:HD12	1.76	0.67
1:C:187:GLU:OE2	1:D:189:ARG:HD3	1.94	0.67
1:C:48:ARG:HH12	1:C:155:ASN:ND2	1.93	0.66
1:D:141:ALA:HB2	1:D:173:ALA:HB3	1.78	0.66
1:B:4:LYS:HG3	1:B:9:GLU:HG3	1.77	0.65
1:A:48:ARG:HH22	1:A:155:ASN:HD22	1.43	0.65
1:D:124:LYS:O	1:D:128:GLU:HG3	1.97	0.65
1:D:314:THR:HG22	1:D:315:GLU:H	1.61	0.65
1:C:189:ARG:HD3	1:D:187:GLU:OE2	1.96	0.65
1:C:167:ALA:HB1	1:C:230:VAL:HG12	1.77	0.65
1:A:152:THR:HG22	1:A:153:HIS:H	1.62	0.65
1:D:140:GLY:C	1:D:142:GLN:H	2.00	0.65
1:C:182:ARG:HA	1:C:208:GLU:HB3	1.79	0.65
1:D:329:ILE:HD12	1:D:329:ILE:N	2.12	0.65
1:D:294:CYS:HB2	1:D:299:ILE:HD13	1.78	0.64
1:C:124:LYS:O	1:C:128:GLU:HG3	1.98	0.64
1:A:151:LEU:HD11	1:A:186:ASP:OD1	1.98	0.63
1:D:193:GLN:HE22	1:D:245:LYS:HE3	1.62	0.63
1:B:48:ARG:HH22	1:B:155:ASN:HD22	1.44	0.63
1:A:172:ARG:NH2	1:A:201:GLU:OE2	2.31	0.63
1:B:137:GLY:HA2	1:B:170:VAL:HA	1.80	0.63
1:C:227:ASP:O	1:C:261:PRO:HD2	1.97	0.63
1:C:277:SER:HB3	1:C:280:GLU:HG3	1.81	0.63
1:C:9:GLU:HB3	1:C:16:LYS:HB2	1.81	0.63
1:C:202:LEU:HD23	1:C:209:VAL:HG11	1.80	0.63
1:D:184:PHE:CD1	1:D:210:TYR:HB2	2.34	0.63
1:D:316:ASN:HB2	1:D:333:PHE:CD1	2.33	0.63
1:C:187:GLU:HG2	1:C:213:THR:HA	1.81	0.62
1:C:132:VAL:HG13	1:C:325:GLU:CB	2.30	0.62
1:A:137:GLY:HA2	1:A:170:VAL:HA	1.81	0.62
1:C:140:GLY:C	1:C:142:GLN:H	2.02	0.62
1:A:51:PRO:HB2	1:A:161:THR:HG22	1.80	0.62
1:A:294:CYS:HB2	1:A:299:ILE:HD13	1.81	0.62
1:D:329:ILE:HG22	1:D:330:ARG:N	2.15	0.61
1:C:329:ILE:N	1:C:329:ILE:HD12	2.15	0.61
1:D:167:ALA:HB1	1:D:230:VAL:HG12	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:HE2	1:A:310:ALA:O	2.01	0.60
1:C:211:VAL:HB	1:D:306:VAL:HG12	1.83	0.60
1:B:171:ILE:HD13	1:B:183:VAL:CG2	2.31	0.60
1:B:39:ALA:HB2	1:B:84:LEU:HD12	1.84	0.60
1:C:247:GLY:N	1:C:312:ASP:OD2	2.35	0.60
1:C:148:SER:HB2	1:C:227:ASP:OD2	2.02	0.60
1:B:221:MSE:HE2	1:B:260:ILE:HD12	1.83	0.60
1:C:191:TYR:HD2	1:C:193:GLN:HG3	1.67	0.60
1:C:340:ILE:N	1:C:340:ILE:HD12	2.16	0.60
1:D:132:VAL:HG13	1:D:325:GLU:CB	2.30	0.60
1:C:221:MSE:HG2	1:C:258:ASN:HD22	1.66	0.59
1:D:150:ILE:HG21	1:D:230:VAL:HG23	1.84	0.59
1:B:134:LYS:HA	1:B:164:TYR:CE2	2.37	0.59
1:A:297:ASN:ND2	1:B:297:ASN:ND2	2.51	0.59
1:D:193:GLN:NE2	1:D:245:LYS:HE3	2.17	0.59
1:A:65:LEU:HD22	1:A:118:LEU:HD12	1.84	0.59
1:A:51:PRO:CB	1:A:161:THR:HG22	2.33	0.59
1:D:48:ARG:HH12	1:D:155:ASN:ND2	1.98	0.59
1:D:89:PRO:HG2	1:D:284:GLU:HB2	1.85	0.59
1:D:187:GLU:HG2	1:D:213:THR:HA	1.85	0.58
1:C:304:VAL:HG22	1:C:305:LYS:N	2.17	0.58
1:D:133:ASN:HA	1:D:136:ILE:HG22	1.84	0.58
1:A:113:ASN:O	1:A:117:ILE:HG13	2.03	0.58
1:C:301:PRO:HD3	1:D:195:ALA:O	2.03	0.58
1:C:306:VAL:HG12	1:D:211:VAL:HB	1.86	0.58
1:B:113:ASN:O	1:B:117:ILE:HG13	2.02	0.58
1:D:202:LEU:HD23	1:D:209:VAL:CG1	2.33	0.58
1:B:51:PRO:CB	1:B:161:THR:HG22	2.34	0.58
1:B:287:ARG:HB2	1:B:289:GLU:OE1	2.03	0.58
1:C:202:LEU:HD23	1:C:209:VAL:CG1	2.33	0.58
1:C:314:THR:HG22	1:C:315:GLU:N	2.19	0.58
1:D:152:THR:HG23	1:D:230:VAL:O	2.04	0.57
1:C:152:THR:HG23	1:C:230:VAL:O	2.04	0.57
1:D:227:ASP:O	1:D:261:PRO:HD2	2.04	0.57
1:C:324:THR:HG22	1:C:325:GLU:N	2.18	0.57
1:B:135:ALA:HA	1:B:138:LYS:HE3	1.86	0.57
1:D:128:GLU:O	1:D:132:VAL:HG23	2.05	0.57
1:C:221:MSE:HB3	1:C:258:ASN:ND2	2.19	0.57
1:D:333:PHE:C	1:D:335:GLU:H	2.08	0.57
1:D:314:THR:HG22	1:D:315:GLU:N	2.19	0.57
1:D:247:GLY:N	1:D:312:ASP:OD2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ASP:OD1	1:D:274:THR:N	2.38	0.57
1:D:324:THR:HG22	1:D:325:GLU:N	2.21	0.56
1:B:172:ARG:NH2	1:B:201:GLU:OE2	2.38	0.56
1:C:291:VAL:HB	1:C:306:VAL:HG21	1.87	0.56
1:C:151:LEU:HD11	1:C:186:ASP:OD1	2.05	0.56
1:C:262:PHE:HD2	1:C:319:ILE:HG22	1.70	0.56
1:D:39:ALA:HB2	1:D:84:LEU:HD12	1.85	0.56
1:C:305:LYS:O	1:D:210:TYR:HA	2.06	0.56
1:C:195:ALA:O	1:D:301:PRO:HD3	2.05	0.56
1:D:324:THR:HG23	1:D:325:GLU:OE1	2.06	0.56
1:C:309:PRO:HD2	1:D:216:MSE:SE	2.56	0.56
1:D:250:SER:O	1:D:254:LEU:HB2	2.06	0.56
1:A:324:THR:HG22	1:A:325:GLU:N	2.20	0.55
1:A:221:MSE:HE2	1:A:260:ILE:HD12	1.86	0.55
1:B:45:MSE:HE2	1:B:286:ARG:NE	2.22	0.55
1:C:314:THR:HG22	1:C:315:GLU:H	1.72	0.55
1:B:298:ARG:HH21	1:B:302:GLU:HA	1.71	0.55
1:C:167:ALA:HB2	1:C:231:VAL:O	2.06	0.55
1:B:324:THR:HG22	1:B:325:GLU:N	2.21	0.55
1:A:171:ILE:HD13	1:A:183:VAL:CG2	2.35	0.55
1:D:316:ASN:HA	1:D:319:ILE:HG12	1.88	0.55
1:A:59:PHE:O	1:A:62:VAL:HG22	2.06	0.55
1:D:140:GLY:O	1:D:142:GLN:N	2.40	0.55
1:C:262:PHE:CD2	1:C:319:ILE:HG22	2.42	0.55
1:B:124:LYS:HG2	1:B:128:GLU:OE2	2.07	0.54
1:D:171:ILE:HG22	1:D:207:ILE:HD13	1.89	0.54
1:A:48:ARG:NH2	1:A:155:ASN:HD22	2.05	0.54
1:D:151:LEU:HD11	1:D:186:ASP:OD1	2.07	0.54
1:A:134:LYS:HA	1:A:164:TYR:CE2	2.42	0.54
1:C:140:GLY:O	1:C:142:GLN:N	2.41	0.54
1:C:134:LYS:HA	1:C:164:TYR:CE2	2.43	0.54
1:D:304:VAL:HG22	1:D:305:LYS:N	2.23	0.54
1:A:187:GLU:CD	1:B:189:ARG:HE	2.11	0.54
1:B:4:LYS:HG3	1:B:9:GLU:CG	2.38	0.54
1:C:141:ALA:HB2	1:C:173:ALA:HB3	1.88	0.54
1:D:191:TYR:HD2	1:D:193:GLN:HG3	1.72	0.54
1:A:298:ARG:NH2	1:A:302:GLU:HA	2.22	0.54
1:C:184:PHE:CD1	1:C:210:TYR:HB2	2.42	0.54
1:B:202:LEU:HB3	1:B:209:VAL:CG2	2.32	0.54
1:B:48:ARG:NH2	1:B:155:ASN:HD22	2.04	0.54
1:A:301:PRO:HD3	1:B:195:ALA:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:N	1:C:143:LEU:HD12	2.23	0.54
1:C:249:TYR:O	1:C:253:VAL:HG23	2.07	0.54
1:D:253:VAL:HG12	1:D:253:VAL:O	2.07	0.54
1:A:195:ALA:O	1:B:301:PRO:HD3	2.08	0.54
1:B:48:ARG:HD2	2:B:411:SO4:O3	2.08	0.53
1:A:48:ARG:HD2	2:A:401:SO4:O3	2.08	0.53
1:C:39:ALA:HB2	1:C:84:LEU:HD12	1.90	0.53
1:C:133:ASN:HA	1:C:136:ILE:HG22	1.90	0.53
1:B:152:THR:HG22	1:B:153:HIS:N	2.22	0.53
1:A:287:ARG:HB2	1:A:289:GLU:OE1	2.08	0.53
1:C:304:VAL:HG22	1:C:305:LYS:H	1.73	0.53
1:A:82:GLU:OE1	1:A:82:GLU:HA	2.08	0.53
1:C:191:TYR:HB3	1:C:193:GLN:OE1	2.08	0.53
1:A:297:ASN:HD21	1:B:297:ASN:ND2	2.07	0.53
1:B:152:THR:HG23	1:B:230:VAL:O	2.09	0.53
1:C:210:TYR:HA	1:D:305:LYS:O	2.08	0.53
1:C:220:LEU:HD21	1:D:307:LEU:HD13	1.91	0.53
1:C:82:GLU:O	1:C:86:ARG:HG3	2.09	0.53
1:B:128:GLU:O	1:B:132:VAL:HG23	2.09	0.53
1:B:186:ASP:O	1:B:194:GLY:HA3	2.09	0.52
1:B:82:GLU:OE1	1:B:82:GLU:HA	2.09	0.52
1:C:221:MSE:HE3	1:C:254:LEU:O	2.09	0.52
1:B:193:GLN:NE2	1:B:193:GLN:H	1.90	0.52
1:D:221:MSE:HE2	1:D:254:LEU:HD12	1.90	0.52
1:D:260:ILE:N	1:D:260:ILE:HD12	2.25	0.52
1:C:329:ILE:C	1:C:330:ARG:HG2	2.29	0.52
1:D:329:ILE:C	1:D:330:ARG:HG2	2.29	0.52
1:D:156:ALA:HB1	1:D:166:THR:OG1	2.09	0.52
1:D:252:ALA:C	1:D:254:LEU:H	2.13	0.52
1:B:34:THR:HG22	1:B:36:GLU:N	2.14	0.52
1:C:59:PHE:O	1:C:62:VAL:HG22	2.09	0.52
1:B:75:ASP:O	1:B:79:GLN:HG3	2.10	0.52
1:D:324:THR:CG2	1:D:325:GLU:N	2.73	0.52
1:A:23:LEU:HB3	1:A:24:PRO:HA	1.91	0.52
1:C:316:ASN:O	1:C:319:ILE:HG12	2.08	0.51
1:D:157:GLY:HA2	1:D:168:LEU:HB2	1.91	0.51
1:C:250:SER:OG	1:D:218:GLY:HA3	2.10	0.51
1:A:81:LYS:NZ	1:A:99:ASN:ND2	2.58	0.51
1:D:191:TYR:HB3	1:D:193:GLN:OE1	2.10	0.51
1:D:331:PRO:HA	1:D:333:PHE:H	1.72	0.51
1:D:333:PHE:O	1:D:335:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:MSE:HE1	1:B:255:ALA:HA	1.92	0.51
1:D:316:ASN:O	1:D:319:ILE:HG12	2.11	0.51
1:B:236:ILE:HG12	1:B:242:THR:HB	1.92	0.51
1:A:216:MSE:HE1	1:B:308:ASN:HA	1.91	0.51
1:A:324:THR:HG22	1:A:326:LYS:N	2.22	0.51
1:A:190:PRO:HB2	1:A:290:GLU:O	2.11	0.51
1:A:144:ILE:HG23	1:A:150:ILE:HD11	1.93	0.51
1:A:168:LEU:HD23	1:A:171:ILE:HD12	1.93	0.51
1:B:316:ASN:HB2	1:B:333:PHE:CD1	2.46	0.51
1:A:187:GLU:OE2	1:B:189:ARG:NE	2.42	0.51
1:C:172:ARG:NH1	1:C:205:ASP:OD2	2.36	0.51
1:A:308:ASN:HA	1:B:216:MSE:HE1	1.93	0.51
1:A:158:ALA:N	1:A:201:GLU:OE2	2.40	0.51
1:B:239:ASN:HB2	1:B:277:SER:HA	1.93	0.51
1:C:157:GLY:HA2	1:C:168:LEU:HB2	1.92	0.50
1:C:21:ARG:HB3	1:C:191:TYR:OH	2.10	0.50
1:B:81:LYS:NZ	1:B:99:ASN:ND2	2.59	0.50
1:C:246:ILE:HA	1:C:312:ASP:OD2	2.11	0.50
1:C:307:LEU:HD13	1:D:220:LEU:HD21	1.93	0.50
1:D:103:LYS:O	1:D:107:GLU:HG3	2.11	0.50
1:A:198:THR:O	1:A:202:LEU:HB2	2.12	0.50
1:C:215:ASN:ND2	1:D:189:ARG:O	2.45	0.50
1:A:144:ILE:CG2	1:A:150:ILE:HD11	2.42	0.50
1:D:334:GLU:HG2	1:D:334:GLU:O	2.11	0.50
1:B:86:ARG:HG2	1:B:86:ARG:O	2.12	0.50
1:A:128:GLU:O	1:A:132:VAL:HG23	2.11	0.50
1:B:324:THR:CG2	1:B:325:GLU:N	2.74	0.50
1:A:189:ARG:NE	1:B:187:GLU:OE2	2.43	0.50
1:B:21:ARG:NE	1:B:46:ILE:HG12	2.27	0.50
1:C:150:ILE:HG21	1:C:230:VAL:HG23	1.93	0.50
1:C:133:ASN:O	1:C:136:ILE:HG22	2.11	0.50
1:A:236:ILE:HG23	1:A:242:THR:HG22	1.94	0.50
1:B:92:VAL:HB	1:B:235:ARG:HD3	1.94	0.50
1:C:169:GLY:HA2	1:C:172:ARG:HD2	1.94	0.49
1:B:17:LEU:HD13	1:B:47:VAL:HB	1.93	0.49
1:C:324:THR:CG2	1:C:325:GLU:N	2.75	0.49
1:A:45:MSE:HE2	1:A:286:ARG:HE	1.77	0.49
1:D:329:ILE:HG22	1:D:330:ARG:H	1.76	0.49
1:A:152:THR:HG22	1:A:153:HIS:N	2.27	0.49
1:D:59:PHE:O	1:D:62:VAL:HG22	2.11	0.49
1:C:260:ILE:HD12	1:C:260:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:CYS:HB2	1:C:299:ILE:HD13	1.94	0.49
1:C:329:ILE:HG22	1:C:330:ARG:N	2.28	0.49
1:A:324:THR:CG2	1:A:325:GLU:N	2.76	0.49
1:C:51:PRO:HB2	1:C:161:THR:HG22	1.93	0.49
1:A:86:ARG:HG2	1:A:86:ARG:O	2.13	0.49
1:D:249:TYR:O	1:D:253:VAL:HG23	2.12	0.49
1:D:332:PRO:O	1:D:334:GLU:N	2.45	0.49
1:D:143:LEU:N	1:D:143:LEU:HD12	2.26	0.49
1:C:251:LEU:O	1:C:255:ALA:HB2	2.12	0.49
1:D:182:ARG:HA	1:D:208:GLU:HB3	1.95	0.49
1:C:218:GLY:HA3	1:D:250:SER:OG	2.13	0.49
1:A:193:GLN:NE2	1:A:193:GLN:N	2.44	0.49
1:C:328:VAL:C	1:C:329:ILE:HD12	2.32	0.49
1:A:4:LYS:HG2	1:A:9:GLU:CG	2.34	0.48
1:C:245:LYS:HG3	1:C:246:ILE:HD12	1.94	0.48
1:D:51:PRO:HB2	1:D:161:THR:HG22	1.95	0.48
1:B:151:LEU:HD11	1:B:186:ASP:OD1	2.13	0.48
1:D:82:GLU:O	1:D:86:ARG:HG3	2.13	0.48
1:A:76:TRP:HD1	1:A:77:MSE:CE	2.25	0.48
1:C:45:MSE:HE2	1:C:286:ARG:HE	1.79	0.48
1:A:324:THR:HG23	1:A:325:GLU:OE1	2.14	0.48
1:A:38:VAL:O	1:A:42:ILE:HG13	2.14	0.48
1:B:168:LEU:HD23	1:B:171:ILE:HD12	1.96	0.48
1:D:333:PHE:C	1:D:335:GLU:N	2.66	0.48
1:A:297:ASN:HD21	1:B:297:ASN:HD21	1.60	0.48
1:A:134:LYS:O	1:A:138:LYS:HE2	2.13	0.48
1:A:239:ASN:HB2	1:A:277:SER:HA	1.96	0.48
1:D:277:SER:HB3	1:D:280:GLU:CG	2.42	0.48
1:A:294:CYS:HG	1:B:294:CYS:CB	2.27	0.47
1:A:221:MSE:HE1	1:A:255:ALA:HA	1.95	0.47
1:A:318:LEU:HD21	1:B:257:ARG:NH2	2.29	0.47
1:A:245:LYS:HA	1:A:245:LYS:HE3	1.96	0.47
1:B:18:LEU:HD12	1:B:28:GLU:O	2.15	0.47
1:B:23:LEU:HB3	1:B:24:PRO:HA	1.95	0.47
1:C:272:ASP:OD1	1:C:274:THR:N	2.46	0.47
1:A:189:ARG:HE	1:B:187:GLU:CD	2.16	0.47
1:C:35:HIS:CD2	1:C:80:VAL:HG13	2.49	0.47
1:B:190:PRO:HB2	1:B:290:GLU:O	2.14	0.47
1:D:172:ARG:NH1	1:D:205:ASP:OD2	2.37	0.47
1:A:202:LEU:HB3	1:A:209:VAL:CG2	2.36	0.47
1:C:155:ASN:O	1:C:160:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:TYR:HB3	1:B:193:GLN:NE2	2.30	0.47
1:B:332:PRO:HB2	1:B:335:GLU:HB3	1.97	0.47
1:D:150:ILE:HG23	1:D:228:ALA:O	2.15	0.46
1:D:304:VAL:HG22	1:D:305:LYS:H	1.80	0.46
1:A:124:LYS:HG2	1:A:128:GLU:OE2	2.15	0.46
1:C:318:LEU:HD21	1:D:257:ARG:NH1	2.29	0.46
1:C:271:ILE:HG23	1:C:271:ILE:O	2.15	0.46
1:C:332:PRO:HB2	1:C:335:GLU:OE2	2.15	0.46
1:D:155:ASN:O	1:D:160:ALA:HB2	2.15	0.46
1:C:191:TYR:O	1:C:192:LEU:HB2	2.15	0.46
1:B:189:ARG:CG	1:B:190:PRO:HA	2.44	0.46
1:A:113:ASN:HA	1:A:116:GLU:OE1	2.15	0.46
1:C:186:ASP:HB3	1:C:214:ASP:OD1	2.15	0.46
1:D:168:LEU:HD11	1:D:198:THR:HG23	1.97	0.46
1:C:89:PRO:HG2	1:C:284:GLU:HB2	1.96	0.46
1:A:186:ASP:HB3	1:A:214:ASP:OD1	2.15	0.46
1:C:213:THR:OG1	1:C:216:MSE:HE3	2.16	0.46
1:B:76:TRP:HD1	1:B:77:MSE:CE	2.29	0.46
1:D:221:MSE:HE3	1:D:254:LEU:C	2.36	0.46
1:B:324:THR:HG23	1:B:325:GLU:OE1	2.16	0.46
1:A:189:ARG:CG	1:A:190:PRO:HA	2.42	0.46
1:D:182:ARG:HB3	1:D:208:GLU:HG2	1.97	0.46
1:A:157:GLY:CA	1:A:168:LEU:HD12	2.35	0.46
1:C:329:ILE:HG22	1:C:333:PHE:CE2	2.51	0.46
1:B:294:CYS:HB2	1:B:299:ILE:HD13	1.98	0.46
1:B:221:MSE:HE2	1:B:260:ILE:CD1	2.46	0.46
1:D:241:ASP:OD2	1:D:278:GLY:N	2.48	0.46
1:C:103:LYS:O	1:C:107:GLU:HG3	2.16	0.46
1:C:216:MSE:SE	1:D:309:PRO:HD2	2.66	0.45
1:C:189:ARG:O	1:D:215:ASN:ND2	2.49	0.45
1:C:91:ALA:HB3	4:C:413:HOH:O	2.16	0.45
1:D:151:LEU:HD12	1:D:184:PHE:O	2.15	0.45
1:A:108:ASN:ND2	1:A:117:ILE:HD13	2.31	0.45
1:C:324:THR:HG23	1:C:325:GLU:OE1	2.16	0.45
1:A:286:ARG:HD3	4:A:455:HOH:O	2.14	0.45
1:A:154:CYS:SG	1:A:155:ASN:N	2.87	0.45
1:C:138:LYS:C	1:C:140:GLY:H	2.19	0.45
1:D:147:GLY:N	1:D:180:ARG:O	2.49	0.45
1:D:35:HIS:CD2	1:D:80:VAL:HG13	2.51	0.45
1:B:49:GLY:O	1:B:50:ALA:C	2.54	0.45
1:D:291:VAL:HB	1:D:306:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLY:HA3	1:B:215:ASN:HB2	1.98	0.45
1:C:2:LYS:CB	1:C:123:LEU:HD21	2.47	0.45
1:B:4:LYS:HG3	1:B:9:GLU:OE1	2.17	0.45
1:C:189:ARG:HB3	1:C:190:PRO:HA	1.99	0.45
1:A:116:GLU:O	1:A:120:ASN:HB2	2.17	0.45
1:A:39:ALA:HB2	1:A:84:LEU:HD12	1.97	0.45
1:C:188:THR:O	1:C:192:LEU:HA	2.17	0.45
1:D:189:ARG:NH2	1:D:293:HIS:O	2.46	0.45
1:C:140:GLY:C	1:C:142:GLN:N	2.69	0.45
1:B:19:ASP:HA	1:B:46:ILE:HG23	1.98	0.45
1:A:19:ASP:OD1	1:A:22:LYS:HG3	2.17	0.45
1:C:167:ALA:CB	1:C:230:VAL:HG12	2.47	0.45
1:D:221:MSE:CG	1:D:258:ASN:HD22	2.26	0.45
1:D:191:TYR:O	1:D:192:LEU:HB2	2.16	0.45
1:B:187:GLU:HB2	1:B:192:LEU:HD22	1.99	0.45
1:A:92:VAL:HB	1:A:235:ARG:HD3	1.99	0.45
1:B:50:ALA:HB3	1:B:51:PRO:CD	2.40	0.45
1:D:144:ILE:O	1:D:179:LYS:HD3	2.16	0.45
1:A:136:ILE:HG23	1:A:323:ILE:HG22	1.99	0.44
1:C:221:MSE:HE3	1:C:255:ALA:HA	1.99	0.44
1:D:188:THR:O	1:D:192:LEU:HA	2.17	0.44
1:A:155:ASN:O	1:A:160:ALA:HB2	2.17	0.44
1:D:248:THR:HB	1:D:312:ASP:OD1	2.18	0.44
1:C:253:VAL:O	1:C:253:VAL:HG12	2.16	0.44
1:D:221:MSE:HB3	1:D:258:ASN:ND2	2.32	0.44
1:B:48:ARG:HH22	1:B:160:ALA:HB2	1.82	0.44
1:C:306:VAL:HB	1:D:211:VAL:O	2.17	0.44
1:D:148:SER:HB2	1:D:227:ASP:OD2	2.16	0.44
1:D:134:LYS:HA	1:D:164:TYR:CE2	2.53	0.44
1:D:154:CYS:SG	1:D:245:LYS:HD2	2.57	0.44
1:C:337:ILE:HA	1:C:340:ILE:HD13	1.99	0.44
1:D:169:GLY:HA2	1:D:172:ARG:HD2	1.99	0.44
1:A:305:LYS:HD3	1:B:210:TYR:CZ	2.53	0.44
1:D:140:GLY:C	1:D:142:GLN:N	2.68	0.44
1:A:221:MSE:HE2	1:A:260:ILE:CD1	2.48	0.44
1:A:218:GLY:HA3	1:B:250:SER:OG	2.18	0.44
1:B:150:ILE:N	1:B:150:ILE:HD12	2.33	0.44
1:A:140:GLY:HA2	1:A:143:LEU:HD23	2.00	0.44
1:B:168:LEU:O	1:B:172:ARG:HG3	2.17	0.44
1:A:186:ASP:O	1:A:194:GLY:HA3	2.18	0.44
1:A:102:GLU:HG2	1:A:106:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TYR:HE1	1:B:70:THR:O	2.00	0.44
1:A:253:VAL:HG11	1:B:254:LEU:HD12	2.00	0.44
1:B:218:GLY:HA2	1:B:254:LEU:HD23	2.00	0.44
1:A:258:ASN:O	1:A:260:ILE:HG13	2.18	0.44
1:B:241:ASP:OD1	1:B:316:ASN:N	2.44	0.44
1:B:68:TYR:CE1	1:B:70:THR:O	2.71	0.44
1:C:336:ASN:O	1:C:336:ASN:ND2	2.51	0.44
1:C:191:TYR:HD2	1:C:193:GLN:CG	2.31	0.43
1:C:189:ARG:NH1	1:D:187:GLU:OE1	2.51	0.43
1:D:89:PRO:CG	1:D:284:GLU:HB2	2.48	0.43
1:A:49:GLY:O	1:A:50:ALA:C	2.55	0.43
1:C:316:ASN:HA	1:C:319:ILE:HG12	1.99	0.43
1:D:335:GLU:HG3	1:D:335:GLU:O	2.18	0.43
1:C:1:MSE:HE2	1:C:9:GLU:OE2	2.19	0.43
1:A:215:ASN:HB2	1:B:247:GLY:HA3	2.01	0.43
1:C:171:ILE:HG22	1:C:207:ILE:HD13	2.00	0.43
1:C:146:ASP:OD2	1:C:179:LYS:HA	2.18	0.43
1:B:287:ARG:HA	1:B:288:PRO:HD3	1.83	0.43
1:C:152:THR:HG22	1:C:153:HIS:H	1.83	0.43
1:C:256:LYS:O	1:C:259:ASN:N	2.39	0.43
1:B:151:LEU:HG	1:B:152:THR:N	2.32	0.43
1:B:189:ARG:HG2	1:B:189:ARG:HH11	1.82	0.43
1:B:186:ASP:HB3	1:B:214:ASP:OD1	2.19	0.43
1:D:2:LYS:CB	1:D:123:LEU:HD21	2.49	0.43
1:D:337:ILE:CG2	1:D:338:LYS:N	2.81	0.43
1:B:100:ARG:HD3	1:B:125:MSE:HE2	1.99	0.43
1:C:154:CYS:SG	1:C:245:LYS:HD2	2.59	0.43
1:D:150:ILE:HG21	1:D:230:VAL:CG2	2.47	0.43
1:C:45:MSE:HE2	1:C:286:ARG:NE	2.33	0.43
1:C:40:HIS:CE1	1:C:44:GLU:HG3	2.54	0.43
1:D:328:VAL:C	1:D:329:ILE:HD12	2.39	0.42
1:C:143:LEU:N	1:C:143:LEU:CD1	2.82	0.42
1:C:156:ALA:HB1	1:C:166:THR:OG1	2.19	0.42
1:C:116:GLU:OE1	1:C:116:GLU:N	2.46	0.42
1:D:325:GLU:HG2	1:D:326:LYS:HG3	2.00	0.42
1:D:271:ILE:O	1:D:271:ILE:HG23	2.20	0.42
1:D:21:ARG:HB3	1:D:191:TYR:OH	2.19	0.42
1:D:329:ILE:CG2	1:D:330:ARG:N	2.81	0.42
1:D:342:GLU:C	1:D:342:GLU:OE2	2.57	0.42
1:D:134:LYS:O	1:D:138:LYS:HG3	2.19	0.42
1:B:81:LYS:NZ	1:B:99:ASN:HD22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ARG:CB	1:D:208:GLU:HG2	2.49	0.42
1:C:250:SER:O	1:C:254:LEU:HB2	2.19	0.42
1:D:133:ASN:O	1:D:136:ILE:HG22	2.19	0.42
1:A:108:ASN:HD22	1:A:117:ILE:HD13	1.84	0.42
1:C:236:ILE:HG12	1:C:242:THR:HB	2.02	0.42
1:C:101:MSE:SE	1:C:121:GLU:HB3	2.69	0.42
1:A:202:LEU:HD23	1:A:209:VAL:HG22	2.02	0.42
1:D:186:ASP:HB3	1:D:214:ASP:OD1	2.18	0.42
1:D:89:PRO:HG2	1:D:90:THR:H	1.85	0.42
1:B:108:ASN:ND2	1:B:117:ILE:HD13	2.35	0.42
1:D:147:GLY:HA2	1:D:180:ARG:O	2.20	0.42
1:D:338:LYS:HD2	1:D:338:LYS:O	2.19	0.42
1:B:113:ASN:HA	1:B:116:GLU:OE1	2.19	0.42
1:D:143:LEU:CD1	1:D:143:LEU:N	2.82	0.42
1:C:320:THR:HG22	1:C:321:ALA:N	2.34	0.42
1:A:340:ILE:HD12	1:A:340:ILE:N	2.35	0.42
1:D:252:ALA:C	1:D:254:LEU:N	2.73	0.42
1:A:100:ARG:HD3	1:A:125:MSE:HE2	2.02	0.42
1:D:45:MSE:HE2	1:D:286:ARG:NE	2.34	0.42
1:C:151:LEU:HD12	1:C:184:PHE:O	2.20	0.42
1:C:249:TYR:OH	1:D:222:LYS:HB2	2.20	0.42
1:B:10:TRP:CD1	1:B:123:LEU:HD11	2.55	0.42
1:B:340:ILE:HD12	1:B:340:ILE:N	2.34	0.42
1:B:88:ARG:HA	1:B:89:PRO:HD3	1.58	0.42
1:C:220:LEU:HD11	1:D:307:LEU:HD12	2.02	0.41
1:C:270:THR:O	1:C:270:THR:HG22	2.19	0.41
1:A:88:ARG:HA	1:A:89:PRO:HD3	1.62	0.41
1:A:187:GLU:HG2	1:A:213:THR:HA	2.01	0.41
1:A:76:TRP:HD1	1:A:77:MSE:HE1	1.85	0.41
1:B:336:ASN:HA	1:B:339:LYS:HD3	2.01	0.41
1:D:324:THR:HB	1:D:327:GLY:O	2.21	0.41
1:C:217:ALA:HB1	1:C:251:LEU:HD21	2.02	0.41
1:B:258:ASN:O	1:B:260:ILE:HG13	2.21	0.41
1:B:20:GLN:OE1	1:B:159:LEU:HB3	2.19	0.41
1:C:147:GLY:HA2	1:C:180:ARG:O	2.20	0.41
1:B:158:ALA:N	1:B:201:GLU:OE2	2.43	0.41
1:D:167:ALA:CB	1:D:230:VAL:HG12	2.49	0.41
1:D:329:ILE:CD1	1:D:329:ILE:N	2.82	0.41
1:B:155:ASN:O	1:B:160:ALA:HB2	2.21	0.41
1:A:270:THR:HG22	1:A:270:THR:O	2.20	0.41
1:A:254:LEU:HD12	1:B:253:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ARG:HG3	1:A:192:LEU:HD21	2.03	0.41
1:A:19:ASP:HA	1:A:46:ILE:HG23	2.02	0.41
1:D:213:THR:OG1	1:D:216:MSE:HE3	2.20	0.41
1:A:21:ARG:NE	1:A:46:ILE:HG12	2.36	0.41
1:C:147:GLY:N	1:C:180:ARG:O	2.53	0.41
1:D:246:ILE:HD12	1:D:246:ILE:N	2.36	0.41
1:D:154:CYS:SG	1:D:155:ASN:N	2.94	0.41
1:A:168:LEU:O	1:A:172:ARG:HG3	2.20	0.41
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.87	0.41
1:A:19:ASP:OD1	1:A:21:ARG:CG	2.66	0.41
1:B:221:MSE:HE1	1:B:255:ALA:CB	2.50	0.41
1:A:108:ASN:O	1:A:111:ARG:HB2	2.21	0.41
1:B:76:TRP:HD1	1:B:77:MSE:HE2	1.86	0.41
1:A:92:VAL:HA	1:A:95:PHE:HD1	1.86	0.41
1:C:115:PHE:HB3	1:C:116:GLU:OE1	2.20	0.41
1:C:132:VAL:CG1	1:C:325:GLU:HB3	2.41	0.41
1:B:92:VAL:HA	1:B:95:PHE:HD1	1.86	0.41
1:D:45:MSE:HE2	1:D:286:ARG:HE	1.86	0.41
1:A:210:TYR:HA	1:B:305:LYS:O	2.21	0.41
1:A:249:TYR:CE1	1:B:222:LYS:HD2	2.56	0.40
1:D:101:MSE:HE1	1:D:118:LEU:O	2.20	0.40
1:C:168:LEU:HD11	1:C:198:THR:HG23	2.01	0.40
1:C:241:ASP:OD2	1:C:278:GLY:N	2.50	0.40
1:D:270:THR:HG22	1:D:270:THR:O	2.20	0.40
1:D:150:ILE:CG2	1:D:230:VAL:HG23	2.50	0.40
1:B:116:GLU:O	1:B:120:ASN:HB2	2.20	0.40
1:C:252:ALA:C	1:C:254:LEU:N	2.75	0.40
1:C:191:TYR:CD2	1:C:193:GLN:HG3	2.52	0.40
1:B:189:ARG:NH1	1:B:189:ARG:HG2	2.37	0.40
1:A:298:ARG:HH21	1:A:302:GLU:CA	2.30	0.40
1:B:213:THR:OG1	1:B:216:MSE:HG3	2.21	0.40
1:A:222:LYS:HD2	1:B:249:TYR:CE1	2.56	0.40
1:D:40:HIS:CE1	1:D:44:GLU:HG3	2.56	0.40
1:C:252:ALA:C	1:C:254:LEU:H	2.24	0.40
1:A:202:LEU:CB	1:A:209:VAL:HG21	2.38	0.40
1:B:245:LYS:CE	1:B:310:ALA:O	2.69	0.40
1:C:216:MSE:H	1:C:216:MSE:HG2	1.45	0.40
1:B:4:LYS:HG3	1:B:9:GLU:CD	2.41	0.40
1:B:221:MSE:CE	1:B:255:ALA:HA	2.50	0.40
1:A:76:TRP:O	1:A:80:VAL:HG23	2.22	0.40
1:B:270:THR:HG22	1:B:270:THR:O	2.21	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	338/347 (97%)	320 (95%)	16 (5%)	2 (1%)	30 56
1	B	338/347 (97%)	313 (93%)	23 (7%)	2 (1%)	30 56
1	C	340/347 (98%)	287 (84%)	46 (14%)	7 (2%)	9 16
1	D	340/347 (98%)	283 (83%)	47 (14%)	10 (3%)	6 9
All	All	1356/1388 (98%)	1203 (89%)	132 (10%)	21 (2%)	13 26

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	320	THR
1	D	320	THR
1	C	141	ALA
1	C	241	ASP
1	D	141	ALA
1	D	241	ASP
1	D	336	ASN
1	A	296	GLY
1	D	333	PHE
1	D	334	GLU
1	B	89	PRO
1	C	332	PRO
1	D	89	PRO
1	A	89	PRO
1	D	90	THR
1	B	50	ALA
1	D	179	LYS
1	C	224	GLY
1	C	273	PRO
1	D	253	VAL

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Mol	Chain	Res	Type
1	C	140	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/275 (102%)	268 (96%)	11 (4%)	39	68
1	B	279/275 (102%)	268 (96%)	11 (4%)	39	68
1	C	281/275 (102%)	269 (96%)	12 (4%)	35	64
1	D	281/275 (102%)	271 (96%)	10 (4%)	42	71
All	All	1120/1100 (102%)	1076 (96%)	44 (4%)	39	68

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	186	ASP
1	A	189	ARG
1	A	193	GLN
1	A	202	LEU
1	A	205	ASP
1	A	225	LEU
1	A	235	ARG
1	A	239	ASN
1	A	254	LEU
1	A	287	ARG
1	B	48	ARG
1	B	84	LEU
1	B	189	ARG
1	B	193	GLN
1	B	202	LEU
1	B	205	ASP
1	B	225	LEU
1	B	235	ARG
1	B	239	ASN

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Mol	Chain	Res	Type
1	B	242	THR
1	B	287	ARG
1	C	48	ARG
1	C	152	THR
1	C	202	LEU
1	C	221	MSE
1	C	223	ARG
1	C	242	THR
1	C	245	LYS
1	C	246	ILE
1	C	254	LEU
1	C	259	ASN
1	C	336	ASN
1	C	342	GLU
1	D	48	ARG
1	D	84	LEU
1	D	152	THR
1	D	202	LEU
1	D	221	MSE
1	D	223	ARG
1	D	242	THR
1	D	246	ILE
1	D	254	LEU
1	D	336	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	108	ASN
1	A	133	ASN
1	A	155	ASN
1	A	193	GLN
1	A	239	ASN
1	A	297	ASN
1	B	79	GLN
1	B	99	ASN
1	B	108	ASN
1	B	133	ASN
1	B	155	ASN
1	B	193	GLN
1	B	239	ASN

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Mol	Chain	Res	Type
1	B	244	ASN
1	B	293	HIS
1	B	297	ASN
1	C	40	HIS
1	C	79	GLN
1	C	99	ASN
1	C	133	ASN
1	C	155	ASN
1	C	258	ASN
1	C	259	ASN
1	C	293	HIS
1	C	297	ASN
1	C	336	ASN
1	D	40	HIS
1	D	79	GLN
1	D	99	ASN
1	D	133	ASN
1	D	155	ASN
1	D	258	ASN
1	D	297	ASN
1	D	336	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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	SO4	A	401	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	B	411	-	4,4,4	0.09	0	6,6,6	0.11	0
2	SO4	C	403	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	D	413	-	4,4,4	0.16	0	6,6,6	0.10	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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	411	-	-	0/0/0/0	0/0/0/0
2	SO4	C	403	-	-	0/0/0/0	0/0/0/0
2	SO4	D	413	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	1	0
2	B	411	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	332/347 (95%)	-0.07	4 (1%)	81	77	14, 32, 52, 68	0
1	B	332/347 (95%)	-0.09	4 (1%)	81	77	14, 32, 52, 69	0
1	C	333/347 (95%)	0.29	21 (6%)	23	17	16, 37, 66, 77	0
1	D	333/347 (95%)	0.29	20 (6%)	25	18	16, 37, 66, 75	0
All	All	1330/1388 (95%)	0.11	49 (3%)	45	37	14, 34, 64, 77	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	327	GLY	4.7
1	D	319	ILE	3.9
1	D	276	ARG	3.9
1	D	181	ILE	3.8
1	D	335	GLU	3.8
1	C	144	ILE	3.7
1	C	258	ASN	3.3
1	D	263	TYR	3.1
1	D	142	GLN	3.0
1	C	260	ILE	3.0
1	D	273	PRO	3.0
1	D	340	ILE	2.9
1	B	110	ASP	2.9
1	C	323	ILE	2.9
1	C	335	GLU	2.8
1	D	138	LYS	2.8
1	C	340	ILE	2.7
1	B	3	LEU	2.6
1	C	280	GLU	2.6
1	C	253	VAL	2.6
1	D	226	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	295	GLY	2.6
1	A	4	LYS	2.6
1	A	113	ASN	2.6
1	C	150	ILE	2.5
1	C	142	GLN	2.5
1	D	249	TYR	2.5
1	C	321	ALA	2.5
1	C	178	GLY	2.5
1	D	314	THR	2.4
1	C	181	ILE	2.4
1	D	275	ILE	2.4
1	C	271	ILE	2.4
1	C	259	ASN	2.4
1	D	223	ARG	2.3
1	C	332	PRO	2.3
1	D	238	LEU	2.3
1	D	144	ILE	2.2
1	C	295	GLY	2.2
1	D	261	PRO	2.2
1	C	324	THR	2.1
1	A	109	ALA	2.1
1	B	126	ALA	2.1
1	C	254	LEU	2.1
1	C	239	ASN	2.1
1	D	336	ASN	2.1
1	C	276	ARG	2.1
1	B	109	ALA	2.1
1	D	259	ASN	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
2	SO4	A	401	5/5	0.97	0.14	-0.65	19,20,20,21	0
2	SO4	C	403	5/5	0.99	0.11	-1.09	8,9,14,16	0
2	SO4	D	413	5/5	0.98	0.11	-1.09	10,11,17,18	0
2	SO4	B	411	5/5	0.99	0.12	-1.51	18,19,20,20	0
3	CL	B	406	1/1	0.99	0.24	-	33,33,33,33	0
3	CL	A	416	1/1	0.97	0.15	-	33,33,33,33	0

6.5 Other polymers

There are no such residues in this entry.