



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:27 PM UTC

PDB ID : 1ZE1 / pdb_00001ze1
Title : Conformational Change of Pseudouridine 55 Synthase upon Its Association with RNA Substrate
Authors : Phannachet, K.; Huang, R.H.
Deposited on : 2005-04-16
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

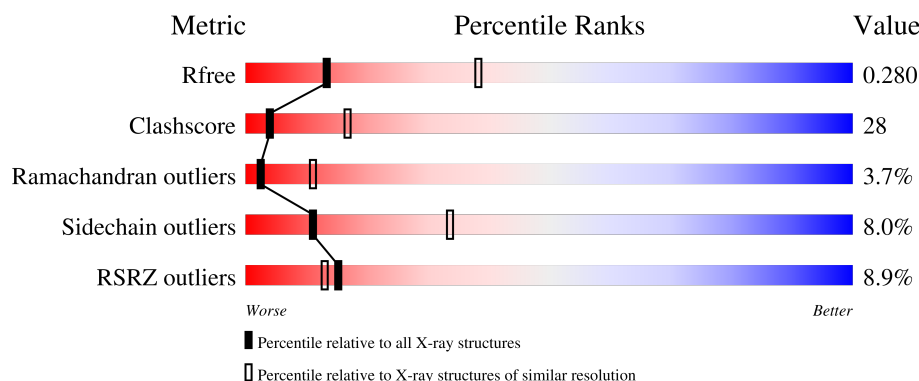
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	
1	B	309	
1	C	309	
1	D	309	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9868 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 tRNA pseudouridine synthase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2489	1591	437	451	10			
1	B	308	Total	C	N	O	S	0	0	0
			2489	1591	437	451	10			
1	C	308	Total	C	N	O	S	0	0	0
			2489	1591	437	451	10			
1	D	284	Total	C	N	O	S	0	0	0
			2289	1460	401	418	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	GLN	ASN	SEE REMARK 999	UNP Q9WZW0
A	297	ARG	GLU	conflict	UNP Q9WZW0
A	307	GLN	ASN	SEE REMARK 999	UNP Q9WZW0
B	296	GLN	ASN	SEE REMARK 999	UNP Q9WZW0
B	297	ARG	GLU	conflict	UNP Q9WZW0
B	307	GLN	ASN	SEE REMARK 999	UNP Q9WZW0
C	296	GLN	ASN	SEE REMARK 999	UNP Q9WZW0
C	297	ARG	GLU	conflict	UNP Q9WZW0
C	307	GLN	ASN	SEE REMARK 999	UNP Q9WZW0
D	296	GLN	ASN	SEE REMARK 999	UNP Q9WZW0
D	297	ARG	GLU	conflict	UNP Q9WZW0
D	307	GLN	ASN	SEE REMARK 999	UNP Q9WZW0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

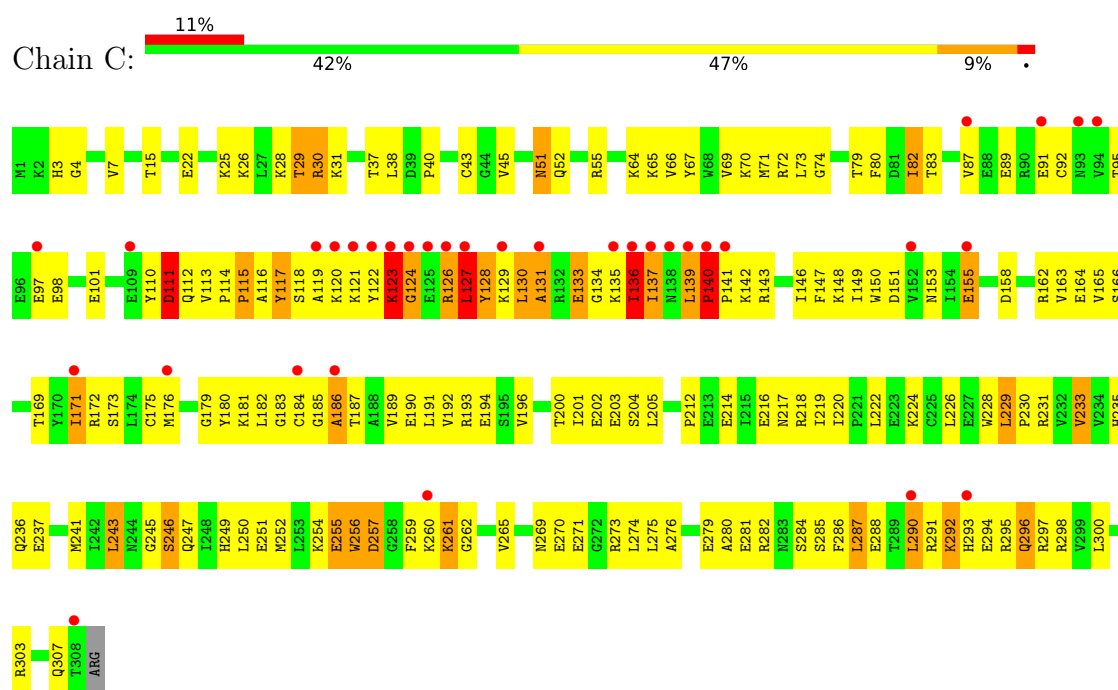
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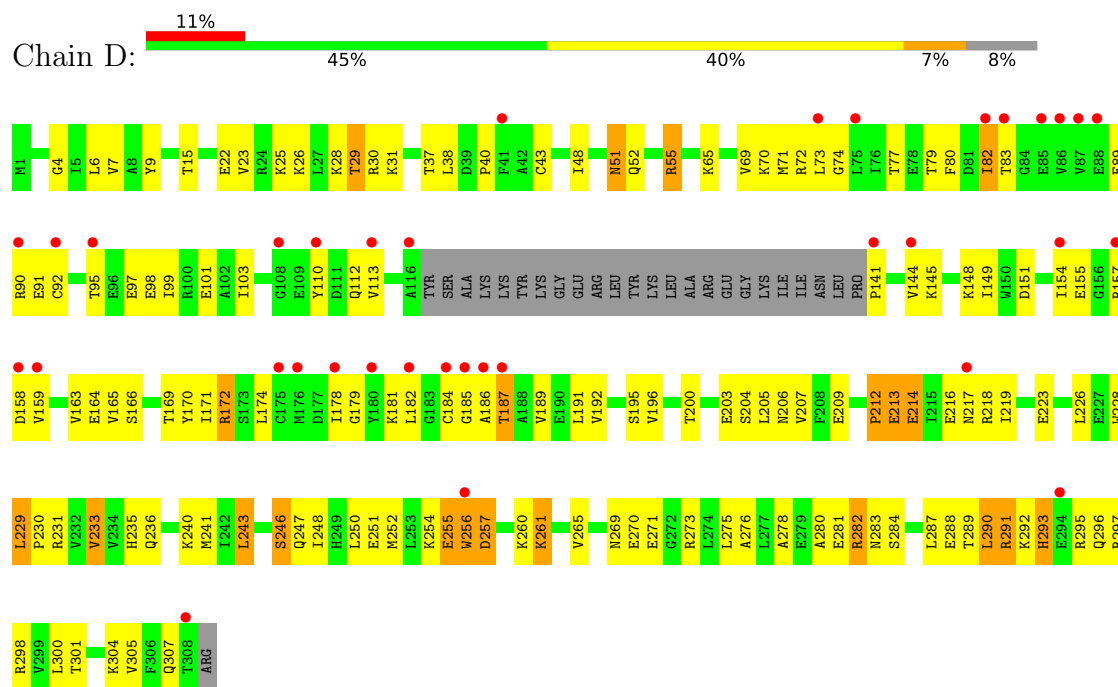
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total 54	O 54	0	0
3	B	14	Total 14	O 14	0	0
3	C	13	Total 13	O 13	0	0
3	D	27	Total 27	O 27	0	0



• Molecule 1: tRNA pseudouridine synthase B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.65Å 64.17Å 176.07Å 87.48° 86.44° 79.35°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 91.4 (50.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.281 0.240 , 0.280	Depositor DCC
R_{free} test set	3254 reflections (8.10%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9868	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MG

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	0.57	0/2536	0.97	6/3415 (0.2%)
1	B	0.48	0/2536	0.92	6/3415 (0.2%)
1	C	0.44	0/2536	0.94	7/3415 (0.2%)
1	D	0.51	0/2331	0.97	9/3140 (0.3%)
All	All	0.50	0/9939	0.95	28/13385 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ARG	N-CA-C	-10.96	95.23	110.35
1	C	137	ILE	N-CA-C	-10.17	95.43	109.46
1	A	125	GLU	N-CA-C	-8.11	100.13	110.19
1	B	286	PHE	N-CA-C	-7.66	103.94	113.20
1	D	293	HIS	N-CA-C	-6.64	101.19	110.35
1	C	131	ALA	N-CA-C	-6.21	104.97	112.54
1	C	126	ARG	N-CA-C	-6.09	105.70	113.01
1	B	117	TYR	N-CA-C	-5.96	100.47	109.95
1	B	181	LYS	N-CA-C	-5.86	104.80	111.07
1	C	182	LEU	N-CA-C	-5.84	106.24	113.19
1	D	4	GLY	N-CA-C	5.70	117.86	110.45
1	D	291	ARG	N-CA-C	-5.67	98.73	110.80
1	A	195	SER	N-CA-C	5.61	117.63	108.76
1	A	110	TYR	N-CA-C	5.61	122.75	113.50
1	B	135	LYS	N-CA-C	-5.54	108.30	114.62
1	D	219	ILE	CA-C-N	-5.54	118.83	122.60
1	D	219	ILE	C-N-CA	-5.54	118.83	122.60
1	D	51	ASN	CB-CA-C	-5.54	109.70	117.23
1	A	181	LYS	N-CA-C	-5.52	105.16	111.07
1	D	240	LYS	N-CA-C	5.46	116.92	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	ASN	CB-CA-C	-5.43	109.85	117.23
1	C	292	LYS	N-CA-C	-5.43	106.85	112.93
1	B	120	LYS	N-CA-C	-5.38	104.97	112.45
1	D	276	ALA	N-CA-C	5.37	115.45	107.88
1	A	285	SER	N-CA-C	-5.37	105.59	111.82
1	C	276	ALA	N-CA-C	5.25	115.29	107.88
1	B	195	SER	N-CA-C	5.24	117.05	108.76
1	D	110	TYR	N-CA-C	5.05	120.16	112.54

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	2489	0	2557	121	0
1	B	2489	0	2557	141	0
1	C	2489	0	2557	177	0
1	D	2289	0	2338	126	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	54	0	0	10	0
3	B	14	0	0	1	0
3	C	13	0	0	6	0
3	D	27	0	0	1	0
All	All	9868	0	10009	553	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 28.

All (553) 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:C:165:VAL:HG21	1:C:169:THR:HG21	1.44	0.99
1:D:73:LEU:HD23	1:D:186:ALA:HB2	1.45	0.98
1:B:72:ARG:HD3	1:B:158:ASP:OD1	1.73	0.89
1:B:135:LYS:H	1:B:139:LEU:HD21	1.37	0.89
1:B:295:ARG:HH11	1:B:297:ARG:HH21	1.20	0.89
1:B:80:PHE:CE2	1:B:176:MET:HE2	2.09	0.88
1:C:52:GLN:HG3	3:C:315:HOH:O	1.73	0.87
1:A:91:GLU:HA	3:A:315:HOH:O	1.72	0.87
1:A:111:ASP:HA	1:A:142:LYS:O	1.75	0.86
1:D:112:GLN:HE22	1:D:170:TYR:H	1.24	0.86
1:D:171:ILE:HD11	1:D:191:LEU:HD22	1.58	0.85
1:C:153:ASN:HD21	1:C:155:GLU:HG2	1.42	0.83
1:C:288:GLU:HG3	1:C:292:LYS:HE2	1.61	0.82
1:D:149:ILE:HG12	1:D:163:VAL:HG12	1.59	0.82
1:A:72:ARG:HD3	1:A:158:ASP:OD1	1.79	0.82
1:B:282:ARG:NH2	1:B:297:ARG:HD3	1.94	0.81
1:A:251:GLU:HG3	1:A:296:GLN:HG3	1.63	0.81
1:C:236:GLN:HG2	1:C:270:GLU:HB2	1.62	0.80
1:C:249:HIS:HB3	1:C:296:GLN:HE22	1.43	0.80
1:B:29:THR:HG21	1:B:51:ASN:HD21	1.46	0.80
1:C:80:PHE:CE1	1:C:176:MET:HG2	2.17	0.80
1:A:29:THR:HG21	1:A:51:ASN:HD21	1.48	0.79
1:B:76:ILE:HG23	1:B:176:MET:HE1	1.63	0.79
1:C:29:THR:HG21	1:C:51:ASN:HD21	1.48	0.78
1:B:136:ILE:HG22	1:B:138:ASN:H	1.49	0.78
1:C:149:ILE:HG12	1:C:163:VAL:HG12	1.66	0.77
1:C:171:ILE:HD12	3:C:311:HOH:O	1.84	0.76
1:B:125:GLU:HG2	1:B:180:TYR:HE2	1.50	0.76
1:D:291:ARG:O	1:D:293:HIS:N	2.17	0.76
1:C:71:MET:HB3	1:C:175:CYS:SG	2.25	0.76
1:C:129:LYS:HD3	1:C:180:TYR:HD1	1.50	0.76
1:D:29:THR:HG21	1:D:51:ASN:HD21	1.50	0.76
1:A:236:GLN:HG2	1:A:270:GLU:HB2	1.68	0.76
1:B:136:ILE:HD13	1:B:139:LEU:HD23	1.69	0.75
1:A:290:LEU:HD21	1:A:297:ARG:HE	1.51	0.74
1:A:231:ARG:O	1:A:257:ASP:HB2	1.88	0.74
1:A:176:MET:SD	1:A:180:TYR:HE1	2.10	0.74
1:B:236:GLN:HG2	1:B:270:GLU:HB2	1.69	0.74
1:C:259:PHE:H	1:C:284:SER:HB2	1.53	0.74
1:A:125:GLU:O	1:A:126:ARG:HB3	1.88	0.74
1:A:76:ILE:HG23	1:A:176:MET:HE1	1.70	0.73
1:C:260:LYS:HD2	3:C:320:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ARG:HE	1:D:297:ARG:HE	1.35	0.73
1:C:114:PRO:HG3	1:C:139:LEU:HB2	1.69	0.73
1:C:307:GLN:H	1:C:307:GLN:CD	1.98	0.72
1:B:135:LYS:N	1:B:139:LEU:HD21	2.04	0.72
1:B:290:LEU:HD11	1:B:297:ARG:HD2	1.71	0.72
1:D:112:GLN:NE2	1:D:170:TYR:H	1.86	0.72
1:C:127:LEU:O	1:C:130:LEU:HD12	1.89	0.72
1:B:149:ILE:HG12	1:B:163:VAL:HG12	1.70	0.71
1:A:149:ILE:HG12	1:A:163:VAL:HG12	1.71	0.71
1:C:80:PHE:CE2	1:C:176:MET:HE3	2.26	0.71
1:D:260:LYS:HD2	1:D:283:ASN:OD1	1.90	0.71
1:A:165:VAL:HG21	1:A:169:THR:HG21	1.73	0.71
1:A:233:VAL:HG13	1:A:255:GLU:HB2	1.74	0.70
1:C:43:CYS:SG	1:C:192:VAL:HG22	2.31	0.70
1:B:136:ILE:HB	1:B:139:LEU:HG	1.73	0.70
1:A:17:HIS:HE1	3:A:328:HOH:O	1.74	0.70
1:B:259:PHE:H	1:B:284:SER:HB3	1.54	0.70
1:C:226:LEU:HB3	1:C:229:LEU:HD12	1.73	0.70
1:D:256:TRP:HE1	1:D:287:LEU:HG	1.57	0.69
1:C:233:VAL:HG13	1:C:255:GLU:HB2	1.75	0.69
1:D:228:TRP:O	1:D:229:LEU:HB2	1.92	0.69
1:B:226:LEU:HB3	1:B:229:LEU:HD12	1.74	0.69
1:C:129:LYS:HD3	1:C:180:TYR:CD1	2.28	0.68
1:B:295:ARG:HD2	1:B:297:ARG:HE	1.59	0.68
1:C:124:GLY:O	1:C:127:LEU:HG	1.92	0.68
1:C:15:THR:HG22	1:C:40:PRO:HG3	1.76	0.68
1:B:231:ARG:O	1:B:257:ASP:HB2	1.93	0.68
1:D:165:VAL:HG21	1:D:169:THR:HG21	1.75	0.68
1:D:112:GLN:HE22	1:D:170:TYR:N	1.92	0.68
1:B:233:VAL:HG13	1:B:255:GLU:HB2	1.76	0.67
1:D:213:GLU:CD	1:D:213:GLU:H	1.99	0.67
1:B:259:PHE:H	1:B:284:SER:CB	2.07	0.67
1:D:226:LEU:HB3	1:D:229:LEU:HD12	1.75	0.67
1:C:72:ARG:HD3	1:C:158:ASP:OD1	1.94	0.67
1:D:15:THR:HG22	1:D:40:PRO:HG3	1.75	0.67
1:D:231:ARG:O	1:D:257:ASP:HB2	1.96	0.66
1:B:125:GLU:HG2	1:B:180:TYR:CE2	2.31	0.66
1:C:128:TYR:CE2	1:C:130:LEU:HA	2.31	0.66
1:D:144:VAL:HG22	1:D:145:LYS:H	1.60	0.66
1:B:43:CYS:SG	1:B:192:VAL:HG22	2.35	0.65
1:C:52:GLN:HE22	1:C:307:GLN:NE2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:H	1:B:139:LEU:HD21	1.61	0.65
1:C:72:ARG:O	1:C:186:ALA:HA	1.95	0.65
1:B:136:ILE:H	1:B:139:LEU:CD2	2.10	0.65
1:D:195:SER:HB3	1:D:200:THR:HG22	1.77	0.65
1:A:307:GLN:HB2	3:A:340:HOH:O	1.96	0.65
1:C:214:GLU:O	1:C:218:ARG:HB2	1.97	0.65
1:B:15:THR:HG22	1:B:40:PRO:HG3	1.79	0.65
1:D:236:GLN:HG2	1:D:270:GLU:HB2	1.78	0.65
1:A:80:PHE:CE2	1:A:176:MET:HE2	2.31	0.64
1:C:179:GLY:HA3	1:C:186:ALA:HB3	1.79	0.64
1:A:228:TRP:O	1:A:229:LEU:HB2	1.98	0.64
1:C:118:SER:HA	1:C:123:LYS:HB3	1.79	0.64
1:C:259:PHE:H	1:C:284:SER:CB	2.11	0.64
1:C:73:LEU:HD23	1:C:186:ALA:HB2	1.80	0.64
1:A:291:ARG:C	1:A:293:HIS:H	2.03	0.64
1:C:126:ARG:C	1:C:128:TYR:H	2.06	0.64
1:C:179:GLY:HA3	1:C:185:GLY:O	1.98	0.64
1:A:1:MET:HE3	1:A:3:HIS:HE1	1.63	0.63
1:A:136:ILE:HG22	1:A:139:LEU:H	1.62	0.63
1:C:153:ASN:ND2	1:C:155:GLU:HG2	2.14	0.63
1:C:150:TRP:NE1	1:C:162:ARG:HD2	2.14	0.63
1:C:249:HIS:CB	1:C:296:GLN:HE22	2.11	0.63
1:B:82:ILE:HG13	1:B:189:VAL:HA	1.80	0.63
1:C:228:TRP:O	1:C:229:LEU:HB2	1.97	0.63
1:B:230:PRO:HB2	1:B:265:VAL:HG12	1.79	0.63
1:B:256:TRP:HE1	1:B:287:LEU:HG	1.64	0.63
1:B:111:ASP:HA	1:B:143:ARG:HA	1.80	0.63
1:B:295:ARG:HD2	1:B:297:ARG:NE	2.14	0.62
1:C:31:LYS:HB3	1:C:51:ASN:HA	1.81	0.62
1:A:149:ILE:HG12	1:A:163:VAL:CG1	2.30	0.62
1:A:15:THR:HG22	1:A:40:PRO:HG3	1.81	0.62
1:B:136:ILE:N	1:B:136:ILE:HD12	2.14	0.62
1:D:99:ILE:HA	1:D:182:LEU:HD21	1.81	0.62
1:B:3:HIS:ND1	1:B:52:GLN:HB2	2.14	0.62
1:D:23:VAL:HG22	1:D:207:VAL:HG11	1.80	0.62
1:D:282:ARG:HH12	1:D:297:ARG:HD2	1.65	0.62
1:A:29:THR:HG23	1:D:251:GLU:OE2	1.99	0.61
1:A:31:LYS:HB3	1:A:51:ASN:HA	1.83	0.61
1:D:7:VAL:HG12	1:D:204:SER:HA	1.81	0.61
1:D:113:VAL:HG12	1:D:141:PRO:N	2.14	0.61
1:A:256:TRP:NE1	1:A:287:LEU:HD22	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ALA:HA	1:C:300:LEU:HD23	1.82	0.61
1:D:284:SER:O	1:D:287:LEU:HB2	2.00	0.61
1:C:128:TYR:OH	1:C:134:GLY:HA3	2.00	0.61
1:B:165:VAL:HG21	1:B:169:THR:HG21	1.81	0.61
1:D:172:ARG:HH11	1:D:172:ARG:HG2	1.66	0.61
1:B:228:TRP:O	1:B:229:LEU:HB2	1.99	0.61
1:D:295:ARG:HE	1:D:297:ARG:NE	1.98	0.61
1:A:226:LEU:HB3	1:A:229:LEU:HD12	1.83	0.61
1:B:307:GLN:O	1:B:307:GLN:HG2	2.01	0.60
1:C:231:ARG:O	1:C:257:ASP:HB2	2.02	0.60
1:C:133:GLU:OE1	1:C:136:ILE:HG13	2.01	0.60
1:D:256:TRP:NE1	1:D:287:LEU:HG	2.16	0.60
1:B:29:THR:HG23	1:C:251:GLU:OE2	2.01	0.60
1:C:288:GLU:HA	1:C:291:ARG:HB3	1.84	0.60
1:A:218:ARG:HD3	3:A:345:HOH:O	2.01	0.60
1:D:31:LYS:HB3	1:D:51:ASN:HA	1.82	0.60
1:A:30:ARG:HB2	1:D:235:HIS:CD2	2.37	0.60
1:B:109:GLU:HG3	1:B:143:ARG:HH11	1.67	0.60
1:A:37:THR:HG22	1:A:38:LEU:N	2.17	0.59
1:B:37:THR:HG22	1:B:38:LEU:N	2.16	0.59
1:B:31:LYS:HB3	1:B:51:ASN:HA	1.83	0.59
1:B:80:PHE:CE1	1:B:176:MET:HG2	2.36	0.59
1:C:116:ALA:O	1:C:117:TYR:HB2	2.02	0.59
1:D:233:VAL:HG13	1:D:255:GLU:HB2	1.85	0.59
1:C:150:TRP:HD1	1:C:151:ASP:OD1	1.85	0.59
1:A:17:HIS:ND1	3:A:331:HOH:O	2.32	0.59
1:D:144:VAL:HG22	1:D:145:LYS:N	2.16	0.59
1:D:195:SER:CB	1:D:200:THR:HG22	2.32	0.59
1:B:295:ARG:HH11	1:B:297:ARG:NH2	1.97	0.59
1:D:103:ILE:HD13	1:D:178:ILE:HG21	1.84	0.58
1:A:1:MET:HE3	1:A:3:HIS:CE1	2.38	0.58
1:A:82:ILE:HG13	1:A:189:VAL:HA	1.85	0.58
1:A:176:MET:SD	1:A:180:TYR:CE1	2.95	0.58
1:A:65:LYS:HE3	1:A:196:VAL:HG13	1.85	0.58
1:A:76:ILE:HG23	1:A:176:MET:CE	2.34	0.58
1:C:37:THR:HG22	1:C:38:LEU:N	2.17	0.58
1:A:293:HIS:C	1:A:295:ARG:H	2.12	0.58
1:B:136:ILE:HB	1:B:139:LEU:CG	2.33	0.58
1:C:69:VAL:HG22	1:C:70:LYS:N	2.17	0.58
1:C:80:PHE:CD2	1:C:176:MET:HE3	2.38	0.58
1:A:261:LYS:O	1:A:280:ALA:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:GLY:HA2	1:C:184:CYS:O	2.02	0.57
1:C:79:THR:O	1:C:80:PHE:HB2	2.03	0.57
1:D:284:SER:HA	1:D:287:LEU:HD23	1.85	0.57
1:C:307:GLN:O	1:C:307:GLN:HG2	2.04	0.57
1:B:131:ALA:HA	1:B:139:LEU:HD23	1.86	0.57
1:C:79:THR:HG22	3:C:319:HOH:O	2.04	0.57
1:D:77:THR:H	1:D:187:THR:HG21	1.70	0.57
1:C:216:GLU:C	1:C:218:ARG:H	2.13	0.57
1:D:79:THR:O	1:D:80:PHE:HB2	2.04	0.57
1:B:109:GLU:HB2	1:B:143:ARG:HD2	1.87	0.57
1:B:165:VAL:HG22	1:B:166:SER:N	2.20	0.57
1:C:200:THR:O	1:C:203:GLU:HG2	2.04	0.57
1:C:284:SER:O	1:C:287:LEU:HB2	2.04	0.57
1:A:63:LEU:HD21	1:A:228:TRP:CZ2	2.40	0.56
1:A:273:ARG:NH1	3:A:329:HOH:O	2.37	0.56
1:C:127:LEU:HD12	1:C:129:LYS:H	1.70	0.56
1:C:273:ARG:HG2	1:C:275:LEU:HD12	1.87	0.56
1:B:17:HIS:HE1	3:B:316:HOH:O	1.87	0.56
1:B:149:ILE:HG12	1:B:163:VAL:CG1	2.35	0.56
1:C:3:HIS:ND1	1:C:52:GLN:HB2	2.20	0.56
1:D:37:THR:HG22	1:D:38:LEU:N	2.19	0.56
1:C:140:PRO:HB2	1:C:141:PRO:HD2	1.85	0.56
1:B:80:PHE:CZ	1:B:176:MET:HG2	2.41	0.56
1:D:174:LEU:O	1:D:178:ILE:HG13	2.06	0.56
1:D:295:ARG:HH21	1:D:297:ARG:CZ	2.18	0.56
1:D:305:VAL:HG12	1:D:307:GLN:HE21	1.69	0.56
1:A:247:GLN:HG3	1:A:298:ARG:CZ	2.36	0.56
1:C:303:ARG:HD3	3:C:316:HOH:O	2.06	0.55
1:A:79:THR:O	1:A:80:PHE:HB2	2.05	0.55
1:B:79:THR:O	1:B:80:PHE:HB2	2.05	0.55
1:A:291:ARG:O	1:A:292:LYS:HB2	2.06	0.55
1:B:69:VAL:HG22	1:B:70:LYS:N	2.21	0.55
1:C:218:ARG:HG3	1:C:218:ARG:HH11	1.71	0.55
1:C:307:GLN:H	1:C:307:GLN:NE2	2.04	0.55
1:D:256:TRP:N	1:D:256:TRP:HE3	2.05	0.55
1:D:261:LYS:O	1:D:280:ALA:HB3	2.07	0.55
1:C:286:PHE:O	1:C:290:LEU:HD22	2.06	0.55
1:C:22:GLU:OE1	1:C:26:LYS:HE3	2.06	0.55
1:D:112:GLN:HE21	1:D:170:TYR:HD1	1.52	0.55
1:A:69:VAL:HG22	1:A:70:LYS:N	2.22	0.55
1:A:80:PHE:CZ	1:A:176:MET:HG2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLN:NE2	1:B:271:GLU:H	2.05	0.55
1:A:3:HIS:ND1	1:A:52:GLN:HB2	2.22	0.54
1:D:216:GLU:C	1:D:218:ARG:H	2.15	0.54
1:A:103:ILE:HD13	1:A:178:ILE:HG21	1.89	0.54
1:B:236:GLN:HE21	1:B:271:GLU:H	1.55	0.54
1:A:100:ARG:HD2	3:A:316:HOH:O	2.07	0.54
1:A:236:GLN:NE2	1:A:271:GLU:H	2.04	0.54
1:C:111:ASP:HA	1:C:142:LYS:O	2.08	0.54
1:C:218:ARG:HG3	1:C:218:ARG:NH1	2.23	0.54
1:D:69:VAL:HG22	1:D:70:LYS:N	2.22	0.54
1:D:298:ARG:HH11	1:D:301:THR:HG23	1.71	0.54
1:D:305:VAL:CG1	1:D:307:GLN:HE21	2.20	0.54
1:C:146:ILE:HD12	1:C:146:ILE:N	2.23	0.54
1:D:223:GLU:CD	1:D:223:GLU:H	2.16	0.54
1:B:90:ARG:HH22	1:B:125:GLU:HG3	1.72	0.54
1:B:247:GLN:HG3	1:B:298:ARG:CZ	2.38	0.54
1:B:24:ARG:HG2	1:C:241:MET:HE2	1.90	0.53
1:D:289:THR:O	1:D:291:ARG:O	2.26	0.53
1:A:230:PRO:HB2	1:A:265:VAL:HG12	1.89	0.53
1:A:256:TRP:H	1:A:256:TRP:HE3	1.57	0.53
1:D:236:GLN:NE2	1:D:271:GLU:H	2.06	0.53
1:B:261:LYS:O	1:B:280:ALA:HB3	2.08	0.53
1:C:7:VAL:HG12	1:C:204:SER:HB3	1.89	0.53
1:C:171:ILE:HD13	1:C:191:LEU:HD21	1.89	0.53
1:C:45:VAL:HG23	1:C:201:ILE:HG22	1.90	0.53
1:D:246:SER:HA	3:D:314:HOH:O	2.08	0.53
1:B:273:ARG:HG2	1:B:275:LEU:HD12	1.89	0.53
1:C:52:GLN:HE22	1:C:307:GLN:HE21	1.57	0.53
1:C:165:VAL:HG21	1:C:169:THR:CG2	2.28	0.53
1:C:230:PRO:HB2	1:C:265:VAL:HG12	1.90	0.53
1:D:95:THR:OG1	1:D:98:GLU:HG3	2.08	0.53
1:D:82:ILE:HD12	1:D:83:THR:H	1.73	0.53
1:C:65:LYS:HG2	1:C:193:ARG:HH11	1.74	0.53
1:A:293:HIS:HB3	1:A:295:ARG:HH11	1.73	0.53
1:D:154:ILE:HG23	1:D:159:VAL:HG12	1.91	0.53
1:C:205:LEU:H	1:C:205:LEU:HD23	1.74	0.52
1:B:95:THR:OG1	1:B:98:GLU:HG3	2.09	0.52
1:A:122:TYR:O	1:A:123:LYS:HD3	2.09	0.52
1:D:256:TRP:HE3	1:D:256:TRP:H	1.57	0.52
1:D:295:ARG:NE	1:D:297:ARG:HE	2.04	0.52
1:C:135:LYS:O	1:C:137:ILE:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ARG:CZ	1:C:298:ARG:H	2.22	0.52
1:D:256:TRP:N	1:D:256:TRP:CE3	2.77	0.52
1:C:129:LYS:O	1:C:131:ALA:N	2.43	0.52
1:C:95:THR:OG1	1:C:98:GLU:HG3	2.09	0.52
1:A:165:VAL:HG22	1:A:166:SER:N	2.25	0.52
1:A:273:ARG:HG2	1:A:275:LEU:HD12	1.91	0.52
1:C:237:GLU:HB2	3:C:317:HOH:O	2.08	0.52
1:D:65:LYS:HG3	1:D:196:VAL:HG22	1.90	0.52
1:D:230:PRO:HB2	1:D:265:VAL:HG12	1.92	0.52
1:A:76:ILE:CG2	1:A:176:MET:HE1	2.38	0.52
1:B:25:LYS:O	1:B:28:LYS:HD2	2.10	0.52
1:A:22:GLU:OE1	1:A:26:LYS:HE3	2.10	0.52
1:A:125:GLU:O	1:A:126:ARG:CB	2.54	0.52
1:A:148:LYS:HB3	1:B:90:ARG:HA	1.92	0.52
1:A:200:THR:HB	1:A:202:GLU:OE2	2.10	0.52
1:B:103:ILE:HD13	1:B:178:ILE:HG21	1.91	0.52
1:C:70:LYS:HB3	1:C:190:GLU:HB2	1.92	0.52
1:C:249:HIS:HB3	1:C:296:GLN:NE2	2.20	0.52
1:B:82:ILE:HD12	1:B:83:THR:H	1.75	0.51
1:B:256:TRP:N	1:B:256:TRP:HE3	2.08	0.51
1:C:121:LYS:O	1:C:122:TYR:HB2	2.09	0.51
1:A:236:GLN:HE21	1:A:271:GLU:H	1.57	0.51
1:A:256:TRP:HE3	1:A:256:TRP:N	2.07	0.51
1:C:29:THR:HG21	1:C:51:ASN:ND2	2.24	0.51
1:D:22:GLU:OE1	1:D:26:LYS:HE3	2.09	0.51
1:B:139:LEU:O	1:B:140:PRO:C	2.52	0.51
1:D:179:GLY:HA3	1:D:185:GLY:HA2	1.93	0.51
1:D:256:TRP:HE1	1:D:287:LEU:CG	2.22	0.51
1:A:256:TRP:N	1:A:256:TRP:CE3	2.79	0.51
1:A:256:TRP:HE1	1:A:287:LEU:HD22	1.75	0.51
1:B:241:MET:O	1:B:246:SER:HB3	2.11	0.51
1:C:25:LYS:O	1:C:28:LYS:HD2	2.10	0.51
1:C:256:TRP:HE1	1:C:287:LEU:HB3	1.75	0.51
1:D:181:LYS:NZ	1:D:181:LYS:HB3	2.26	0.51
1:D:241:MET:O	1:D:246:SER:HB3	2.10	0.51
1:A:25:LYS:O	1:A:28:LYS:HD2	2.11	0.51
1:C:67:TYR:CD2	1:C:191:LEU:HD11	2.46	0.51
1:C:181:LYS:C	1:C:183:GLY:H	2.18	0.51
1:A:43:CYS:SG	1:A:192:VAL:HG22	2.50	0.51
1:C:282:ARG:HE	1:C:286:PHE:HD2	1.57	0.51
1:C:126:ARG:O	1:C:128:TYR:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ARG:NH1	1:D:301:THR:HG23	2.26	0.50
1:B:22:GLU:OE1	1:B:26:LYS:HE3	2.12	0.50
1:B:136:ILE:N	1:B:139:LEU:HD21	2.26	0.50
1:B:145:LYS:O	1:B:165:VAL:HG23	2.11	0.50
1:A:260:LYS:HB3	3:A:350:HOH:O	2.11	0.50
1:B:136:ILE:H	1:B:136:ILE:HD12	1.76	0.50
1:D:256:TRP:HE1	1:D:287:LEU:CB	2.24	0.50
1:B:136:ILE:CD1	1:B:139:LEU:HD23	2.39	0.50
1:C:121:LYS:NZ	1:C:135:LYS:HG2	2.26	0.50
1:B:176:MET:SD	1:B:180:TYR:HE1	2.35	0.50
1:C:201:ILE:HG13	1:C:202:GLU:N	2.27	0.50
1:C:285:SER:C	1:C:287:LEU:H	2.19	0.50
1:A:236:GLN:CD	1:A:271:GLU:HG3	2.36	0.50
1:C:148:LYS:HE3	1:C:150:TRP:CZ3	2.47	0.50
1:B:82:ILE:HG21	1:B:189:VAL:HG13	1.93	0.49
1:B:236:GLN:HE22	1:B:269:ASN:ND2	2.10	0.49
1:C:236:GLN:NE2	1:C:271:GLU:H	2.10	0.49
1:C:293:HIS:ND1	1:C:294:GLU:N	2.60	0.49
1:D:72:ARG:HB2	1:D:189:VAL:HG21	1.94	0.49
1:B:256:TRP:N	1:B:256:TRP:CE3	2.80	0.49
1:C:256:TRP:N	1:C:256:TRP:CE3	2.81	0.49
1:B:131:ALA:HA	1:B:139:LEU:CD2	2.42	0.49
1:C:241:MET:O	1:C:246:SER:HB3	2.13	0.49
1:C:256:TRP:HE1	1:C:287:LEU:HG	1.77	0.49
1:D:273:ARG:HG2	1:D:275:LEU:HD12	1.95	0.49
1:B:76:ILE:CG2	1:B:176:MET:HE1	2.38	0.49
1:B:226:LEU:O	1:B:228:TRP:O	2.30	0.49
1:D:295:ARG:HE	1:D:297:ARG:HH21	1.60	0.49
1:A:24:ARG:HG2	1:D:241:MET:HE2	1.94	0.49
1:B:307:GLN:H	1:B:307:GLN:CD	2.21	0.49
1:C:256:TRP:N	1:C:256:TRP:HE3	2.10	0.49
1:C:261:LYS:O	1:C:280:ALA:HB3	2.13	0.49
1:A:80:PHE:CE1	1:A:176:MET:HG2	2.48	0.49
1:B:109:GLU:HG3	1:B:143:ARG:NH1	2.27	0.49
1:C:235:HIS:ND1	1:C:254:LYS:HD2	2.28	0.49
1:C:82:ILE:HD12	1:C:83:THR:H	1.76	0.49
1:C:260:LYS:HE3	1:C:261:LYS:H	1.78	0.49
1:A:28:LYS:O	1:D:252:MET:HG3	2.13	0.48
1:D:154:ILE:HA	1:D:159:VAL:HG12	1.95	0.48
1:B:293:HIS:O	1:B:294:GLU:C	2.56	0.48
1:C:165:VAL:HG22	1:C:166:SER:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LEU:HD23	1:D:206:ASN:N	2.28	0.48
1:B:131:ALA:HA	1:B:136:ILE:HD13	1.96	0.48
1:B:211:ALA:O	1:B:214:GLU:HB3	2.13	0.48
1:B:288:GLU:O	1:B:292:LYS:HG2	2.13	0.48
1:D:260:LYS:HE3	1:D:261:LYS:H	1.79	0.48
1:A:125:GLU:HG2	1:A:126:ARG:H	1.77	0.48
1:A:241:MET:O	1:A:246:SER:HB3	2.14	0.48
1:B:235:HIS:ND1	1:B:254:LYS:HD2	2.28	0.48
1:B:256:TRP:HE1	1:B:287:LEU:CG	2.26	0.48
1:C:26:LYS:HB3	1:C:212:PRO:HG3	1.96	0.48
1:C:256:TRP:HE1	1:C:287:LEU:CG	2.27	0.48
1:A:291:ARG:C	1:A:293:HIS:N	2.70	0.48
1:A:124:GLY:C	1:A:125:GLU:O	2.50	0.48
1:A:236:GLN:NE2	1:A:271:GLU:HG3	2.29	0.48
1:B:200:THR:HB	1:B:202:GLU:OE2	2.13	0.48
1:C:113:VAL:HB	1:C:114:PRO:HD2	1.95	0.48
1:B:74:GLY:O	1:B:89:GLU:HG3	2.14	0.48
1:B:256:TRP:HE3	1:B:256:TRP:H	1.62	0.48
1:C:74:GLY:O	1:C:89:GLU:HG3	2.14	0.48
1:C:127:LEU:CD1	1:C:129:LYS:H	2.26	0.48
1:C:65:LYS:HE3	1:C:196:VAL:HG13	1.96	0.48
1:C:162:ARG:NH1	1:C:194:GLU:OE1	2.46	0.48
1:B:7:VAL:HG12	1:B:204:SER:HA	1.96	0.47
1:C:64:LYS:HE2	1:C:147:PHE:CZ	2.49	0.47
1:D:236:GLN:HE22	1:D:269:ASN:CG	2.22	0.47
1:B:29:THR:HG21	1:B:51:ASN:ND2	2.20	0.47
1:B:287:LEU:N	1:B:287:LEU:HD22	2.29	0.47
1:C:171:ILE:HD13	1:C:191:LEU:CD2	2.44	0.47
1:D:74:GLY:O	1:D:89:GLU:HG3	2.14	0.47
1:A:95:THR:OG1	1:A:98:GLU:HG3	2.14	0.47
1:B:117:TYR:CE1	1:B:124:GLY:HA2	2.49	0.47
1:C:236:GLN:HE22	1:C:269:ASN:CG	2.21	0.47
1:A:82:ILE:HD12	1:A:83:THR:H	1.79	0.47
1:B:236:GLN:HE22	1:B:269:ASN:CG	2.23	0.47
1:B:284:SER:HA	1:B:287:LEU:HD21	1.95	0.47
1:C:236:GLN:HE21	1:C:271:GLU:H	1.62	0.47
1:A:63:LEU:HD13	1:A:197:GLY:HA3	1.96	0.47
1:B:236:GLN:CD	1:B:271:GLU:HG3	2.40	0.47
1:A:148:LYS:HG3	1:A:150:TRP:CZ3	2.50	0.47
1:A:235:HIS:ND1	1:A:254:LYS:HD2	2.30	0.47
1:A:216:GLU:C	1:A:218:ARG:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:GLY:O	1:C:186:ALA:HB3	2.14	0.47
1:D:280:ALA:HA	1:D:300:LEU:HD23	1.97	0.47
1:B:43:CYS:HG	1:B:192:VAL:HG22	1.79	0.46
1:C:4:GLY:HA3	1:C:220:ILE:O	2.15	0.46
1:C:256:TRP:HE1	1:C:287:LEU:CB	2.29	0.46
1:A:261:LYS:N	3:A:350:HOH:O	2.47	0.46
1:A:110:TYR:O	1:A:111:ASP:HB2	2.15	0.46
1:A:211:ALA:O	1:A:214:GLU:HB3	2.15	0.46
1:D:247:GLN:HG3	1:D:298:ARG:CZ	2.45	0.46
1:C:171:ILE:HD12	1:C:171:ILE:H	1.80	0.46
1:D:236:GLN:HE21	1:D:271:GLU:H	1.63	0.46
1:D:248:ILE:HB	1:D:300:LEU:HB2	1.97	0.46
1:A:251:GLU:HB2	1:A:296:GLN:OE1	2.16	0.46
1:C:259:PHE:N	1:C:284:SER:HB2	2.28	0.46
1:D:226:LEU:O	1:D:228:TRP:O	2.33	0.46
1:A:148:LYS:CB	1:B:90:ARG:HA	2.45	0.46
1:A:284:SER:HA	1:A:287:LEU:HD13	1.98	0.46
1:C:303:ARG:NH1	1:C:303:ARG:HG3	2.30	0.46
1:D:295:ARG:HE	1:D:297:ARG:NH2	2.13	0.46
1:D:90:ARG:HD2	1:D:184:CYS:O	2.16	0.46
1:B:76:ILE:HG23	1:B:176:MET:CE	2.40	0.45
1:B:260:LYS:HD2	1:B:283:ASN:OD1	2.16	0.45
1:C:231:ARG:HG3	1:C:231:ARG:HH11	1.81	0.45
1:B:29:THR:CG2	1:B:51:ASN:HD21	2.23	0.45
1:C:80:PHE:C	1:C:187:THR:HG23	2.41	0.45
1:D:282:ARG:HH12	1:D:297:ARG:CD	2.28	0.45
1:A:7:VAL:HG21	1:A:203:GLU:OE2	2.15	0.45
1:B:65:LYS:HE3	1:B:196:VAL:HG13	1.98	0.45
1:C:256:TRP:HE3	1:C:256:TRP:H	1.63	0.45
1:D:203:GLU:O	1:D:218:ARG:NH2	2.50	0.45
1:B:136:ILE:HG22	1:B:137:ILE:N	2.31	0.45
1:C:43:CYS:HG	1:C:192:VAL:HG22	1.80	0.45
1:D:171:ILE:C	1:D:171:ILE:HD12	2.42	0.45
1:D:205:LEU:HD23	1:D:205:LEU:C	2.42	0.45
1:A:7:VAL:HG12	1:A:204:SER:HA	1.99	0.45
1:A:296:GLN:HE21	1:A:296:GLN:HB3	1.41	0.45
1:B:29:THR:HG22	1:B:30:ARG:H	1.82	0.45
1:B:121:LYS:O	1:B:122:TYR:HB2	2.16	0.45
1:C:126:ARG:C	1:C:128:TYR:N	2.71	0.45
1:C:236:GLN:CD	1:C:271:GLU:HG3	2.41	0.45
1:B:296:GLN:OE1	1:B:296:GLN:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ALA:HB1	1:D:301:THR:O	2.16	0.45
1:A:293:HIS:C	1:A:295:ARG:N	2.75	0.45
1:B:216:GLU:C	1:B:218:ARG:H	2.23	0.45
1:D:295:ARG:HG2	1:D:295:ARG:HH11	1.82	0.45
1:B:63:LEU:HD13	1:B:197:GLY:HA3	1.98	0.44
1:B:28:LYS:O	1:C:252:MET:HG3	2.15	0.44
1:C:110:TYR:CE1	1:C:112:GLN:HB3	2.52	0.44
1:C:128:TYR:CD2	1:C:130:LEU:HA	2.51	0.44
1:D:9:TYR:N	1:D:205:LEU:O	2.38	0.44
1:D:165:VAL:HG22	1:D:166:SER:N	2.32	0.44
1:D:172:ARG:HG2	1:D:172:ARG:NH1	2.33	0.44
1:D:282:ARG:HH22	1:D:297:ARG:CZ	2.30	0.44
1:B:143:ARG:HG3	1:B:144:VAL:N	2.32	0.44
1:C:262:GLY:O	1:C:279:GLU:HG3	2.18	0.44
1:A:5:ILE:HD13	1:A:225:CYS:SG	2.58	0.44
1:C:82:ILE:HG13	1:C:189:VAL:HA	2.00	0.44
1:A:250:LEU:HD12	1:A:290:LEU:HB3	1.99	0.44
1:C:219:ILE:HG22	1:C:220:ILE:N	2.31	0.44
1:A:110:TYR:CE1	1:A:112:GLN:HB3	2.53	0.44
1:A:145:LYS:O	1:A:165:VAL:HG23	2.17	0.44
1:A:289:THR:O	1:A:293:HIS:HD2	2.01	0.44
1:C:7:VAL:O	1:C:204:SER:HA	2.17	0.44
1:B:117:TYR:O	1:B:118:SER:HB2	2.18	0.44
1:B:137:ILE:HG23	1:B:138:ASN:ND2	2.33	0.44
1:B:243:LEU:HD12	1:B:243:LEU:HA	1.81	0.44
1:D:38:LEU:HD23	1:D:38:LEU:HA	1.87	0.44
1:D:72:ARG:HA	1:D:157:ARG:O	2.17	0.44
1:D:26:LYS:HB3	1:D:212:PRO:HG3	1.99	0.44
1:D:43:CYS:SG	1:D:192:VAL:HG22	2.58	0.44
1:B:37:THR:CG2	1:B:38:LEU:N	2.81	0.43
1:A:231:ARG:NE	3:A:349:HOH:O	2.50	0.43
1:A:277:LEU:O	1:A:303:ARG:HB3	2.19	0.43
1:B:135:LYS:H	1:B:139:LEU:CD2	2.18	0.43
1:A:74:GLY:HA2	1:A:184:CYS:O	2.19	0.43
1:C:97:GLU:O	1:C:101:GLU:HB2	2.18	0.43
1:C:173:SER:O	1:C:176:MET:HB3	2.18	0.43
1:D:235:HIS:ND1	1:D:254:LYS:HD2	2.34	0.43
1:A:29:THR:HG21	1:A:51:ASN:ND2	2.26	0.43
1:A:100:ARG:CZ	1:B:85:GLU:OE1	2.66	0.43
1:B:148:LYS:HG3	1:B:150:TRP:CZ3	2.53	0.43
1:B:282:ARG:CZ	1:B:297:ARG:HD3	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:O	1:B:139:LEU:HG	2.17	0.43
1:C:181:LYS:C	1:C:183:GLY:N	2.76	0.43
1:C:171:ILE:H	1:C:171:ILE:CD1	2.29	0.43
1:C:256:TRP:NE1	1:C:287:LEU:HG	2.34	0.43
1:B:233:VAL:HG13	1:B:255:GLU:CB	2.48	0.43
1:B:236:GLN:NE2	1:B:271:GLU:HG3	2.34	0.43
1:C:66:VAL:HG22	1:C:164:GLU:HG3	2.01	0.43
1:C:236:GLN:NE2	1:C:269:ASN:HB2	2.34	0.43
1:C:247:GLN:HG3	1:C:298:ARG:CZ	2.49	0.43
1:D:291:ARG:C	1:D:293:HIS:N	2.76	0.43
1:A:37:THR:CG2	1:A:38:LEU:N	2.81	0.43
1:A:74:GLY:O	1:A:89:GLU:HG3	2.19	0.43
1:B:136:ILE:C	1:B:139:LEU:HG	2.44	0.43
1:B:235:HIS:CE1	1:B:254:LYS:HD2	2.53	0.43
1:B:290:LEU:HD11	1:B:297:ARG:CD	2.46	0.43
1:C:220:ILE:HG22	1:C:224:LYS:HB2	2.00	0.43
1:D:97:GLU:O	1:D:101:GLU:HB2	2.19	0.43
1:D:191:LEU:HD12	1:D:192:VAL:N	2.34	0.43
1:C:123:LYS:H	1:C:123:LYS:HG3	1.47	0.42
1:B:287:LEU:HD22	1:B:287:LEU:H	1.84	0.42
1:D:154:ILE:HG23	1:D:159:VAL:CG1	2.49	0.42
1:A:150:TRP:HD1	1:A:151:ASP:OD1	2.02	0.42
1:A:282:ARG:HH12	1:A:297:ARG:HD2	1.83	0.42
1:B:218:ARG:HD2	1:B:218:ARG:HA	1.87	0.42
1:C:236:GLN:HE22	1:C:269:ASN:ND2	2.18	0.42
1:D:144:VAL:HG23	1:D:169:THR:OG1	2.18	0.42
1:C:290:LEU:HB2	1:C:295:ARG:HB3	2.02	0.42
1:C:296:GLN:HE21	1:C:296:GLN:C	2.27	0.42
1:A:289:THR:O	1:A:291:ARG:O	2.37	0.42
1:A:121:LYS:HE2	1:A:121:LYS:HB2	1.84	0.42
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.90	0.42
1:C:279:GLU:HB2	1:C:303:ARG:NH1	2.35	0.42
1:D:25:LYS:O	1:D:28:LYS:HD2	2.20	0.42
1:B:260:LYS:HE3	1:B:261:LYS:H	1.84	0.42
1:C:288:GLU:OE2	1:C:292:LYS:HG3	2.19	0.42
1:D:71:MET:HG3	1:D:159:VAL:CG2	2.49	0.42
1:D:103:ILE:HD13	1:D:178:ILE:CG2	2.49	0.42
1:A:97:GLU:O	1:A:101:GLU:HB2	2.20	0.42
1:A:110:TYR:O	1:A:111:ASP:O	2.38	0.42
1:B:90:ARG:HH22	1:B:125:GLU:CG	2.33	0.42
1:B:303:ARG:O	1:B:304:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:GLN:CD	1:D:271:GLU:HG3	2.45	0.42
1:A:165:VAL:HG21	1:A:169:THR:CG2	2.47	0.41
1:C:37:THR:CG2	1:C:38:LEU:N	2.82	0.41
1:C:69:VAL:CG2	1:C:70:LYS:N	2.83	0.41
1:C:87:VAL:HG21	1:C:117:TYR:CE2	2.55	0.41
1:C:118:SER:O	1:C:119:ALA:HB3	2.18	0.41
1:D:148:LYS:HG2	1:D:164:GLU:HB3	2.02	0.41
1:B:154:ILE:HA	1:B:159:VAL:HG12	2.02	0.41
1:B:43:CYS:O	1:B:192:VAL:HA	2.19	0.41
1:B:258:GLY:HA2	1:B:284:SER:OG	2.20	0.41
1:C:69:VAL:HG22	1:C:70:LYS:H	1.83	0.41
1:C:222:LEU:HB3	1:C:274:LEU:HD23	2.02	0.41
1:C:256:TRP:HB3	1:C:257:ASP:H	1.68	0.41
1:D:282:ARG:NH1	1:D:297:ARG:HD2	2.33	0.41
1:A:110:TYR:OH	1:A:112:GLN:NE2	2.54	0.41
1:B:218:ARG:HH11	1:B:218:ARG:HG2	1.86	0.41
1:C:115:PRO:HG3	1:C:172:ARG:HE	1.86	0.41
1:C:303:ARG:HG3	1:C:303:ARG:HH11	1.84	0.41
1:D:69:VAL:HG22	1:D:70:LYS:H	1.86	0.41
1:D:243:LEU:HD12	1:D:243:LEU:HA	1.86	0.41
1:D:205:LEU:HD23	1:D:206:ASN:C	2.45	0.41
1:A:203:GLU:O	1:A:203:GLU:HG2	2.20	0.41
1:B:97:GLU:O	1:B:101:GLU:HB2	2.20	0.41
1:B:121:LYS:HG2	1:B:122:TYR:CD1	2.55	0.41
1:D:72:ARG:HB2	1:D:189:VAL:CG2	2.50	0.41
1:A:206:ASN:OD1	1:A:208:PHE:HB2	2.20	0.41
1:D:65:LYS:HE3	1:D:196:VAL:HG13	2.03	0.41
1:B:99:ILE:O	1:B:103:ILE:HG12	2.21	0.41
1:B:165:VAL:CG2	1:B:166:SER:N	2.83	0.41
1:C:80:PHE:CZ	1:C:176:MET:HE3	2.55	0.41
1:C:243:LEU:HD12	1:C:243:LEU:HA	1.92	0.41
1:C:287:LEU:O	1:C:291:ARG:HB2	2.21	0.41
1:A:6:LEU:HB3	1:A:48:ILE:HB	2.03	0.41
1:A:233:VAL:HG13	1:A:255:GLU:CB	2.46	0.41
1:B:262:GLY:O	1:B:279:GLU:HG3	2.20	0.41
1:C:291:ARG:C	1:C:293:HIS:H	2.28	0.41
1:D:6:LEU:HB3	1:D:48:ILE:HB	2.03	0.41
1:D:37:THR:CG2	1:D:38:LEU:N	2.84	0.41
1:C:111:ASP:HA	1:C:143:ARG:HA	2.02	0.41
1:C:128:TYR:O	1:C:129:LYS:C	2.63	0.41
1:D:191:LEU:HD12	1:D:192:VAL:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HD13	1:A:178:ILE:HD13	2.03	0.40
1:A:236:GLN:HE22	1:A:269:ASN:CG	2.29	0.40
1:D:290:LEU:C	1:D:291:ARG:O	2.60	0.40
1:C:52:GLN:NE2	1:C:307:GLN:HE21	2.17	0.40
1:D:295:ARG:HE	1:D:297:ARG:CZ	2.33	0.40
1:B:30:ARG:HB2	1:C:235:HIS:CD2	2.57	0.40
1:C:29:THR:HG22	1:C:30:ARG:H	1.85	0.40
1:C:235:HIS:CE1	1:C:254:LYS:HD2	2.57	0.40
1:D:80:PHE:HA	1:D:187:THR:HG22	2.03	0.40
1:C:162:ARG:HH11	1:C:162:ARG:HG2	1.87	0.40
1:C:216:GLU:O	1:C:218:ARG:N	2.54	0.40
1:D:52:GLN:O	1:D:55:ARG:HG3	2.21	0.40
1:D:216:GLU:C	1:D:218:ARG:N	2.79	0.40
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.82	0.40
1:A:243:LEU:HD21	1:A:273:ARG:NH2	2.36	0.40
1:B:6:LEU:HD13	1:B:6:LEU:C	2.46	0.40
1:B:24:ARG:HG2	1:C:241:MET:CE	2.51	0.40
1:C:285:SER:C	1:C:287:LEU:N	2.79	0.40
1:D:214:GLU:O	1:D:218:ARG:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	306/309 (99%)	263 (86%)	34 (11%)	9 (3%)	3	15
1	B	306/309 (99%)	257 (84%)	39 (13%)	10 (3%)	3	13
1	C	306/309 (99%)	244 (80%)	43 (14%)	19 (6%)	1	3
1	D	280/309 (91%)	235 (84%)	39 (14%)	6 (2%)	5	21
All	All	1198/1236 (97%)	999 (83%)	155 (13%)	44 (4%)	2	11

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	LYS
1	B	261	LYS
1	B	285	SER
1	C	117	TYR
1	C	130	LEU
1	C	136	ILE
1	C	261	LYS
1	D	261	LYS
1	A	117	TYR
1	A	257	ASP
1	A	283	ASN
1	A	284	SER
1	B	257	ASP
1	C	127	LEU
1	C	257	ASP
1	D	257	ASP
1	A	111	ASP
1	B	246	SER
1	B	294	GLU
1	C	111	ASP
1	A	229	LEU
1	A	245	GLY
1	B	140	PRO
1	B	229	LEU
1	C	115	PRO
1	C	120	LYS
1	C	128	TYR
1	C	229	LEU
1	C	246	SER
1	D	217	ASN
1	D	229	LEU
1	A	246	SER
1	B	118	SER
1	C	123	LYS
1	C	124	GLY
1	C	139	LEU
1	D	292	LYS
1	C	186	ALA
1	C	217	ASN
1	D	246	SER
1	C	245	GLY
1	B	245	GLY

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Mol	Chain	Res	Type
1	C	140	PRO
1	B	134	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	272/273 (100%)	254 (93%)	18 (7%)	15	43
1	B	272/273 (100%)	254 (93%)	18 (7%)	15	43
1	C	272/273 (100%)	249 (92%)	23 (8%)	10	31
1	D	252/273 (92%)	226 (90%)	26 (10%)	7	23
All	All	1068/1092 (98%)	983 (92%)	85 (8%)	11	34

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	30	ARG
1	A	55	ARG
1	A	82	ILE
1	A	91	GLU
1	A	92	CYS
1	A	132	ARG
1	A	138	ASN
1	A	155	GLU
1	A	163	VAL
1	A	233	VAL
1	A	243	LEU
1	A	250	LEU
1	A	255	GLU
1	A	256	TRP
1	A	281	GLU
1	A	282	ARG
1	A	296	GLN
1	B	29	THR

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Mol	Chain	Res	Type
1	B	30	ARG
1	B	55	ARG
1	B	82	ILE
1	B	91	GLU
1	B	92	CYS
1	B	135	LYS
1	B	136	ILE
1	B	139	LEU
1	B	155	GLU
1	B	163	VAL
1	B	233	VAL
1	B	243	LEU
1	B	250	LEU
1	B	255	GLU
1	B	256	TRP
1	B	281	GLU
1	B	296	GLN
1	C	29	THR
1	C	30	ARG
1	C	55	ARG
1	C	82	ILE
1	C	91	GLU
1	C	92	CYS
1	C	111	ASP
1	C	123	LYS
1	C	127	LEU
1	C	133	GLU
1	C	136	ILE
1	C	140	PRO
1	C	155	GLU
1	C	171	ILE
1	C	233	VAL
1	C	243	LEU
1	C	250	LEU
1	C	255	GLU
1	C	256	TRP
1	C	281	GLU
1	C	287	LEU
1	C	290	LEU
1	C	296	GLN
1	D	29	THR
1	D	30	ARG

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Mol	Chain	Res	Type
1	D	55	ARG
1	D	82	ILE
1	D	91	GLU
1	D	92	CYS
1	D	151	ASP
1	D	155	GLU
1	D	158	ASP
1	D	172	ARG
1	D	187	THR
1	D	209	GLU
1	D	212	PRO
1	D	213	GLU
1	D	214	GLU
1	D	233	VAL
1	D	243	LEU
1	D	250	LEU
1	D	255	GLU
1	D	256	TRP
1	D	281	GLU
1	D	282	ARG
1	D	288	GLU
1	D	290	LEU
1	D	296	GLN
1	D	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	199	HIS
1	A	236	GLN
1	A	296	GLN
1	B	17	HIS
1	B	138	ASN
1	B	199	HIS
1	B	236	GLN
1	B	293	HIS
1	C	34	HIS
1	C	51	ASN
1	C	93	ASN
1	C	138	ASN
1	C	153	ASN

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Mol	Chain	Res	Type
1	C	206	ASN
1	C	236	GLN
1	C	296	GLN
1	C	307	GLN
1	D	34	HIS
1	D	51	ASN
1	D	112	GLN
1	D	236	GLN
1	D	307	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	308/309 (99%)	0.34	23 (7%) 20 16	16, 32, 60, 82	0
1	B	308/309 (99%)	0.47	16 (5%) 33 26	23, 41, 77, 83	0
1	C	308/309 (99%)	0.72	34 (11%) 10 9	27, 50, 90, 97	0
1	D	284/309 (91%)	0.57	35 (12%) 8 7	13, 40, 84, 95	0
All	All	1208/1236 (97%)	0.52	108 (8%) 15 13	13, 40, 80, 97	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	TYR	6.7
1	C	139	LEU	6.0
1	C	129	LYS	5.5
1	A	87	VAL	4.9
1	D	86	VAL	4.3
1	D	116	ALA	4.2
1	A	97	GLU	3.9
1	D	87	VAL	3.8
1	D	185	GLY	3.6
1	A	90	ARG	3.6
1	A	227	GLU	3.6
1	B	308	THR	3.6
1	A	294	GLU	3.5
1	C	136	ILE	3.5
1	D	92	CYS	3.5
1	D	113	VAL	3.3
1	B	91	GLU	3.2
1	B	121	LYS	3.2
1	A	88	GLU	3.2
1	C	127	LEU	3.2
1	D	108	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	101	GLU	3.2
1	D	82	ILE	3.2
1	D	90	ARG	3.1
1	D	110	TYR	3.0
1	A	116	ALA	3.0
1	C	119	ALA	3.0
1	B	89	GLU	2.9
1	D	180	TYR	2.9
1	B	90	ARG	2.9
1	D	186	ALA	2.9
1	A	82	ILE	2.9
1	B	176	MET	2.8
1	C	123	LYS	2.8
1	D	187	THR	2.8
1	D	184	CYS	2.8
1	C	137	ILE	2.8
1	D	73	LEU	2.7
1	C	293	HIS	2.7
1	D	141	PRO	2.7
1	D	41	PHE	2.7
1	C	138	ASN	2.7
1	A	110	TYR	2.6
1	C	184	CYS	2.6
1	B	136	ILE	2.6
1	A	89	GLU	2.6
1	C	260	LYS	2.5
1	C	94	VAL	2.5
1	D	176	MET	2.5
1	A	92	CYS	2.5
1	D	159	VAL	2.5
1	A	256	TRP	2.5
1	A	128	TYR	2.5
1	B	92	CYS	2.5
1	A	78	GLU	2.4
1	B	80	PHE	2.4
1	C	120	LYS	2.4
1	C	122	TYR	2.4
1	C	93	ASN	2.4
1	A	91	GLU	2.4
1	C	176	MET	2.4
1	C	290	LEU	2.4
1	C	140	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	91	GLU	2.3
1	C	155	GLU	2.3
1	A	111	ASP	2.3
1	C	141	PRO	2.3
1	C	135	LYS	2.3
1	D	182	LEU	2.3
1	C	126	ARG	2.3
1	C	124	GLY	2.3
1	C	87	VAL	2.2
1	A	74	GLY	2.2
1	D	178	ILE	2.2
1	B	87	VAL	2.2
1	A	108	GLY	2.2
1	C	131	ALA	2.2
1	D	75	LEU	2.2
1	B	94	VAL	2.2
1	B	140	PRO	2.2
1	D	95	THR	2.2
1	B	122	TYR	2.2
1	C	152	VAL	2.2
1	D	158	ASP	2.2
1	C	109	GLU	2.2
1	C	125	GLU	2.2
1	D	308	THR	2.1
1	D	175	CYS	2.1
1	C	171	ILE	2.1
1	A	35	GLY	2.1
1	D	83	THR	2.1
1	D	157	ARG	2.1
1	B	135	LYS	2.1
1	C	121	LYS	2.1
1	C	97	GLU	2.1
1	D	294	GLU	2.1
1	B	181	LYS	2.1
1	D	144	VAL	2.0
1	D	217	ASN	2.0
1	C	308	THR	2.0
1	C	186	ALA	2.0
1	D	85	GLU	2.0
1	D	88	GLU	2.0
1	A	86	VAL	2.0
1	B	86	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	154	ILE	2.0
1	A	209	GLU	2.0
1	D	256	TRP	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	MG	C	310	1/1	0.77	0.17	47,47,47,47	0
2	MG	D	310	1/1	0.86	0.17	41,41,41,41	0
2	MG	A	310	1/1	0.95	0.12	14,14,14,14	0
2	MG	B	310	1/1	0.97	0.03	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.