Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 05:23 PM EST

PDB ID	:	3I3Y
Title	:	Crystal structure of Ribokinase in Complex with D-Ribose from Klebsiella pneumoniae
Authors	:	Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-07-01
Resolution	:	2.15 Å(reported)

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

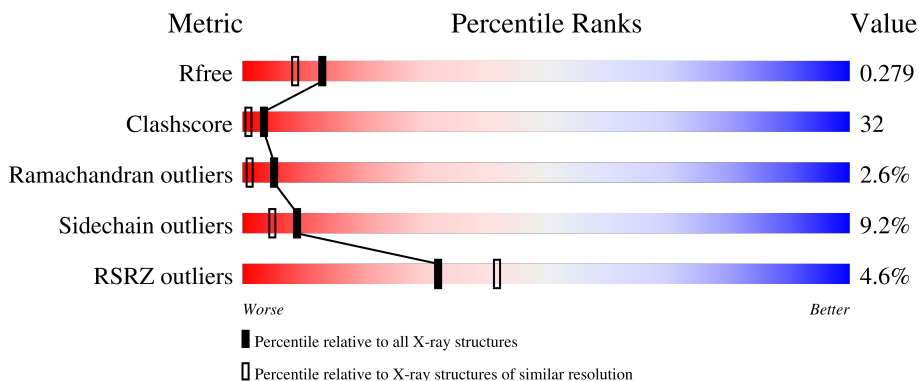|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.15 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	Percentile Ranks	Value
Rfree		0.279
Clashscore		32
Ramachandran outliers		2.6%
Sidechain outliers		9.2%
RSRZ outliers		4.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	299	4% — 52% / 37% / 5% · 5%
1	B	299	4% — 49% / 41% / · 6%
1	C	299	2% — 62% / 30% / · 5%
1	D	299	6% — 49% / 38% / 7% · 5%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8707 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 Carbohydrate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	Se	0	0	0
			2121	1333	372	408	3	5			
1	B	282	Total	C	N	O	S	Se	0	0	0
			2099	1322	368	401	3	5			
1	C	285	Total	C	N	O	S	Se	0	0	0
			2121	1333	372	408	3	5			
1	D	285	Total	C	N	O	S	Se	0	0	0
			2121	1333	372	408	3	5			

There are 44 discrepancies between the modelled and reference sequences:
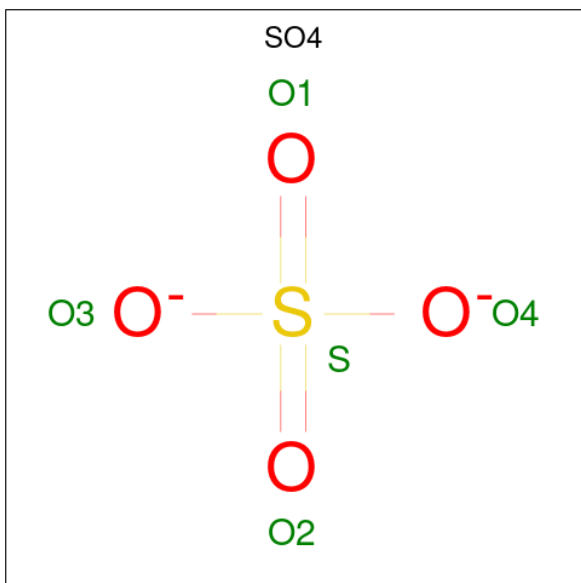
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MSE	-	expression tag	UNP A6T989
A	-2	SER	-	expression tag	UNP A6T989
A	-1	LEU	-	expression tag	UNP A6T989
A	290	GLU	-	expression tag	UNP A6T989
A	291	GLY	-	expression tag	UNP A6T989
A	292	HIS	-	expression tag	UNP A6T989
A	293	HIS	-	expression tag	UNP A6T989
A	294	HIS	-	expression tag	UNP A6T989
A	295	HIS	-	expression tag	UNP A6T989
A	296	HIS	-	expression tag	UNP A6T989
A	297	HIS	-	expression tag	UNP A6T989
B	-3	MSE	-	expression tag	UNP A6T989
B	-2	SER	-	expression tag	UNP A6T989
B	-1	LEU	-	expression tag	UNP A6T989
B	290	GLU	-	expression tag	UNP A6T989
B	291	GLY	-	expression tag	UNP A6T989
B	292	HIS	-	expression tag	UNP A6T989
B	293	HIS	-	expression tag	UNP A6T989
B	294	HIS	-	expression tag	UNP A6T989
B	295	HIS	-	expression tag	UNP A6T989
B	296	HIS	-	expression tag	UNP A6T989

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Chain	Residue	Modelled	Actual	Comment	Reference
B	297	HIS	-	expression tag	UNP A6T989
C	-3	MSE	-	expression tag	UNP A6T989
C	-2	SER	-	expression tag	UNP A6T989
C	-1	LEU	-	expression tag	UNP A6T989
C	290	GLU	-	expression tag	UNP A6T989
C	291	GLY	-	expression tag	UNP A6T989
C	292	HIS	-	expression tag	UNP A6T989
C	293	HIS	-	expression tag	UNP A6T989
C	294	HIS	-	expression tag	UNP A6T989
C	295	HIS	-	expression tag	UNP A6T989
C	296	HIS	-	expression tag	UNP A6T989
C	297	HIS	-	expression tag	UNP A6T989
D	-3	MSE	-	expression tag	UNP A6T989
D	-2	SER	-	expression tag	UNP A6T989
D	-1	LEU	-	expression tag	UNP A6T989
D	290	GLU	-	expression tag	UNP A6T989
D	291	GLY	-	expression tag	UNP A6T989
D	292	HIS	-	expression tag	UNP A6T989
D	293	HIS	-	expression tag	UNP A6T989
D	294	HIS	-	expression tag	UNP A6T989
D	295	HIS	-	expression tag	UNP A6T989
D	296	HIS	-	expression tag	UNP A6T989
D	297	HIS	-	expression tag	UNP A6T989

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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
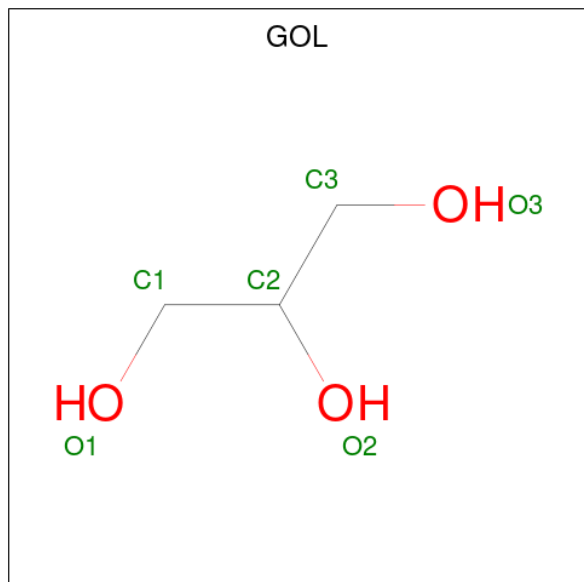
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 6	C 3	O 3	0	0

- Molecule 4 is alpha-D-ribofuranose (three-letter code: RIB) (formula: $C_5H_{10}O_5$).

RIB
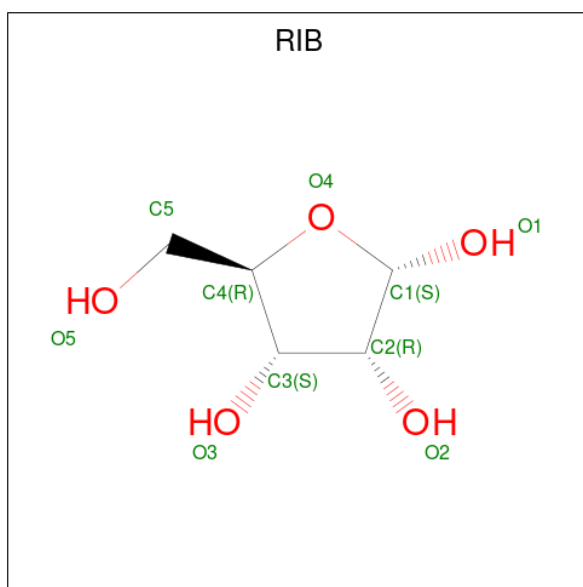
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 10	C 5	O 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total 60	O 60	0	0
5	B	41	Total 41	O 41	0	0
5	C	60	Total 60	O 60	0	0
5	D	38	Total 38	O 38	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Carbohydrate kinase
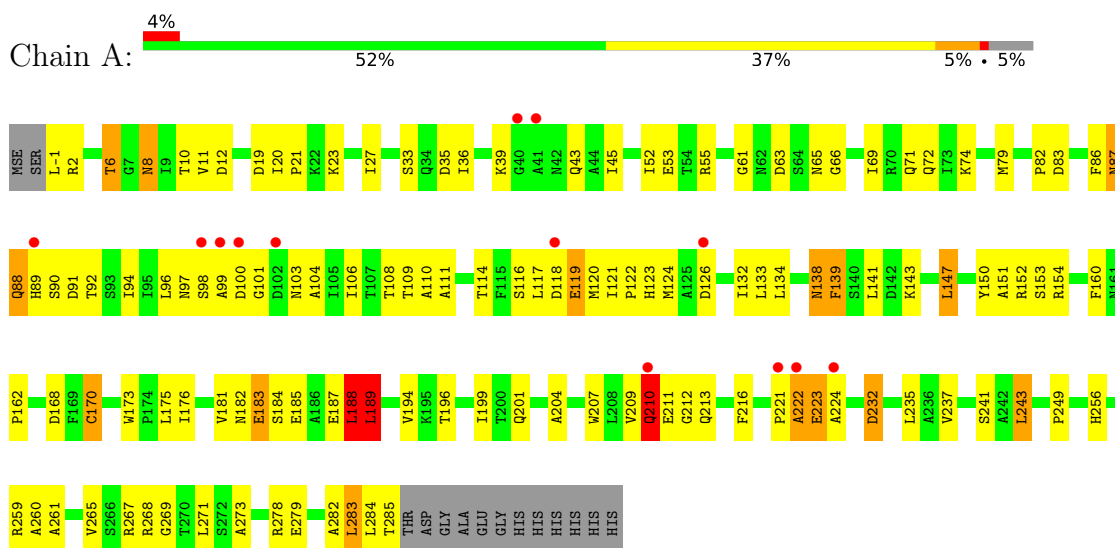
- Molecule 1: Carbohydrate kinase

- Molecule 1: Carbohydrate kinase

• Molecule 1: Carbohydrate kinase

Chain D:
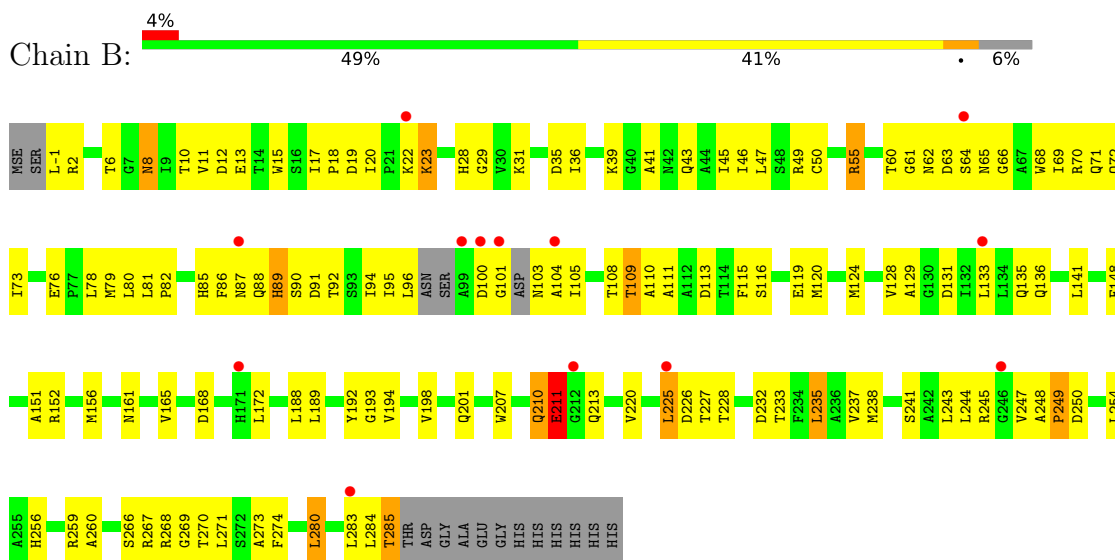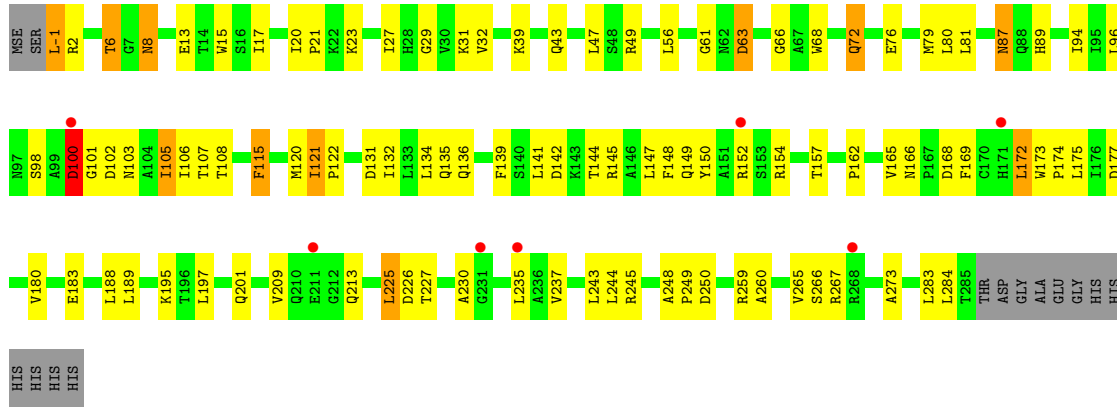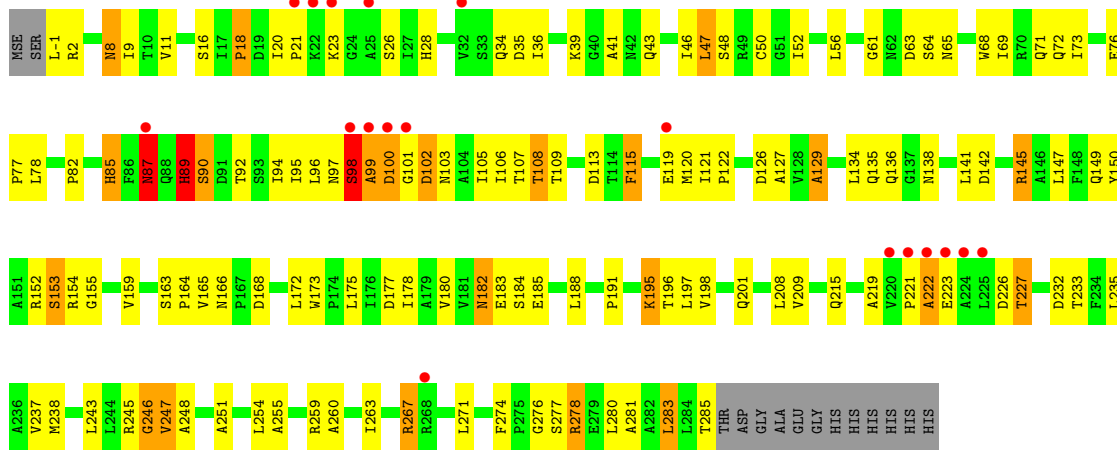
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.49Å 105.90Å 121.15Å 90.00° 99.45° 90.00°	Depositor
Resolution (Å)	34.97 – 2.15 34.97 – 2.05	Depositor EDS
% Data completeness (in resolution range)	91.3 (34.97-2.15) 91.3 (34.97-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	0.50 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.276 0.251 , 0.279	Depositor DCC
R_{free} test set	4236 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.9	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8707	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, RIB, SO4

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	0.39	0/2155	0.72	0/2931
1	B	0.36	0/2131	0.66	0/2895
1	C	0.36	0/2155	0.68	0/2931
1	D	0.36	0/2155	0.69	0/2931
All	All	0.37	0/8596	0.69	0/11688

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 (i)

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	2121	0	2122	165	0
1	B	2099	0	2105	152	0
1	C	2121	0	2122	100	0
1	D	2121	0	2122	163	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	5	0	0	0	0
3	C	6	0	8	0	0
4	D	10	0	0	0	0

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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	60	0	0	12	0
5	B	41	0	0	7	0
5	C	60	0	0	1	0
5	D	38	0	0	6	0
All	All	8707	0	8479	544	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 32.

All (544) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLY:H	1:A:89:HIS:CD2	1.66	1.13
1:A:10:THR:HG23	1:A:91:ASP:HA	1.34	1.10
1:D:195:LYS:H	1:D:195:LYS:HD2	0.95	1.09
1:A:181:VAL:HG13	1:A:185:GLU:HB2	1.42	1.01
1:D:259:ARG:HB3	1:D:283:LEU:HD11	1.45	0.98
1:A:61:GLY:N	1:A:89:HIS:HD2	1.63	0.95
1:C:6:THR:HG21	1:C:147:LEU:HD13	1.43	0.95
1:A:6:THR:HG23	1:A:120:MSE:HE1	1.49	0.93
1:A:61:GLY:H	1:A:89:HIS:HD2	0.93	0.93
1:D:195:LYS:HD2	1:D:195:LYS:N	1.81	0.93
1:B:70:ARG:HD3	1:B:85:HIS:NE2	1.86	0.89
1:B:63:ASP:H	1:B:89:HIS:HE1	1.22	0.87
1:A:188:LEU:O	1:A:189:LEU:HB2	1.71	0.86
1:A:45:ILE:HD13	1:A:271:LEU:HD11	1.56	0.86
1:B:228:THR:HG21	1:B:270:THR:HG22	1.57	0.86
1:A:19:ASP:HA	1:A:97:ASN:HD22	1.40	0.86
1:C:20:ILE:O	1:C:20:ILE:HD12	1.78	0.83
1:A:100:ASP:HB3	1:C:23:LYS:NZ	1.93	0.83
1:D:43:GLN:NE2	1:D:136:GLN:HE21	1.77	0.83
1:B:63:ASP:H	1:B:89:HIS:CE1	1.97	0.83
1:D:195:LYS:CD	1:D:195:LYS:H	1.80	0.83
1:B:63:ASP:HB3	1:B:89:HIS:CE1	2.13	0.82
1:C:79:MSE:HE2	1:C:81:LEU:HD21	1.59	0.82
1:C:166:ASN:HD21	1:C:168:ASP:HB2	1.43	0.82
1:A:20:ILE:HG13	1:A:97:ASN:HD21	1.46	0.80
1:D:177:ASP:HA	1:D:195:LYS:HD3	1.62	0.80
1:A:209:VAL:O	1:A:210:GLN:HB2	1.79	0.80
1:D:141:LEU:HD11	1:D:172:LEU:HD11	1.65	0.79
1:A:66:GLY:CA	1:A:89:HIS:NE2	2.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ARG:HG2	5:D:325:HOH:O	1.83	0.78
1:B:8:ASN:H	1:B:8:ASN:HD22	1.31	0.77
1:C:-1:LEU:HD12	1:C:2:ARG:N	2.00	0.77
1:C:152:ARG:CZ	1:C:175:LEU:HA	2.14	0.77
1:B:63:ASP:N	1:B:89:HIS:HE1	1.82	0.76
1:D:11:VAL:HG21	1:D:65:ASN:HB3	1.65	0.76
1:A:194:VAL:O	1:A:210:GLN:HG2	1.86	0.76
1:C:6:THR:HG23	1:C:139:PHE:HE2	1.49	0.76
1:D:145:ARG:HH11	1:D:145:ARG:CB	2.00	0.75
1:D:16:SER:HA	1:D:97:ASN:HB3	1.69	0.74
1:B:220:VAL:HG21	1:B:259:ARG:HG3	1.69	0.74
1:B:79:MSE:HE2	1:B:81:LEU:HD21	1.69	0.74
1:B:65:ASN:HB2	1:B:89:HIS:CD2	2.23	0.73
1:C:152:ARG:NH1	1:C:175:LEU:HA	2.03	0.73
1:A:-1:LEU:N	5:A:349:HOH:O	2.20	0.73
1:D:43:GLN:HE22	1:D:136:GLN:HE21	1.37	0.73
1:A:117:LEU:H	1:A:143:LYS:HZ2	1.37	0.73
1:B:39:LYS:HE2	1:B:232:ASP:OD1	1.86	0.73
1:B:23:LYS:HD3	1:D:101:GLY:HA3	1.71	0.73
1:B:141:LEU:HD11	1:B:172:LEU:HD11	1.71	0.72
1:B:68:TRP:O	1:B:72:GLN:HG2	1.89	0.72
1:C:68:TRP:HE1	1:C:72:GLN:NE2	1.88	0.72
1:B:124:MSE:HE3	1:B:156:MSE:HE1	1.72	0.71
1:B:63:ASP:HB3	1:B:89:HIS:NE2	2.06	0.71
1:B:28:HIS:CE1	1:D:138:ASN:HD22	2.09	0.70
1:B:23:LYS:NZ	1:D:101:GLY:HA3	2.06	0.70
1:D:238:MSE:HG3	1:D:254:LEU:HD12	1.72	0.70
1:A:282:ALA:O	1:A:285:THR:HG22	1.92	0.70
1:A:65:ASN:CB	1:A:89:HIS:HE1	2.04	0.70
1:B:210:GLN:HB2	5:B:307:HOH:O	1.91	0.70
1:A:117:LEU:C	1:A:119:GLU:H	1.94	0.70
1:D:71:GLN:NE2	1:D:72:GLN:HE21	1.90	0.70
1:D:141:LEU:HD22	1:D:168:ASP:HB3	1.74	0.69
1:A:224:ALA:HA	1:A:265:VAL:HG12	1.74	0.69
1:D:82:PRO:HD3	1:D:115:PHE:CZ	2.26	0.69
1:C:68:TRP:HE1	1:C:72:GLN:HE22	1.40	0.69
1:B:285:THR:HG22	5:B:328:HOH:O	1.92	0.69
1:B:95:ILE:HG23	1:B:104:ALA:HB3	1.75	0.68
1:B:70:ARG:HD3	1:B:85:HIS:CE1	2.28	0.68
1:A:196:THR:HG21	1:A:249:PRO:HG2	1.75	0.68
1:A:121:ILE:HD12	1:A:124:MSE:HE3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LEU:HA	1:D:159:VAL:HG13	1.74	0.68
1:C:49:ARG:HD2	1:C:76:GLU:OE1	1.93	0.68
1:C:105:ILE:C	1:C:105:ILE:HD12	2.14	0.67
1:C:225:LEU:HD21	1:C:266:SER:C	2.14	0.67
1:A:241:SER:OG	1:A:256:HIS:HD2	1.76	0.67
1:A:100:ASP:HB3	1:C:23:LYS:HZ2	1.58	0.67
1:A:36:ILE:HD11	1:A:72:GLN:HB2	1.74	0.67
1:A:183:GLU:CD	1:A:201:GLN:HG2	2.15	0.66
1:D:109:THR:HG23	1:D:113:ASP:OD2	1.95	0.66
1:B:63:ASP:CG	1:B:64:SER:H	1.99	0.66
1:D:121:ILE:HG13	1:D:122:PRO:CD	2.26	0.66
1:B:94:ILE:HD12	1:B:94:ILE:N	2.11	0.66
1:B:60:THR:HG23	1:B:85:HIS:HD1	1.60	0.65
1:A:66:GLY:N	1:A:89:HIS:NE2	2.43	0.65
1:A:117:LEU:HD22	1:A:143:LYS:NZ	2.12	0.65
1:A:210:GLN:O	1:A:211:GLU:HB2	1.97	0.65
1:C:17:ILE:O	1:C:98:SER:HA	1.97	0.65
1:D:99:ALA:O	1:D:100:ASP:HB3	1.96	0.65
1:D:61:GLY:HA3	1:D:89:HIS:O	1.97	0.65
1:B:100:ASP:HB3	1:D:23:LYS:NZ	2.12	0.65
1:B:247:VAL:O	1:B:248:ALA:HB3	1.96	0.64
1:B:19:ASP:HB3	1:B:100:ASP:OD1	1.97	0.64
1:C:154:ARG:HH11	1:C:154:ARG:HG2	1.62	0.64
1:B:70:ARG:CD	1:B:85:HIS:NE2	2.60	0.64
1:B:20:ILE:HD13	1:D:21:PRO:O	1.96	0.64
1:A:283:LEU:HD12	1:A:283:LEU:C	2.18	0.64
1:A:108:THR:HG23	1:C:15:TRP:CZ3	2.33	0.64
1:B:109:THR:HG22	1:D:28:HIS:HE1	1.63	0.64
1:A:23:LYS:NZ	1:C:100:ASP:HB2	2.13	0.63
1:A:43:GLN:HG3	1:A:232:ASP:HB2	1.80	0.63
1:C:225:LEU:CD2	1:C:225:LEU:H	2.12	0.63
1:A:100:ASP:CB	1:C:23:LYS:NZ	2.62	0.63
1:A:187:GLU:O	1:A:188:LEU:HG	1.98	0.63
1:B:11:VAL:HG11	1:B:65:ASN:CG	2.19	0.63
1:B:63:ASP:CG	1:B:64:SER:N	2.52	0.63
1:C:43:GLN:HE21	1:C:134:LEU:HD21	1.63	0.63
1:C:6:THR:O	1:C:6:THR:HG22	1.97	0.63
1:D:39:LYS:HB3	1:D:136:GLN:HG2	1.81	0.63
1:B:28:HIS:HE1	1:D:138:ASN:HD22	1.46	0.62
1:B:63:ASP:CA	1:B:89:HIS:HE1	2.11	0.62
1:A:139:PHE:HB2	5:A:314:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:PHE:HB3	1:C:120:MSE:HE3	1.82	0.62
1:A:61:GLY:N	1:A:89:HIS:CD2	2.47	0.62
1:A:6:THR:HG23	1:A:120:MSE:CE	2.27	0.62
1:B:36:ILE:HD11	1:B:72:GLN:HB2	1.81	0.62
1:B:109:THR:O	1:B:111:ALA:N	2.31	0.61
1:B:165:VAL:HG21	1:B:188:LEU:HD23	1.82	0.61
1:D:152:ARG:O	1:D:153:SER:HB3	1.98	0.61
1:B:60:THR:HG23	1:B:85:HIS:ND1	2.14	0.61
1:D:115:PHE:HB3	1:D:120:MSE:HE3	1.80	0.61
1:D:152:ARG:O	1:D:153:SER:CB	2.46	0.61
1:D:237:VAL:HG21	1:D:260:ALA:CB	2.29	0.61
1:B:124:MSE:CE	1:B:156:MSE:SE	2.99	0.61
1:D:247:VAL:HG22	1:D:248:ALA:H	1.64	0.61
1:A:104:ALA:HB1	1:C:21:PRO:HB2	1.83	0.61
1:D:121:ILE:HG13	1:D:122:PRO:N	2.15	0.61
1:A:121:ILE:HD11	1:A:150:TYR:CE1	2.36	0.61
1:B:17:ILE:HB	1:B:18:PRO:HD2	1.81	0.61
1:B:66:GLY:H	1:B:89:HIS:CE1	2.18	0.61
1:B:225:LEU:HD21	1:B:266:SER:O	2.01	0.60
1:D:8:ASN:HD22	1:D:8:ASN:H	1.47	0.60
1:A:138:ASN:O	1:A:139:PHE:CG	2.54	0.60
1:A:66:GLY:HA2	1:A:89:HIS:NE2	2.15	0.60
1:B:8:ASN:H	1:B:8:ASN:ND2	1.98	0.60
1:D:36:ILE:CD1	1:D:72:GLN:HG3	2.31	0.60
1:A:117:LEU:O	1:A:119:GLU:N	2.32	0.60
1:C:68:TRP:NE1	1:C:72:GLN:NE2	2.50	0.60
1:A:65:ASN:HB2	1:A:89:HIS:HE1	1.65	0.59
1:D:43:GLN:NE2	1:D:136:GLN:NE2	2.50	0.59
1:B:105:ILE:N	1:B:105:ILE:HD12	2.18	0.59
1:B:241:SER:OG	1:B:256:HIS:HD2	1.85	0.59
1:B:244:LEU:HD12	1:B:284:LEU:HD13	1.83	0.59
1:A:43:GLN:HG3	1:A:232:ASP:CB	2.32	0.59
1:C:141:LEU:HD22	1:C:168:ASP:HB3	1.84	0.59
1:B:17:ILE:HG22	1:B:29:GLY:HA3	1.84	0.59
1:A:12:ASP:OD1	1:A:92:THR:HG22	2.03	0.58
1:C:-1:LEU:CD1	1:C:131:ASP:HA	2.32	0.58
1:B:28:HIS:NE2	1:D:164:PRO:HG3	2.18	0.58
1:A:82:PRO:HB3	1:A:123:HIS:NE2	2.18	0.58
1:A:86:PHE:C	1:A:87:ASN:OD1	2.41	0.58
1:C:165:VAL:HG23	1:C:189:LEU:HD11	1.84	0.58
1:C:21:PRO:HG3	1:C:27:ILE:CD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLN:O	1:D:152:ARG:O	2.21	0.58
1:C:39:LYS:HB3	1:C:136:GLN:HG2	1.84	0.58
1:D:121:ILE:HG13	1:D:122:PRO:HD3	1.84	0.58
1:D:135:GLN:HE22	1:D:147:LEU:HD12	1.68	0.58
1:D:247:VAL:HG22	1:D:248:ALA:N	2.18	0.58
1:A:10:THR:HG22	1:A:11:VAL:N	2.17	0.58
1:B:201:GLN:HE21	1:B:207:TRP:HD1	1.52	0.58
1:D:87:ASN:N	1:D:87:ASN:HD22	2.01	0.58
1:A:10:THR:CG2	1:A:11:VAL:N	2.67	0.57
1:B:15:TRP:CE2	1:D:94:ILE:HD11	2.40	0.57
1:A:222:ALA:O	1:A:223:GLU:HB2	2.05	0.57
1:C:6:THR:HG22	1:C:135:GLN:HG2	1.85	0.57
1:A:100:ASP:CB	1:C:23:LYS:HZ3	2.17	0.57
1:D:9:ILE:HG21	1:D:69:ILE:HG21	1.86	0.57
1:C:235:LEU:HD12	1:C:235:LEU:O	2.04	0.57
1:A:117:LEU:HD22	1:A:143:LYS:HZ2	1.70	0.57
1:B:109:THR:CG2	1:D:28:HIS:HE1	2.17	0.57
1:C:115:PHE:O	1:C:120:MSE:HE3	2.04	0.57
1:A:121:ILE:HD11	1:A:150:TYR:CZ	2.40	0.57
1:A:106:ILE:HD11	1:C:21:PRO:HG2	1.86	0.57
1:A:222:ALA:O	1:A:223:GLU:CB	2.53	0.57
1:A:20:ILE:HG13	1:A:97:ASN:ND2	2.18	0.56
1:A:2:ARG:HD2	5:A:308:HOH:O	2.04	0.56
1:B:141:LEU:HD11	1:B:172:LEU:CD1	2.35	0.56
1:C:87:ASN:HD22	1:C:87:ASN:H	1.53	0.56
1:D:2:ARG:HH11	1:D:2:ARG:HG2	1.70	0.56
1:D:43:GLN:O	1:D:47:LEU:HB2	2.05	0.56
1:D:36:ILE:HD11	1:D:72:GLN:HG3	1.87	0.56
1:A:173:TRP:CE3	1:A:176:ILE:HD12	2.40	0.56
1:B:8:ASN:N	1:B:8:ASN:HD22	1.94	0.56
1:A:261:ALA:O	1:A:265:VAL:HG23	2.04	0.56
1:A:121:ILE:HD11	1:A:150:TYR:CD1	2.40	0.56
1:A:182:ASN:OD1	1:A:185:GLU:HG3	2.05	0.56
1:B:23:LYS:HD3	1:D:102:ASP:H	1.69	0.56
1:B:95:ILE:HG22	1:B:104:ALA:O	2.06	0.56
1:C:180:VAL:HG21	1:C:235:LEU:HD13	1.88	0.56
1:B:65:ASN:O	1:B:69:ILE:HG13	2.06	0.56
1:C:8:ASN:H	1:C:8:ASN:HD22	1.53	0.56
1:A:237:VAL:HG21	1:A:260:ALA:CB	2.36	0.56
1:B:22:LYS:HB2	1:B:22:LYS:NZ	2.20	0.56
1:B:104:ALA:C	1:B:105:ILE:HD12	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:SER:HB2	1:D:100:ASP:H	1.71	0.55
1:D:141:LEU:HD11	1:D:172:LEU:CD1	2.35	0.55
1:A:181:VAL:HG12	1:A:182:ASN:O	2.06	0.55
1:D:99:ALA:O	1:D:100:ASP:CB	2.54	0.55
1:B:210:GLN:HA	1:B:210:GLN:HE21	1.72	0.55
1:D:105:ILE:HG22	1:D:106:ILE:N	2.22	0.55
1:D:165:VAL:HG21	1:D:188:LEU:HD23	1.89	0.55
1:D:255:ALA:O	1:D:259:ARG:HD3	2.07	0.55
1:B:61:GLY:O	1:B:85:HIS:ND1	2.40	0.55
1:B:17:ILE:HD13	1:B:95:ILE:HD11	1.88	0.55
1:A:11:VAL:HG23	1:A:69:ILE:HD11	1.89	0.54
1:A:8:ASN:H	1:A:8:ASN:HD22	1.55	0.54
1:B:100:ASP:C	1:D:23:LYS:HZ2	2.10	0.54
1:C:166:ASN:ND2	1:C:168:ASP:HB2	2.17	0.54
1:B:63:ASP:HB3	1:B:89:HIS:HE2	1.72	0.54
1:D:115:PHE:CG	1:D:120:MSE:HE3	2.42	0.54
1:D:127:ALA:O	1:D:154:ARG:NH2	2.41	0.54
1:A:168:ASP:C	1:A:170:CYS:N	2.61	0.54
1:B:63:ASP:CB	1:B:89:HIS:CE1	2.87	0.54
1:A:23:LYS:O	1:C:103:ASN:O	2.26	0.54
1:D:245:ARG:O	1:D:246:GLY:C	2.46	0.54
1:B:245:ARG:NH2	1:B:250:ASP:OD2	2.40	0.54
1:A:221:PRO:O	1:A:222:ALA:HB2	2.08	0.54
1:D:182:ASN:N	1:D:182:ASN:ND2	2.54	0.54
1:A:222:ALA:O	1:A:223:GLU:HG3	2.09	0.53
1:B:105:ILE:O	1:D:26:SER:HA	2.08	0.53
1:D:150:TYR:CZ	1:D:154:ARG:HD3	2.43	0.53
1:A:184:SER:O	1:A:187:GLU:O	2.26	0.53
1:B:226:ASP:HB3	1:B:267:ARG:O	2.08	0.53
1:D:152:ARG:HH11	1:D:152:ARG:HG2	1.72	0.53
1:A:188:LEU:O	1:A:189:LEU:CB	2.50	0.53
1:B:100:ASP:HB3	1:D:23:LYS:HZ2	1.72	0.53
1:B:136:GLN:HA	1:B:161:ASN:O	2.08	0.53
1:B:270:THR:OG1	1:B:271:LEU:N	2.42	0.53
1:D:227:THR:HG21	5:D:323:HOH:O	2.09	0.53
1:A:121:ILE:HG23	1:A:122:PRO:HD3	1.88	0.53
1:B:211:GLU:H	1:B:211:GLU:CD	2.10	0.53
1:A:52:ILE:HD12	1:A:243:LEU:HD23	1.91	0.53
1:D:105:ILE:N	1:D:105:ILE:HD12	2.24	0.53
1:A:152:ARG:NH1	1:A:175:LEU:HA	2.23	0.52
1:A:2:ARG:HG2	1:A:53:GLU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASN:N	1:A:87:ASN:OD1	2.43	0.52
1:B:66:GLY:N	1:B:89:HIS:ND1	2.57	0.52
1:C:6:THR:O	1:C:6:THR:CG2	2.56	0.52
1:A:6:THR:HG22	1:A:6:THR:O	2.08	0.52
1:B:20:ILE:HG21	1:D:20:ILE:HG22	1.92	0.52
1:A:117:LEU:C	1:A:119:GLU:N	2.62	0.52
1:A:65:ASN:O	1:A:69:ILE:HG13	2.10	0.52
1:B:65:ASN:HB2	1:B:89:HIS:CG	2.45	0.52
1:C:43:GLN:NE2	1:C:136:GLN:HE21	2.08	0.52
1:B:41:ALA:O	1:B:45:ILE:HG13	2.10	0.51
1:D:107:THR:HG22	1:D:108:THR:O	2.09	0.51
1:A:98:SER:O	1:A:99:ALA:C	2.49	0.51
1:B:271:LEU:HA	1:B:274:PHE:CD2	2.45	0.51
1:D:182:ASN:ND2	1:D:185:GLU:OE1	2.44	0.51
1:A:141:LEU:HD22	1:A:168:ASP:HB3	1.91	0.51
1:A:20:ILE:HD11	5:A:313:HOH:O	2.11	0.51
1:A:39:LYS:HE3	5:A:355:HOH:O	2.10	0.51
1:B:95:ILE:CG2	1:B:104:ALA:HB3	2.38	0.51
1:B:116:SER:HB2	1:B:119:GLU:OE2	2.10	0.51
1:C:6:THR:CG2	1:C:139:PHE:HE2	2.22	0.51
1:B:23:LYS:CD	1:D:101:GLY:HA3	2.39	0.51
1:D:2:ARG:NH1	5:D:304:HOH:O	2.42	0.51
1:B:124:MSE:HE2	1:B:156:MSE:SE	2.60	0.51
1:C:244:LEU:CD1	1:C:284:LEU:HD13	2.41	0.51
1:D:87:ASN:N	1:D:87:ASN:ND2	2.58	0.51
1:A:117:LEU:CD2	1:A:143:LYS:HD3	2.41	0.51
1:B:101:GLY:O	1:B:103:ASN:ND2	2.44	0.51
1:B:95:ILE:O	1:B:95:ILE:HG23	2.10	0.51
1:B:201:GLN:NE2	1:B:207:TRP:CD1	2.79	0.51
1:C:166:ASN:HB3	1:C:169:PHE:CD1	2.46	0.51
1:B:109:THR:HG22	1:D:28:HIS:CE1	2.44	0.51
1:A:117:LEU:HA	5:A:336:HOH:O	2.10	0.51
1:D:82:PRO:HD3	1:D:115:PHE:HZ	1.73	0.51
1:D:2:ARG:NH2	1:D:126:ASP:O	2.44	0.51
1:B:6:THR:OG1	1:B:135:GLN:HG2	2.10	0.50
1:D:87:ASN:ND2	5:D:318:HOH:O	2.44	0.50
1:D:173:TRP:CZ2	1:D:191:PRO:HG3	2.47	0.50
1:A:114:THR:O	1:A:114:THR:HG22	2.10	0.50
1:A:117:LEU:O	1:A:118:ASP:HB2	2.11	0.50
1:A:121:ILE:HB	5:A:336:HOH:O	2.10	0.50
1:C:79:MSE:CE	1:C:81:LEU:HD21	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:ALA:O	1:D:155:GLY:O	2.29	0.50
1:D:46:ILE:CD1	1:D:233:THR:HA	2.40	0.50
1:C:177:ASP:HA	1:C:195:LYS:HZ2	1.77	0.50
1:C:188:LEU:O	1:C:188:LEU:HD23	2.11	0.50
1:A:168:ASP:C	1:A:170:CYS:H	2.15	0.50
1:A:183:GLU:OE1	1:A:201:GLN:HG2	2.11	0.50
1:A:116:SER:C	1:A:117:LEU:O	2.49	0.50
1:C:32:VAL:O	1:C:32:VAL:HG22	2.12	0.50
1:D:180:VAL:HG21	1:D:235:LEU:CD2	2.41	0.50
1:A:108:THR:HG22	1:C:29:GLY:O	2.12	0.50
1:A:279:GLU:HG3	5:B:329:HOH:O	2.12	0.49
1:A:133:LEU:HD22	1:A:151:ALA:HB2	1.93	0.49
1:B:192:TYR:O	1:B:194:VAL:N	2.42	0.49
1:C:154:ARG:NH1	1:C:154:ARG:HG2	2.27	0.49
1:D:9:ILE:HG21	1:D:69:ILE:CG2	2.41	0.49
1:A:268:ARG:HG2	1:A:269:GLY:N	2.26	0.49
1:A:20:ILE:N	1:A:97:ASN:ND2	2.60	0.49
1:A:278:ARG:NH2	1:B:131:ASP:OD1	2.44	0.49
1:A:121:ILE:CG2	1:A:122:PRO:HD3	2.42	0.49
1:B:10:THR:HB	1:B:91:ASP:HA	1.94	0.49
1:B:11:VAL:CG1	1:B:91:ASP:HB3	2.43	0.49
1:B:135:GLN:HB2	1:B:148:PHE:CZ	2.47	0.49
1:D:267:ARG:HH11	1:D:267:ARG:HG2	1.78	0.49
1:B:245:ARG:O	1:B:247:VAL:HG13	2.13	0.49
1:C:63:ASP:HB3	1:C:66:GLY:H	1.77	0.49
1:D:177:ASP:HA	1:D:195:LYS:CD	2.39	0.49
1:D:52:ILE:HD12	1:D:52:ILE:N	2.28	0.49
1:C:87:ASN:HD22	1:C:87:ASN:N	2.09	0.49
1:A:210:GLN:O	1:A:213:GLN:HG2	2.12	0.48
1:D:178:ILE:HG12	1:D:196:THR:HB	1.94	0.48
1:A:10:THR:CG2	1:A:91:ASP:HA	2.24	0.48
1:D:98:SER:O	1:D:99:ALA:CB	2.61	0.48
1:B:13:GLU:OE2	1:B:31:LYS:HE3	2.13	0.48
1:C:225:LEU:HD22	1:C:225:LEU:H	1.77	0.48
1:C:79:MSE:HE2	1:C:81:LEU:HD11	1.96	0.48
1:D:36:ILE:N	1:D:36:ILE:HD12	2.28	0.48
1:D:71:GLN:NE2	1:D:72:GLN:NE2	2.60	0.48
1:A:20:ILE:N	1:A:97:ASN:HD21	2.10	0.48
1:B:141:LEU:HD22	1:B:168:ASP:HB3	1.95	0.48
1:D:141:LEU:CD1	1:D:172:LEU:HD11	2.42	0.48
1:D:182:ASN:H	1:D:182:ASN:ND2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LEU:H	1:B:225:LEU:HD23	1.76	0.48
1:D:9:ILE:HG12	1:D:41:ALA:HB2	1.96	0.48
1:B:267:ARG:HB2	1:B:273:ALA:HB1	1.95	0.48
1:D:50:CYS:SG	1:D:280:LEU:HD13	2.53	0.48
1:D:9:ILE:HD11	1:D:56:LEU:HD21	1.96	0.48
1:A:138:ASN:O	1:A:139:PHE:CD1	2.67	0.48
1:A:181:VAL:O	1:A:199:ILE:HA	2.14	0.48
1:D:183:GLU:OE1	1:D:201:GLN:HG2	2.14	0.48
1:A:117:LEU:HD22	1:A:143:LYS:HD3	1.96	0.48
1:A:121:ILE:HD11	1:A:150:TYR:CE2	2.49	0.48
1:B:226:ASP:OD2	1:B:269:GLY:N	2.44	0.48
1:A:10:THR:HG23	1:A:91:ASP:CA	2.23	0.47
1:A:117:LEU:CA	5:A:336:HOH:O	2.62	0.47
1:A:181:VAL:HG13	1:A:185:GLU:CB	2.29	0.47
1:B:46:ILE:HD13	1:B:233:THR:HA	1.96	0.47
1:B:6:THR:HG1	1:B:135:GLN:HG2	1.79	0.47
1:C:152:ARG:NH1	1:C:175:LEU:HD23	2.28	0.47
1:D:180:VAL:HG11	1:D:235:LEU:HD23	1.96	0.47
1:A:117:LEU:HD22	1:A:143:LYS:CD	2.45	0.47
1:A:187:GLU:O	1:A:188:LEU:O	2.32	0.47
1:C:105:ILE:HD12	1:C:106:ILE:N	2.29	0.47
1:C:121:ILE:HG12	1:C:122:PRO:HD3	1.95	0.47
1:D:36:ILE:HD11	1:D:68:TRP:CE2	2.49	0.47
1:A:65:ASN:HB2	1:A:89:HIS:CE1	2.47	0.47
1:B:225:LEU:HD12	1:B:268:ARG:NH2	2.29	0.47
1:A:33:SER:CB	1:A:268:ARG:NH2	2.78	0.47
1:A:11:VAL:O	1:A:91:ASP:HB2	2.14	0.47
1:B:22:LYS:NZ	1:B:22:LYS:CB	2.78	0.47
1:D:65:ASN:O	1:D:69:ILE:HG13	2.15	0.47
1:D:8:ASN:N	1:D:8:ASN:HD22	2.08	0.47
1:B:43:GLN:HE22	1:B:161:ASN:HD22	1.62	0.47
1:D:115:PHE:CB	1:D:120:MSE:HE3	2.42	0.47
1:B:94:ILE:CD1	1:B:94:ILE:N	2.76	0.47
1:C:152:ARG:NH2	1:C:174:PRO:O	2.47	0.47
1:D:165:VAL:HG22	1:D:166:ASN:N	2.30	0.47
1:A:204:ALA:O	1:A:216:PHE:HZ	1.98	0.47
1:A:65:ASN:HB3	1:A:89:HIS:HE1	1.77	0.47
1:B:213:GLN:HB2	5:B:307:HOH:O	2.14	0.47
1:D:175:LEU:N	1:D:175:LEU:HD22	2.30	0.47
1:B:20:ILE:CG2	1:D:20:ILE:CG2	2.93	0.46
1:B:238:MSE:HE3	1:B:249:PRO:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:HD3	1:A:79:MSE:HE2	1.97	0.46
1:D:134:LEU:HD13	1:D:159:VAL:HG13	1.98	0.46
1:B:63:ASP:N	1:B:89:HIS:CE1	2.68	0.46
1:C:135:GLN:HE22	1:C:144:THR:HA	1.79	0.46
1:D:119:GLU:HG2	5:D:305:HOH:O	2.16	0.46
1:D:183:GLU:H	1:D:183:GLU:HG2	1.55	0.46
1:D:9:ILE:HD11	1:D:56:LEU:CD2	2.45	0.46
1:A:188:LEU:HG	1:A:188:LEU:O	2.14	0.46
1:B:11:VAL:HG12	1:B:91:ASP:HB3	1.97	0.46
1:D:215:GLN:OE1	1:D:251:ALA:HB2	2.14	0.46
1:B:22:LYS:O	1:B:23:LYS:O	2.34	0.46
1:B:87:ASN:OD1	1:B:88:GLN:N	2.38	0.46
1:C:6:THR:HG23	1:C:139:PHE:CE2	2.39	0.46
1:D:267:ARG:HG2	1:D:267:ARG:NH1	2.31	0.46
1:C:-1:LEU:HD12	1:C:2:ARG:H	1.76	0.46
1:C:94:ILE:HG22	1:C:96:LEU:HD22	1.97	0.46
1:D:182:ASN:ND2	1:D:185:GLU:CD	2.69	0.46
1:D:226:ASP:HB3	1:D:267:ARG:O	2.15	0.46
1:B:70:ARG:CD	1:B:85:HIS:CE1	2.97	0.46
1:B:82:PRO:HG3	1:B:86:PHE:CZ	2.50	0.46
1:C:121:ILE:N	1:C:122:PRO:CD	2.79	0.46
1:D:150:TYR:OH	1:D:154:ARG:NH1	2.49	0.46
1:B:15:TRP:CZ2	1:D:94:ILE:HD11	2.52	0.45
1:D:219:ALA:O	1:D:221:PRO:HD3	2.16	0.45
1:D:2:ARG:HG2	1:D:2:ARG:NH1	2.31	0.45
1:D:90:SER:O	1:D:92:THR:HG23	2.17	0.45
1:A:121:ILE:HD11	1:A:150:TYR:CG	2.51	0.45
1:C:152:ARG:HH11	1:C:175:LEU:HD23	1.82	0.45
1:D:163:SER:HB2	1:D:185:GLU:OE2	2.17	0.45
1:D:281:ALA:O	1:D:285:THR:HG23	2.16	0.45
1:A:121:ILE:HG23	1:A:122:PRO:CD	2.46	0.45
1:A:124:MSE:HE1	1:A:147:LEU:HD12	1.99	0.45
1:A:160:PHE:CD2	1:A:176:ILE:HD13	2.52	0.45
1:D:145:ARG:HB2	1:D:145:ARG:HH11	1.77	0.45
1:D:271:LEU:HA	1:D:274:PHE:CD2	2.52	0.45
1:A:194:VAL:HG12	1:A:196:THR:H	1.82	0.45
1:A:132:ILE:HD11	1:A:243:LEU:HD11	1.98	0.45
1:C:237:VAL:HG21	1:C:260:ALA:CB	2.47	0.45
1:C:267:ARG:HB2	1:C:273:ALA:HB1	1.97	0.45
1:A:150:TYR:O	1:A:153:SER:HB3	2.17	0.45
1:A:212:GLY:N	5:A:320:HOH:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:MSE:HE3	1:B:156:MSE:CE	2.43	0.45
1:B:39:LYS:CE	1:B:232:ASP:OD1	2.61	0.45
1:C:152:ARG:NH2	5:C:357:HOH:O	2.31	0.45
1:A:232:ASP:HB3	5:A:355:HOH:O	2.17	0.45
1:A:23:LYS:NZ	1:C:100:ASP:CB	2.79	0.45
1:B:23:LYS:HZ2	1:D:101:GLY:HA3	1.79	0.45
1:D:276:GLY:O	1:D:277:SER:C	2.55	0.45
1:D:71:GLN:HE22	1:D:72:GLN:HE21	1.60	0.45
1:A:209:VAL:CG1	1:A:210:GLN:N	2.80	0.44
1:A:43:GLN:OE1	1:A:134:LEU:HD21	2.18	0.44
1:C:56:LEU:HD23	1:C:80:LEU:HD13	2.00	0.44
1:B:109:THR:OG1	1:B:113:ASP:CG	2.56	0.44
1:C:63:ASP:OD1	1:C:89:HIS:HA	2.17	0.44
1:D:152:ARG:HG2	1:D:152:ARG:NH1	2.33	0.44
1:D:11:VAL:CG2	1:D:65:ASN:HB3	2.42	0.44
1:A:282:ALA:HB3	5:A:311:HOH:O	2.16	0.44
1:B:211:GLU:N	5:B:307:HOH:O	2.51	0.44
1:C:166:ASN:HB3	1:C:169:PHE:CE1	2.52	0.44
1:D:197:LEU:HB3	1:D:209:VAL:HB	1.99	0.44
1:D:221:PRO:O	1:D:222:ALA:HB2	2.17	0.44
1:D:43:GLN:HG3	1:D:232:ASP:HB3	1.99	0.44
1:B:86:PHE:HB2	1:B:87:ASN:H	1.49	0.44
1:D:152:ARG:HE	1:D:175:LEU:HA	1.83	0.44
1:A:224:ALA:CB	1:A:265:VAL:CG1	2.96	0.44
1:B:128:VAL:HG12	1:B:129:ALA:O	2.17	0.44
1:B:11:VAL:HG11	1:B:65:ASN:OD1	2.18	0.44
1:C:132:ILE:HG12	1:C:157:THR:HB	2.00	0.44
1:D:76:GLU:C	1:D:78:LEU:H	2.20	0.44
1:D:145:ARG:HH11	1:D:145:ARG:CG	2.29	0.44
1:D:98:SER:O	1:D:99:ALA:HB2	2.17	0.44
1:A:141:LEU:O	1:A:141:LEU:HD12	2.18	0.44
1:B:247:VAL:O	1:B:248:ALA:CB	2.61	0.44
1:B:55:ARG:HB2	1:B:55:ARG:HE	1.61	0.44
1:A:121:ILE:HD11	1:A:150:TYR:CD2	2.53	0.44
1:B:-1:LEU:HD23	1:B:-1:LEU:C	2.38	0.44
1:B:237:VAL:HG21	1:B:260:ALA:CB	2.48	0.44
1:C:145:ARG:O	1:C:149:GLN:HG3	2.18	0.44
1:A:43:GLN:CG	1:A:232:ASP:HB2	2.47	0.43
1:C:135:GLN:HB2	1:C:148:PHE:CZ	2.53	0.43
1:A:106:ILE:CD1	1:C:21:PRO:HG2	2.48	0.43
1:D:154:ARG:HB3	1:D:154:ARG:HE	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ASN:HD21	1:D:185:GLU:CD	2.21	0.43
1:D:237:VAL:HG21	1:D:260:ALA:HB1	1.99	0.43
1:C:31:LYS:NZ	1:C:31:LYS:HB2	2.33	0.43
1:A:194:VAL:O	1:A:210:GLN:CG	2.63	0.43
1:B:10:THR:HG22	1:B:90:SER:HB2	2.00	0.43
1:C:13:GLU:OE2	1:C:31:LYS:HD3	2.18	0.43
1:A:63:ASP:OD1	1:A:89:HIS:NE2	2.52	0.43
1:D:145:ARG:HH11	1:D:145:ARG:HB3	1.82	0.43
1:D:208:LEU:HB2	1:D:254:LEU:CD2	2.49	0.43
1:D:61:GLY:C	1:D:63:ASP:H	2.22	0.43
1:C:173:TRP:N	1:C:174:PRO:HD2	2.34	0.43
1:C:197:LEU:HB3	1:C:209:VAL:HB	2.01	0.43
1:C:225:LEU:HD23	1:C:225:LEU:H	1.82	0.43
1:C:248:ALA:O	1:C:249:PRO:C	2.55	0.43
1:C:17:ILE:HD13	1:C:96:LEU:HD12	2.00	0.43
1:A:109:THR:O	1:A:110:ALA:HB3	2.18	0.43
1:A:21:PRO:HD3	1:A:27:ILE:HD11	2.00	0.43
1:B:11:VAL:O	1:B:11:VAL:HG13	2.19	0.43
1:B:23:LYS:HZ3	1:D:101:GLY:HA3	1.84	0.43
1:C:115:PHE:CB	1:C:120:MSE:HE3	2.49	0.43
1:D:18:PRO:HA	1:D:99:ALA:HB2	2.01	0.43
1:B:225:LEU:HD21	1:B:266:SER:C	2.38	0.43
1:D:94:ILE:HG22	1:D:96:LEU:HD22	2.00	0.43
1:A:187:GLU:O	1:A:188:LEU:CG	2.67	0.42
1:D:198:VAL:HG21	1:D:238:MSE:SE	2.69	0.42
1:C:259:ARG:HB3	1:C:283:LEU:HD11	2.00	0.42
1:A:106:ILE:N	1:A:106:ILE:HD12	2.34	0.42
1:A:259:ARG:HD2	1:A:283:LEU:HB2	2.01	0.42
1:B:116:SER:O	1:B:120:MSE:HG3	2.19	0.42
1:C:141:LEU:HD11	1:C:172:LEU:HD13	2.00	0.42
1:C:230:ALA:HB2	1:C:265:VAL:CG1	2.49	0.42
1:C:8:ASN:N	1:C:8:ASN:HD22	2.14	0.42
1:A:267:ARG:HD2	1:A:273:ALA:O	2.20	0.42
1:B:49:ARG:HD3	1:B:76:GLU:OE1	2.19	0.42
1:D:105:ILE:CG2	1:D:106:ILE:N	2.83	0.42
1:A:109:THR:O	1:A:111:ALA:N	2.47	0.42
1:A:185:GLU:O	1:A:189:LEU:HB2	2.19	0.42
1:B:22:LYS:HB2	1:B:22:LYS:HZ2	1.83	0.42
1:D:135:GLN:HE22	1:D:147:LEU:CD1	2.33	0.42
1:D:46:ILE:HD12	1:D:233:THR:HA	2.00	0.42
1:A:12:ASP:OD1	1:A:92:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LEU:HD12	1:A:188:LEU:C	2.40	0.42
1:A:209:VAL:HG12	1:A:210:GLN:N	2.33	0.42
1:A:12:ASP:HB3	1:A:94:ILE:HD11	2.02	0.42
1:B:43:GLN:O	1:B:47:LEU:HB2	2.20	0.42
1:D:63:ASP:OD1	1:D:64:SER:N	2.49	0.42
1:A:235:LEU:C	1:A:235:LEU:HD23	2.40	0.42
1:B:198:VAL:HG21	1:B:238:MSE:SE	2.70	0.42
1:B:50:CYS:SG	1:B:280:LEU:HG	2.59	0.42
1:D:48:SER:OG	1:D:77:PRO:HG2	2.19	0.42
1:B:28:HIS:NE2	1:D:164:PRO:CG	2.82	0.42
1:B:20:ILE:HG21	1:D:20:ILE:CG2	2.48	0.42
1:C:107:THR:HG22	1:C:108:THR:O	2.20	0.42
1:D:121:ILE:N	1:D:122:PRO:HD2	2.34	0.42
1:D:35:ASP:OD1	1:D:36:ILE:N	2.51	0.42
1:B:20:ILE:HG13	1:B:20:ILE:H	1.58	0.41
1:B:228:THR:CG2	1:B:270:THR:HG22	2.40	0.41
1:D:9:ILE:HD13	1:D:73:ILE:CD1	2.50	0.41
1:A:121:ILE:CG2	1:A:122:PRO:CD	2.97	0.41
1:B:213:GLN:N	5:B:307:HOH:O	2.43	0.41
1:B:45:ILE:O	1:B:49:ARG:HG3	2.20	0.41
1:C:79:MSE:HE2	1:C:81:LEU:CD2	2.41	0.41
1:C:87:ASN:O	1:C:87:ASN:ND2	2.53	0.41
1:D:95:ILE:CG2	1:D:103:ASN:HD22	2.33	0.41
1:B:12:ASP:OD2	1:B:92:THR:CG2	2.68	0.41
1:D:182:ASN:N	1:D:182:ASN:HD22	2.18	0.41
1:A:121:ILE:HA	1:A:124:MSE:HE3	2.02	0.41
1:A:150:TYR:CZ	1:A:154:ARG:HD2	2.56	0.41
1:A:96:LEU:HD12	1:A:97:ASN:N	2.35	0.41
1:B:210:GLN:C	5:B:307:HOH:O	2.58	0.41
1:C:225:LEU:HD23	1:C:226:ASP:N	2.36	0.41
1:D:43:GLN:HE21	1:D:134:LEU:HD21	1.86	0.41
1:D:235:LEU:HD13	1:D:235:LEU:C	2.41	0.41
1:D:85:HIS:CD2	1:D:85:HIS:H	2.38	0.41
1:A:96:LEU:HA	1:A:103:ASN:OD1	2.21	0.41
1:C:235:LEU:C	1:C:235:LEU:HD12	2.41	0.41
1:B:133:LEU:HD22	1:B:151:ALA:HB2	2.02	0.41
1:B:55:ARG:HG2	1:B:81:LEU:HD12	2.02	0.41
1:C:245:ARG:HH22	1:C:250:ASP:CG	2.24	0.41
1:D:263:ILE:O	1:D:267:ARG:HD3	2.21	0.41
1:B:235:LEU:C	1:B:235:LEU:HD12	2.41	0.41
1:B:238:MSE:HG3	1:B:254:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-1:LEU:HD23	1:B:2:ARG:N	2.36	0.41
1:B:73:ILE:HG13	1:B:80:LEU:HD22	2.03	0.41
1:C:169:PHE:O	1:C:172:LEU:HB2	2.21	0.41
1:A:183:GLU:H	1:A:183:GLU:HG2	1.52	0.41
1:A:222:ALA:O	1:A:223:GLU:CG	2.69	0.41
1:A:90:SER:O	1:A:91:ASP:HB3	2.21	0.41
1:D:180:VAL:HG21	1:D:235:LEU:HD22	2.02	0.41
1:A:6:THR:HG21	1:A:147:LEU:HG	2.02	0.40
1:A:207:TRP:CZ3	1:A:216:PHE:HB2	2.57	0.40
1:B:210:GLN:HB2	1:B:211:GLU:OE1	2.21	0.40
1:D:135:GLN:HG3	5:D:300:HOH:O	2.20	0.40
1:C:150:TYR:OH	1:C:154:ARG:HD2	2.21	0.40
1:A:212:GLY:CA	5:A:320:HOH:O	2.69	0.40
1:A:283:LEU:HD12	1:A:284:LEU:N	2.36	0.40
1:B:12:ASP:OD2	1:B:92:THR:HG22	2.22	0.40
1:C:21:PRO:HG3	1:C:27:ILE:HG12	2.03	0.40
1:C:61:GLY:C	1:C:63:ASP:H	2.24	0.40
1:D:129:ALA:O	1:D:155:GLY:C	2.60	0.40
1:D:276:GLY:C	1:D:278:ARG:N	2.70	0.40
1:A:173:TRP:CE3	1:A:173:TRP:HA	2.56	0.40
1:C:201:GLN:HB2	1:C:201:GLN:HE21	1.65	0.40
1:A:96:LEU:HD12	1:A:96:LEU:C	2.41	0.40
1:B:76:GLU:C	1:B:78:LEU:H	2.25	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	283/299 (95%)	247 (87%)	27 (10%)	9 (3%)	4	0
1	B	276/299 (92%)	252 (91%)	19 (7%)	5 (2%)	8	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	283/299 (95%)	268 (95%)	12 (4%)	3 (1%)	14	8
1	D	283/299 (95%)	253 (89%)	18 (6%)	12 (4%)	3	0
All	All	1125/1196 (94%)	1020 (91%)	76 (7%)	29 (3%)	5	1

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY
1	A	210	GLN
1	A	222	ALA
1	A	223	GLU
1	B	23	LYS
1	B	110	ALA
1	D	98	SER
1	D	99	ALA
1	D	100	ASP
1	A	88	GLN
1	A	189	LEU
1	B	193	GLY
1	C	101	GLY
1	D	246	GLY
1	C	100	ASP
1	D	129	ALA
1	D	222	ALA
1	D	278	ARG
1	A	139	PHE
1	A	162	PRO
1	A	188	LEU
1	D	87	ASN
1	D	89	HIS
1	B	211	GLU
1	C	162	PRO
1	D	153	SER
1	B	249	PRO
1	D	247	VAL
1	D	18	PRO

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	223/228 (98%)	203 (91%)	20 (9%)	9	5
1	B	220/228 (96%)	199 (90%)	21 (10%)	8	4
1	C	223/228 (98%)	204 (92%)	19 (8%)	10	6
1	D	223/228 (98%)	201 (90%)	22 (10%)	8	4
All	All	889/912 (98%)	807 (91%)	82 (9%)	9	5

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	8	ASN
1	A	35	ASP
1	A	71	GLN
1	A	74	LYS
1	A	83	ASP
1	A	87	ASN
1	A	88	GLN
1	A	119	GLU
1	A	126	ASP
1	A	138	ASN
1	A	147	LEU
1	A	170	CYS
1	A	183	GLU
1	A	188	LEU
1	A	189	LEU
1	A	210	GLN
1	A	232	ASP
1	A	243	LEU
1	A	283	LEU
1	B	8	ASN
1	B	35	ASP
1	B	55	ARG
1	B	62	ASN
1	B	71	GLN
1	B	89	HIS
1	B	96	LEU
1	B	108	THR

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Mol	Chain	Res	Type
1	B	109	THR
1	B	115	PHE
1	B	152	ARG
1	B	189	LEU
1	B	210	GLN
1	B	211	GLU
1	B	225	LEU
1	B	227	THR
1	B	235	LEU
1	B	243	LEU
1	B	280	LEU
1	B	283	LEU
1	B	285	THR
1	C	-1	LEU
1	C	6	THR
1	C	8	ASN
1	C	47	LEU
1	C	63	ASP
1	C	72	GLN
1	C	87	ASN
1	C	100	ASP
1	C	102	ASP
1	C	105	ILE
1	C	115	PHE
1	C	121	ILE
1	C	142	ASP
1	C	172	LEU
1	C	183	GLU
1	C	213	GLN
1	C	225	LEU
1	C	227	THR
1	C	243	LEU
1	D	-1	LEU
1	D	8	ASN
1	D	34	GLN
1	D	47	LEU
1	D	85	HIS
1	D	87	ASN
1	D	89	HIS
1	D	90	SER
1	D	98	SER
1	D	102	ASP

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Mol	Chain	Res	Type
1	D	108	THR
1	D	115	PHE
1	D	142	ASP
1	D	145	ARG
1	D	182	ASN
1	D	184	SER
1	D	195	LYS
1	D	223	GLU
1	D	227	THR
1	D	243	LEU
1	D	267	ARG
1	D	283	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	71	GLN
1	A	85	HIS
1	A	97	ASN
1	A	135	GLN
1	A	161	ASN
1	A	215	GLN
1	A	256	HIS
1	B	8	ASN
1	B	62	ASN
1	B	71	GLN
1	B	72	GLN
1	B	88	GLN
1	B	89	HIS
1	B	135	GLN
1	B	161	ASN
1	B	171	HIS
1	B	201	GLN
1	B	210	GLN
1	B	256	HIS
1	C	8	ASN
1	C	43	GLN
1	C	72	GLN
1	C	85	HIS
1	C	87	ASN
1	C	88	GLN

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Mol	Chain	Res	Type
1	C	135	GLN
1	C	138	ASN
1	C	161	ASN
1	C	166	ASN
1	C	201	GLN
1	D	8	ASN
1	D	28	HIS
1	D	34	GLN
1	D	43	GLN
1	D	71	GLN
1	D	87	ASN
1	D	88	GLN
1	D	103	ASN
1	D	135	GLN
1	D	138	ASN
1	D	161	ASN
1	D	171	HIS
1	D	182	ASN
1	D	210	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	SO4	C	1	-	4,4,4	0.23	0	6,6,6	0.13	0
4	RIB	D	311	-	10,10,10	1.31	2 (20%)	13,14,14	1.52	3 (23%)
3	GOL	C	501	-	5,5,5	0.29	0	5,5,5	0.36	0
2	SO4	D	298	-	4,4,4	0.29	0	6,6,6	0.13	0
2	SO4	B	298	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	C	298	-	4,4,4	0.23	0	6,6,6	0.14	0
2	SO4	B	300	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	B	299	-	4,4,4	0.28	0	6,6,6	0.06	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
4	RIB	D	311	-	-	0/2/18/18	0/1/1/1
3	GOL	C	501	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	311	RIB	O1-C1	2.38	1.47	1.39
4	D	311	RIB	O4-C1	2.22	1.45	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	311	RIB	C1-C2-C3	3.07	106.14	102.30
4	D	311	RIB	O4-C4-C3	2.67	110.39	105.11
4	D	311	RIB	O4-C1-C2	2.19	107.16	104.46

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 ⓘ

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(Å²)	Q<0.9
1	A	280/299 (93%)	0.38	13 (4%)	32	42	25, 39, 57, 71	0
1	B	277/299 (92%)	0.29	13 (4%)	31	41	26, 39, 61, 83	0
1	C	280/299 (93%)	0.25	7 (2%)	57	65	27, 38, 52, 62	0
1	D	280/299 (93%)	0.49	18 (6%)	19	26	27, 43, 64, 80	0
All	All	1117/1196 (93%)	0.35	51 (4%)	32	42	25, 39, 60, 83	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	ALA	6.0
1	D	221	PRO	5.6
1	D	222	ALA	4.9
1	B	99	ALA	4.6
1	C	100	ASP	4.6
1	D	100	ASP	4.6
1	D	220	VAL	4.3
1	A	100	ASP	4.1
1	A	118	ASP	3.9
1	B	100	ASP	3.9
1	A	210	GLN	3.3
1	B	104	ALA	3.2
1	D	99	ALA	3.0
1	D	87	ASN	3.0
1	B	101	GLY	2.9
1	C	235	LEU	2.9
1	A	98	SER	2.7
1	D	21	PRO	2.7
1	B	87	ASN	2.6
1	A	102	ASP	2.6
1	C	152	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	223	GLU	2.5
1	D	23	LYS	2.5
1	A	126	ASP	2.4
1	C	171	HIS	2.4
1	B	283	LEU	2.4
1	D	224	ALA	2.4
1	B	212	GLY	2.4
1	C	211	GLU	2.4
1	A	89	HIS	2.4
1	B	22	LYS	2.3
1	A	40	GLY	2.3
1	A	224	ALA	2.3
1	D	268	ARG	2.3
1	A	221	PRO	2.2
1	B	246	GLY	2.2
1	B	171	HIS	2.2
1	A	41	ALA	2.2
1	B	64	SER	2.2
1	D	22	LYS	2.1
1	D	25	ALA	2.1
1	D	101	GLY	2.1
1	B	225	LEU	2.1
1	C	231	GLY	2.1
1	D	98	SER	2.1
1	A	222	ALA	2.1
1	D	119	GLU	2.1
1	D	225	LEU	2.0
1	D	32	VAL	2.0
1	B	133	LEU	2.0
1	C	268	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	RIB	D	311	10/10	0.81	0.23	53,55,58,59	0
3	GOL	C	501	6/6	0.89	0.28	41,43,44,48	0
2	SO4	B	299	5/5	0.90	0.15	82,83,83,84	0
2	SO4	B	300	5/5	0.91	0.20	89,90,90,91	0
2	SO4	C	1	5/5	0.92	0.23	74,74,76,77	0
2	SO4	D	298	5/5	0.95	0.14	62,62,64,64	0
2	SO4	B	298	5/5	0.95	0.16	72,72,73,74	0
2	SO4	C	298	5/5	0.97	0.20	42,45,46,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.