Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:40 am BST

PDB ID	:	1UMF
Title	:	crystal structure of chorismate synthase
Authors	:	Ahn, H.J.; Yoon, H.J.; Lee, B.; Suh, S.W.
Deposited on	:	2003-09-30
Resolution	:	2.25 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 following versions of software and data (see references ⓘ) were used in the production of this report:

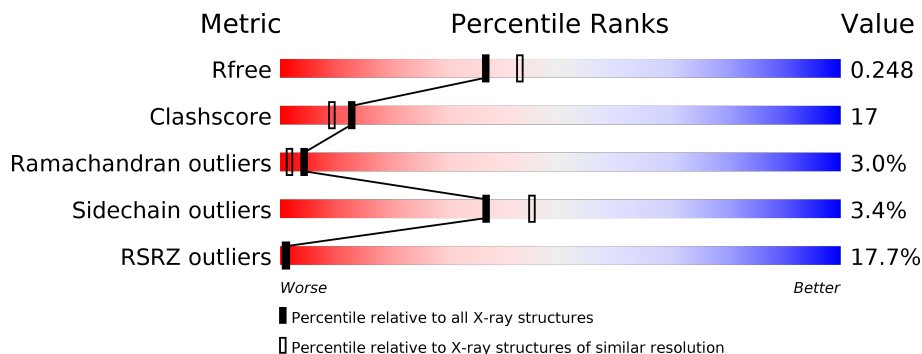|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.25 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		0.248
Clashscore		17
Ramachandran outliers		3.0%
Sidechain outliers		3.4%
RSRZ outliers		17.7%

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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 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	365	13% — 76% — 21% •
1	B	365	22% — 70% — 27% •
1	C	365	23% — 67% — 29% •
1	D	365	13% — 69% — 27% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11756 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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total 2816	C 1768	N 502	O 532	S 14	36	0	0
1	B	365	Total 2816	C 1768	N 502	O 532	S 14	36	0	0
1	C	365	Total 2816	C 1768	N 502	O 532	S 14	36	0	0
1	D	365	Total 2816	C 1768	N 502	O 532	S 14	36	0	0

- Molecule 2 is water.

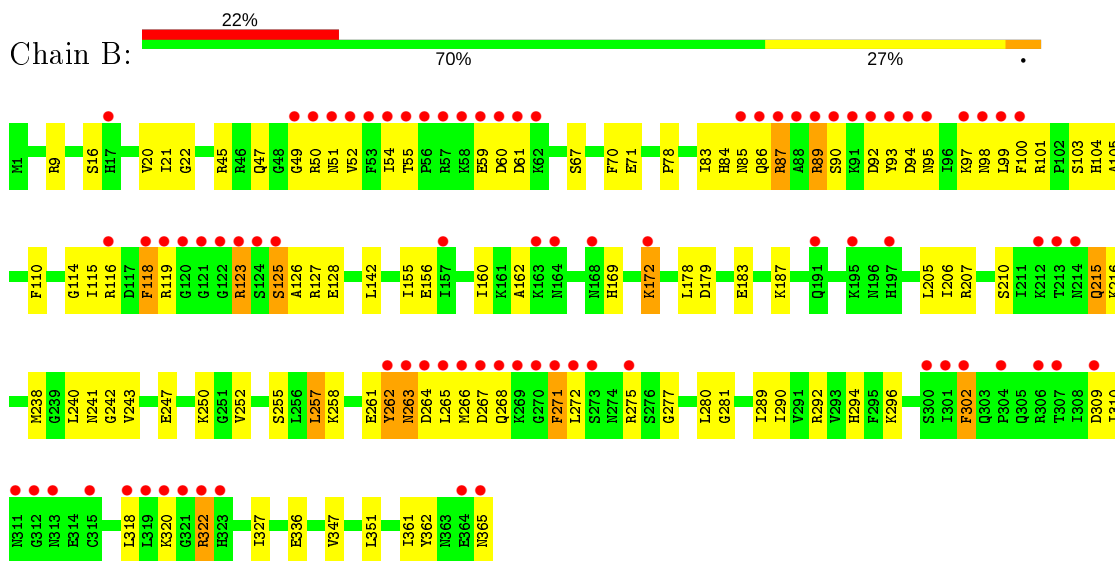| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	173	Total 173	O 173	0	0
2	B	82	Total 82	O 82	0	0
2	C	90	Total 90	O 90	0	0
2	D	147	Total 147	O 147	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
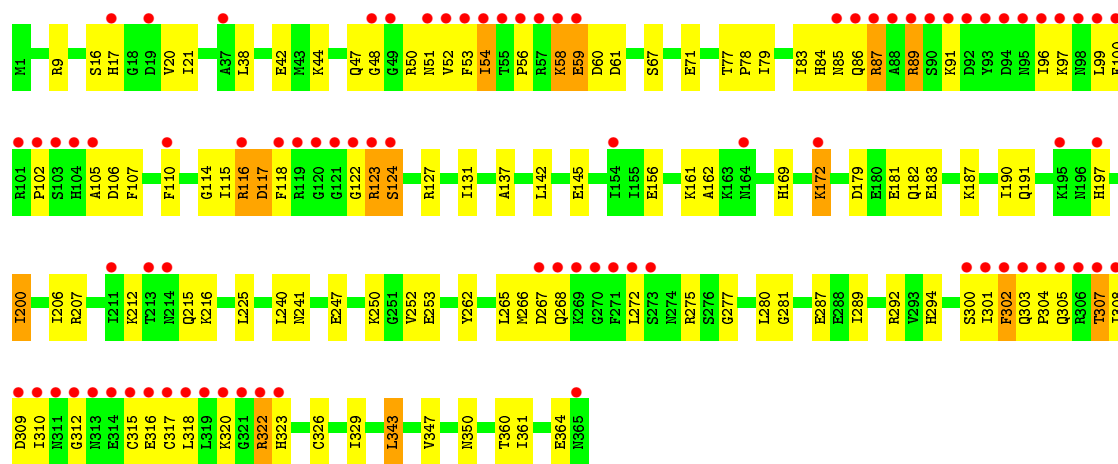
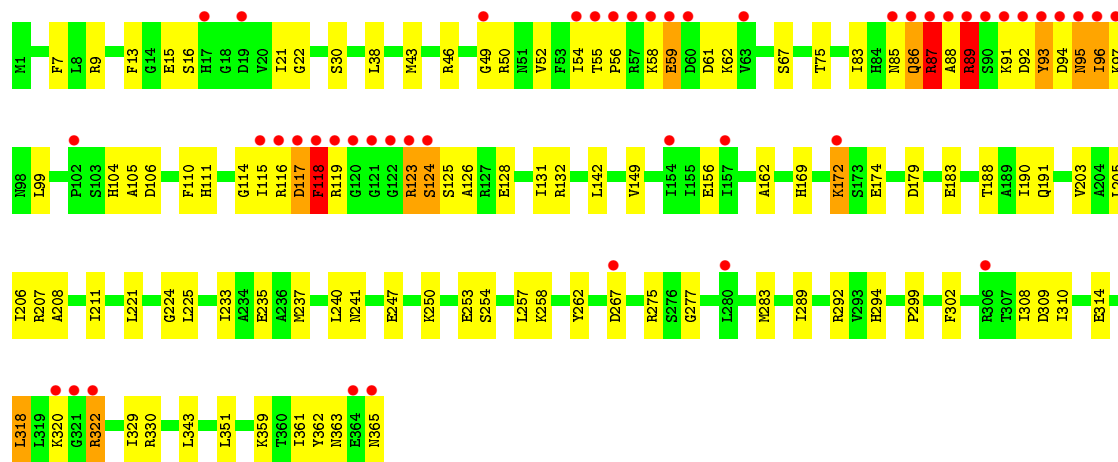- Molecule 1: Chorismate synthase

- Molecule 1: Chorismate synthase

- Molecule 1: Chorismate synthase

• Molecule 1: Chorismate synthase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	146.48Å 146.48Å 132.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.13 – 2.25 21.13 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.5 (21.13-2.25) 98.7 (21.13-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.51 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.248 0.202 , 0.248	Depositor DCC
R_{free} test set	6567 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 63.3	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.34$	Xtriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11756	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.37	0/2857	0.64	3/3833 (0.1%)
1	B	0.33	0/2857	0.60	2/3833 (0.1%)
1	C	0.33	0/2857	0.59	2/3833 (0.1%)
1	D	0.34	0/2857	0.62	2/3833 (0.1%)
All	All	0.34	0/11428	0.61	9/15332 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	89	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	C	87	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	D	89	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	A	89	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	A	87	ARG	NE-CZ-NH2	7.29	123.95	120.30
1	B	89	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	B	87	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	D	87	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	8	LEU	N-CA-C	-5.36	96.52	111.00

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	2816	0	2852	80	0
1	B	2816	0	2852	99	1
1	C	2816	0	2852	123	6
1	D	2816	0	2852	106	5
2	A	173	0	0	6	0
2	B	82	0	0	4	0
2	C	90	0	0	1	0
2	D	147	0	0	5	0
All	All	11756	0	11408	372	7

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 17.

All (372) 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:197:HIS:HB3	1:C:302:PHE:HB3	1.40	0.99
1:C:307:THR:HG23	1:C:308:ILE:H	1.34	0.92
1:B:47:GLN:HE22	1:B:60:ASP:HB3	1.35	0.89
1:C:102:PRO:HG2	1:C:305:GLN:HB3	1.56	0.88
1:A:322:ARG:HH11	1:A:322:ARG:H	1.21	0.86
1:A:318:LEU:HD12	1:A:320:LYS:HE3	1.55	0.85
1:D:322:ARG:HB2	1:D:322:ARG:HH11	1.40	0.84
1:D:104:HIS:HB3	1:D:123:ARG:NH2	1.93	0.82
1:D:105:ALA:N	1:D:123:ARG:HH22	1.77	0.82
1:B:238:MET:HE3	1:B:243:VAL:O	1.80	0.81
1:A:128:GLU:HG3	1:D:225:LEU:HD13	1.62	0.81
1:D:322:ARG:HB2	1:D:322:ARG:NH1	1.95	0.81
1:D:105:ALA:H	1:D:123:ARG:HH12	1.29	0.80
1:B:281:GLY:HA3	1:C:105:ALA:HB2	1.64	0.80
1:B:105:ALA:HB3	1:B:123:ARG:HH22	1.49	0.78
1:D:105:ALA:H	1:D:123:ARG:NH1	1.82	0.77
1:D:115:ILE:HD12	1:D:115:ILE:O	1.84	0.77
1:B:250:LYS:HE2	1:B:257:LEU:HD21	1.66	0.76
1:B:67:SER:HB3	1:D:16:SER:HB3	1.66	0.76
1:C:305:GLN:HB2	1:C:317:CYS:SG	2.25	0.76
1:B:54:ILE:HB	1:B:59:GLU:HG3	1.69	0.75
1:D:21:ILE:HG13	1:D:131:ILE:HD11	1.68	0.75
1:D:123:ARG:HG2	1:D:124:SER:N	2.00	0.74
1:D:169:HIS:CD2	1:D:172:LYS:HE3	2.22	0.74
1:C:322:ARG:H	1:C:322:ARG:HD3	1.53	0.73
1:A:361:ILE:HD11	1:B:361:ILE:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HD2	2:A:491:HOH:O	1.88	0.73
1:C:47:GLN:HE22	1:C:60:ASP:HB2	1.53	0.73
1:B:302:PHE:HE2	1:B:318:LEU:HD11	1.55	0.72
1:B:318:LEU:HD12	1:B:320:LYS:HE3	1.70	0.72
1:C:48:GLY:HA2	1:C:52:VAL:HG21	1.69	0.72
1:C:117:ASP:CG	1:C:118:PHE:H	1.93	0.72
1:D:50:ARG:HD3	1:D:52:VAL:O	1.91	0.71
1:B:169:HIS:HA	1:B:172:LYS:HE3	1.72	0.71
1:A:322:ARG:HB2	1:A:322:ARG:NH1	2.08	0.69
1:D:104:HIS:HB3	1:D:123:ARG:HH22	1.55	0.69
1:D:116:ARG:H	1:D:116:ARG:HD2	1.56	0.69
1:D:247:GLU:OE1	1:D:294:HIS:HE1	1.76	0.69
1:B:320:LYS:H	1:B:320:LYS:HD2	1.58	0.68
1:A:75:THR:HA	1:C:115:ILE:HD12	1.73	0.68
1:A:21:ILE:HG13	1:A:131:ILE:HD11	1.76	0.68
1:B:262:TYR:HD1	1:B:263:ASN:N	1.92	0.68
1:A:302:PHE:HE2	1:A:318:LEU:HD11	1.56	0.68
1:D:97:LYS:HA	2:D:463:HOH:O	1.93	0.68
1:C:197:HIS:CB	1:C:302:PHE:HB3	2.22	0.67
1:C:320:LYS:HD2	1:C:320:LYS:H	1.58	0.67
1:A:262:TYR:O	1:A:275:ARG:HD3	1.94	0.67
1:A:361:ILE:HD12	1:B:351:LEU:HD22	1.76	0.67
1:C:247:GLU:HB2	1:C:292:ARG:HB2	1.76	0.67
1:C:97:LYS:NZ	1:C:97:LYS:HB2	2.09	0.67
1:C:247:GLU:OE2	1:C:252:VAL:HG22	1.95	0.67
1:C:322:ARG:HB2	1:C:322:ARG:NH1	2.11	0.66
1:D:105:ALA:N	1:D:123:ARG:NH2	2.44	0.66
1:D:116:ARG:HE	1:D:310:ILE:HD12	1.60	0.66
1:B:247:GLU:OE2	1:B:252:VAL:HG22	1.96	0.66
1:A:97:LYS:NZ	1:A:97:LYS:HB2	2.10	0.65
1:D:99:LEU:HA	1:D:309:ASP:HA	1.77	0.65
1:B:169:HIS:HE1	1:B:183:GLU:OE2	1.79	0.65
1:C:197:HIS:HB2	1:C:303:GLN:HG3	1.78	0.65
1:D:85:ASN:ND2	1:D:86:GLN:HG3	2.12	0.65
1:B:101:ARG:HH11	1:B:101:ARG:HG3	1.62	0.64
1:C:322:ARG:HD3	1:C:322:ARG:N	2.11	0.64
1:C:361:ILE:HD12	1:D:351:LEU:HD22	1.80	0.64
1:C:21:ILE:HG13	1:C:131:ILE:HD11	1.80	0.64
1:D:162:ALA:HB1	1:D:179:ASP:HB2	1.79	0.64
1:B:128:GLU:HG3	1:C:225:LEU:HD13	1.81	0.63
1:B:206:ILE:HD12	1:B:206:ILE:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HOH:O	1:D:258:LYS:HE3	1.99	0.62
1:C:322:ARG:H	1:C:322:ARG:HH11	1.48	0.62
1:D:206:ILE:HD12	1:D:206:ILE:N	2.14	0.62
1:C:212:LYS:HD3	1:C:215:GLN:HG2	1.82	0.62
1:C:100:PHE:CE2	1:C:310:ILE:HA	2.34	0.61
1:C:308:ILE:HD11	1:C:312:GLY:HA2	1.83	0.61
1:A:330:ARG:HB3	1:A:330:ARG:HH21	1.65	0.61
1:C:308:ILE:HG12	1:C:309:ASP:N	2.16	0.61
1:B:262:TYR:CD1	1:B:263:ASN:N	2.68	0.61
1:C:320:LYS:HD2	1:C:320:LYS:N	2.16	0.61
1:A:322:ARG:HH11	1:A:322:ARG:N	1.96	0.60
1:D:169:HIS:O	1:D:172:LYS:HD3	2.01	0.60
1:D:58:LYS:HG3	1:D:59:GLU:HG2	1.84	0.60
1:C:307:THR:HG23	1:C:308:ILE:N	2.11	0.60
1:D:190:ILE:HD11	1:D:329:ILE:HD11	1.84	0.60
1:A:322:ARG:HH11	1:A:322:ARG:HB2	1.68	0.59
1:D:207:ARG:HG2	1:D:208:ALA:N	2.17	0.59
1:D:318:LEU:HD13	1:D:320:LYS:HE3	1.83	0.59
1:D:54:ILE:CG2	1:D:58:LYS:HD2	2.33	0.59
1:A:123:ARG:HG3	1:A:124:SER:H	1.65	0.59
1:A:320:LYS:H	1:A:320:LYS:HD2	1.68	0.59
1:A:225:LEU:HD13	1:D:128:GLU:HG3	1.84	0.58
1:D:169:HIS:HE1	1:D:183:GLU:OE2	1.86	0.58
1:A:47:GLN:HE22	1:A:60:ASP:CG	2.06	0.58
1:B:16:SER:HB3	1:D:67:SER:HB3	1.84	0.58
1:A:16:SER:HB3	1:C:67:SER:HB3	1.84	0.58
1:D:322:ARG:CB	1:D:322:ARG:HH11	2.16	0.58
1:B:322:ARG:HD3	1:B:322:ARG:N	2.19	0.58
1:C:48:GLY:HA2	1:C:52:VAL:CG2	2.33	0.58
1:D:106:ASP:H	1:D:123:ARG:NH2	2.00	0.58
1:D:361:ILE:O	1:D:365:ASN:HB2	2.04	0.57
1:B:267:ASP:O	1:B:268:GLN:HG3	2.03	0.57
1:B:118:PHE:O	1:B:119:ARG:HD2	2.05	0.57
1:B:264:ASP:C	1:B:265:LEU:HD12	2.25	0.57
1:D:54:ILE:HG22	1:D:58:LYS:HD2	1.87	0.57
1:A:161:LYS:HE2	2:A:409:HOH:O	2.04	0.57
1:B:247:GLU:OE1	1:B:294:HIS:HE1	1.88	0.57
1:C:322:ARG:HB2	1:C:322:ARG:HH11	1.68	0.57
1:D:49:GLY:O	1:D:174:GLU:HA	2.05	0.56
1:A:169:HIS:HE1	1:A:183:GLU:OE2	1.89	0.56
1:A:156:GLU:HB2	1:A:203:VAL:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:ALA:H	1:D:123:ARG:CZ	2.18	0.56
2:B:433:HOH:O	1:D:115:ILE:HD11	2.06	0.56
1:C:59:GLU:O	1:C:59:GLU:HG2	2.06	0.56
1:C:142:LEU:C	1:C:142:LEU:HD23	2.26	0.56
1:D:116:ARG:N	1:D:116:ARG:HD2	2.20	0.56
1:B:104:HIS:CD2	1:B:123:ARG:HH11	2.24	0.56
1:D:253:GLU:O	1:D:257:LEU:HD13	2.06	0.56
1:C:100:PHE:CZ	1:C:310:ILE:HA	2.41	0.56
1:D:116:ARG:HG2	1:D:310:ILE:HD13	1.88	0.55
1:A:264:ASP:OD1	1:A:275:ARG:HD2	2.07	0.55
1:C:304:PRO:HG3	1:C:318:LEU:CD2	2.36	0.55
1:D:247:GLU:HB2	1:D:292:ARG:HB2	1.87	0.55
1:C:162:ALA:HB1	1:C:179:ASP:HB2	1.86	0.55
1:A:101:ARG:NH1	1:A:106:ASP:OD2	2.39	0.55
1:C:206:ILE:N	1:C:206:ILE:HD12	2.21	0.55
1:C:247:GLU:OE1	1:C:294:HIS:HE1	1.88	0.55
1:A:247:GLU:OE1	1:A:294:HIS:HE1	1.90	0.55
1:D:116:ARG:CD	1:D:116:ARG:H	2.18	0.55
1:B:162:ALA:HB1	1:B:179:ASP:HB2	1.89	0.55
1:C:301:ILE:H	1:C:305:GLN:NE2	2.06	0.54
1:A:67:SER:HB3	1:C:16:SER:HB3	1.89	0.54
1:C:44:LYS:HE2	1:C:56:PRO:HG2	1.89	0.54
1:C:85:ASN:O	1:C:86:GLN:HB2	2.07	0.54
1:A:45:ARG:HH22	1:A:336:GLU:CD	2.10	0.54
1:B:97:LYS:HB3	1:B:118:PHE:CE2	2.43	0.54
1:A:162:ALA:HB1	1:A:179:ASP:HB2	1.88	0.54
1:B:115:ILE:HD12	1:D:75:THR:HA	1.90	0.54
1:B:277:GLY:O	1:B:289:ILE:HA	2.08	0.54
1:A:157:ILE:HD13	1:A:190:ILE:HD11	1.89	0.54
1:A:363:ASN:O	1:A:364:GLU:HG3	2.07	0.54
1:B:266:MET:H	1:C:307:THR:HA	1.73	0.53
1:A:99:LEU:HA	1:A:309:ASP:HA	1.90	0.53
1:A:51:ASN:OD1	1:A:52:VAL:HG23	2.08	0.53
1:D:169:HIS:NE2	1:D:172:LYS:HE3	2.22	0.53
1:C:100:PHE:HD1	1:C:106:ASP:HB3	1.73	0.53
1:A:142:LEU:C	1:A:142:LEU:HD23	2.29	0.53
1:A:21:ILE:HG23	1:A:83:ILE:HB	1.90	0.52
1:A:362:TYR:CE2	1:B:347:VAL:HG13	2.45	0.52
1:A:122:GLY:O	1:A:124:SER:N	2.43	0.52
1:C:38:LEU:HD23	1:C:42:GLU:HG2	1.90	0.52
1:C:277:GLY:O	1:C:289:ILE:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TYR:O	1:C:275:ARG:HD2	2.10	0.52
1:A:351:LEU:HD22	1:B:361:ILE:HD12	1.91	0.52
1:C:360:THR:HG23	1:C:364:GLU:OE1	2.09	0.52
1:A:250:LYS:HB3	1:A:254:SER:OG	2.10	0.52
1:D:330:ARG:HG3	2:D:392:HOH:O	2.09	0.52
1:D:320:LYS:HD2	1:D:320:LYS:N	2.26	0.51
1:B:20:VAL:HG22	1:B:84:HIS:ND1	2.26	0.51
1:B:258:LYS:HZ3	1:B:261:GLU:HG3	1.76	0.51
1:C:318:LEU:O	1:C:320:LYS:HD2	2.10	0.51
1:C:302:PHE:N	1:C:323:HIS:HD2	2.09	0.51
1:A:322:ARG:H	1:A:322:ARG:NH1	2.00	0.51
1:D:128:GLU:HG2	2:D:469:HOH:O	2.11	0.51
1:B:99:LEU:HA	1:B:309:ASP:HA	1.92	0.51
1:A:97:LYS:HZ2	1:A:97:LYS:HB2	1.75	0.51
1:C:122:GLY:O	1:C:123:ARG:HG2	2.10	0.51
1:C:77:THR:HB	1:C:78:PRO:CD	2.41	0.51
1:A:363:ASN:C	1:A:364:GLU:HG3	2.31	0.51
1:B:266:MET:HB2	1:C:308:ILE:HG22	1.93	0.50
1:B:261:GLU:O	1:B:275:ARG:NH1	2.39	0.50
1:A:302:PHE:HE2	1:A:318:LEU:CD1	2.25	0.50
1:B:105:ALA:HB3	1:B:123:ARG:NH2	2.22	0.50
1:B:169:HIS:O	1:B:172:LYS:HD3	2.11	0.50
1:A:330:ARG:CB	1:A:330:ARG:HH21	2.24	0.50
1:C:197:HIS:O	1:C:303:GLN:HG3	2.11	0.50
1:B:155:ILE:CG2	1:B:178:LEU:HD12	2.42	0.50
1:B:271:PHE:CZ	1:B:280:LEU:HD22	2.47	0.50
1:D:97:LYS:HB2	1:D:97:LYS:NZ	2.26	0.50
1:B:264:ASP:HB3	1:B:271:PHE:HD2	1.77	0.50
1:C:9:ARG:HD2	2:C:446:HOH:O	2.11	0.50
1:D:106:ASP:N	1:D:123:ARG:NH2	2.60	0.50
1:A:233:ILE:O	1:A:237:MET:HG2	2.12	0.50
1:B:205:LEU:C	1:B:206:ILE:HD12	2.33	0.50
1:C:100:PHE:CD1	1:C:106:ASP:HB3	2.47	0.50
1:D:106:ASP:H	1:D:123:ARG:HH22	1.58	0.50
1:D:95:ASN:O	1:D:96:ILE:HB	2.11	0.50
1:A:180:GLU:HG2	2:A:535:HOH:O	2.11	0.49
1:C:265:LEU:HD22	1:C:265:LEU:N	2.27	0.49
1:C:360:THR:O	1:C:364:GLU:HB2	2.13	0.49
1:B:100:PHE:HB2	1:C:266:MET:HE3	1.94	0.49
1:C:123:ARG:HG3	1:C:124:SER:N	2.27	0.49
1:D:105:ALA:H	1:D:123:ARG:NH2	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PHE:O	1:B:114:GLY:HA2	2.11	0.49
1:D:124:SER:O	1:D:126:ALA:N	2.46	0.49
1:D:320:LYS:H	1:D:320:LYS:HD2	1.77	0.49
1:A:304:PRO:HB3	1:A:316:GLU:OE1	2.13	0.49
1:A:330:ARG:HB3	1:A:330:ARG:NH2	2.28	0.49
1:C:99:LEU:O	1:C:99:LEU:HD12	2.12	0.49
1:B:97:LYS:HB2	1:B:97:LYS:NZ	2.27	0.49
1:D:123:ARG:CG	1:D:124:SER:N	2.75	0.49
1:B:104:HIS:HD2	1:B:123:ARG:HH11	1.60	0.48
1:B:105:ALA:H	1:B:123:ARG:HH12	1.61	0.48
1:C:117:ASP:CG	1:C:118:PHE:N	2.64	0.48
1:C:58:LYS:HD3	1:C:58:LYS:H	1.78	0.48
1:A:54:ILE:HG22	1:A:55:THR:N	2.29	0.48
1:B:142:LEU:C	1:B:142:LEU:HD23	2.34	0.48
1:B:247:GLU:HB2	1:B:292:ARG:HB2	1.94	0.48
1:B:9:ARG:HD2	2:B:386:HOH:O	2.13	0.48
1:C:20:VAL:HG22	1:C:84:HIS:ND1	2.29	0.48
1:C:265:LEU:HB2	1:C:272:LEU:HD12	1.95	0.48
1:A:361:ILE:O	1:A:365:ASN:OXT	2.30	0.48
1:B:302:PHE:CE2	1:B:318:LEU:HD11	2.42	0.47
1:B:54:ILE:HG22	1:B:55:THR:N	2.29	0.47
1:A:318:LEU:O	1:A:320:LYS:HD2	2.14	0.47
1:B:116:ARG:HH11	1:B:116:ARG:HG3	1.78	0.47
1:C:123:ARG:HG3	1:C:123:ARG:HH11	1.79	0.47
1:C:21:ILE:HG23	1:C:83:ILE:HB	1.96	0.47
1:C:316:GLU:HG2	1:C:318:LEU:H	1.80	0.47
1:B:215:GLN:OE1	1:B:216:LYS:N	2.47	0.47
1:C:110:PHE:O	1:C:114:GLY:HA2	2.15	0.47
1:C:145:GLU:OE1	1:D:359:LYS:HE2	2.15	0.47
1:C:267:ASP:HB2	1:C:272:LEU:CD2	2.45	0.47
1:B:101:ARG:O	1:B:104:HIS:HB2	2.14	0.47
1:C:190:ILE:HD11	1:C:329:ILE:HD11	1.96	0.47
1:A:93:TYR:HA	1:A:320:LYS:O	2.15	0.47
1:C:240:LEU:HD23	1:C:241:ASN:N	2.30	0.47
1:C:38:LEU:HD23	1:C:38:LEU:C	2.36	0.47
1:A:302:PHE:CE2	1:A:318:LEU:HD11	2.44	0.47
1:C:100:PHE:CD2	1:C:107:PHE:HA	2.50	0.47
1:D:132:ARG:NH1	2:D:416:HOH:O	2.47	0.47
1:D:205:LEU:C	1:D:206:ILE:HD12	2.36	0.47
1:C:99:LEU:HD23	1:C:315:CYS:HB2	1.96	0.47
1:A:322:ARG:HH11	1:A:322:ARG:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ILE:HD12	1:B:59:GLU:OE2	2.15	0.46
1:D:142:LEU:HD23	1:D:142:LEU:C	2.36	0.46
1:D:85:ASN:HD22	1:D:86:GLN:HG3	1.77	0.46
1:A:247:GLU:HB2	1:A:292:ARG:HB2	1.96	0.46
1:C:309:ASP:HB3	1:C:315:CYS:SG	2.56	0.46
1:D:314:GLU:HG3	2:D:502:HOH:O	2.15	0.46
1:A:170:ALA:HB2	1:A:178:LEU:HD23	1.98	0.46
1:B:98:ASN:O	1:B:310:ILE:HG13	2.15	0.46
1:D:15:GLU:H	1:D:15:GLU:CD	2.18	0.46
1:C:308:ILE:CG1	1:C:312:GLY:HA2	2.45	0.46
1:D:88:ALA:O	1:D:89:ARG:HB2	2.16	0.46
1:A:75:THR:HA	1:C:115:ILE:CD1	2.45	0.46
1:C:161:LYS:O	1:C:182:GLN:HG3	2.16	0.46
1:A:347:VAL:HG13	1:B:362:TYR:CE2	2.50	0.46
1:C:38:LEU:HD22	1:C:137:ALA:HB1	1.97	0.46
1:B:116:ARG:HG2	1:B:310:ILE:HD13	1.99	0.45
1:C:322:ARG:CB	1:C:322:ARG:HH11	2.29	0.45
1:D:117:ASP:O	1:D:119:ARG:HD3	2.16	0.45
1:A:228:LYS:HD3	1:A:282:GLY:HA3	1.98	0.45
1:D:363:ASN:C	1:D:365:ASN:H	2.19	0.45
1:C:58:LYS:N	1:C:58:LYS:HD3	2.31	0.45
1:C:97:LYS:HB2	1:C:97:LYS:HZ2	1.79	0.45
1:D:61:ASP:O	1:D:62:LYS:HB2	2.15	0.45
1:A:47:GLN:HE22	1:A:60:ASP:CB	2.28	0.45
1:C:322:ARG:HH11	1:C:322:ARG:N	2.12	0.45
1:B:101:ARG:NH1	1:B:101:ARG:HG3	2.30	0.45
1:B:207:ARG:HG3	1:B:290:ILE:HD13	1.98	0.45
1:B:322:ARG:HD3	1:B:322:ARG:H	1.81	0.45
1:D:99:LEU:C	1:D:99:LEU:HD12	2.37	0.45
1:C:308:ILE:CD1	1:C:312:GLY:HA2	2.46	0.45
1:C:77:THR:HB	1:C:78:PRO:HD2	1.99	0.45
1:A:322:ARG:N	1:A:322:ARG:HD3	2.32	0.45
1:A:47:GLN:HE22	1:A:60:ASP:HB3	1.81	0.45
1:B:128:GLU:CG	1:C:225:LEU:HD13	2.45	0.45
1:B:265:LEU:HD12	1:B:265:LEU:N	2.32	0.45
1:D:21:ILE:HG23	1:D:83:ILE:HB	1.99	0.45
1:B:361:ILE:O	1:B:365:ASN:HB3	2.17	0.44
1:C:127:ARG:HG2	1:C:127:ARG:NH1	2.31	0.44
1:C:207:ARG:HA	1:C:289:ILE:O	2.17	0.44
1:A:296:LYS:HD2	1:D:262:TYR:CE1	2.52	0.44
1:A:9:ARG:HD2	2:A:416:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ASP:CG	1:C:268:GLN:H	2.21	0.44
1:C:200:ILE:CD1	1:C:326:CYS:HB2	2.47	0.44
1:B:21:ILE:HG23	1:B:83:ILE:HB	1.98	0.44
1:A:128:GLU:CG	1:D:225:LEU:HD13	2.42	0.44
1:B:327:ILE:HA	2:B:399:HOH:O	2.16	0.44
1:C:122:GLY:O	1:C:124:SER:N	2.45	0.44
1:D:188:THR:HA	1:D:191:GLN:NE2	2.33	0.44
1:D:247:GLU:OE1	1:D:294:HIS:CE1	2.65	0.44
1:A:67:SER:O	1:A:79:ILE:HA	2.17	0.44
1:B:105:ALA:HB2	1:C:281:GLY:HA3	2.00	0.44
1:B:93:TYR:HA	1:B:320:LYS:HB2	2.00	0.44
1:A:116:ARG:HH11	1:A:116:ARG:HG3	1.81	0.44
1:B:156:GLU:HG2	2:B:371:HOH:O	2.17	0.44
1:C:99:LEU:HA	1:C:309:ASP:HA	1.99	0.44
1:C:67:SER:O	1:C:79:ILE:HA	2.18	0.44
1:C:116:ARG:NH1	1:C:310:ILE:HG21	2.33	0.44
1:C:127:ARG:HG2	1:C:127:ARG:HH11	1.82	0.43
1:C:47:GLN:NE2	1:C:60:ASP:HB2	2.27	0.43
1:D:262:TYR:O	1:D:275:ARG:HD2	2.19	0.43
1:A:361:ILE:HD11	1:B:361:ILE:CD1	2.45	0.43
1:B:61:ASP:OD2	1:B:85:ASN:HB3	2.18	0.43
1:B:97:LYS:HB3	1:B:118:PHE:CD2	2.53	0.43
1:C:216:LYS:NZ	1:C:287:GLU:OE1	2.50	0.43
1:C:304:PRO:HG3	1:C:318:LEU:HD23	1.99	0.43
1:B:116:ARG:NH1	1:B:116:ARG:HG3	2.33	0.43
1:C:99:LEU:C	1:C:99:LEU:HD12	2.38	0.43
1:A:2:ASN:OD1	1:C:9:ARG:NH1	2.52	0.43
1:B:92:ASP:C	1:B:94:ASP:H	2.22	0.43
1:D:206:ILE:CD1	1:D:206:ILE:N	2.82	0.43
1:C:183:GLU:HG2	1:C:187:LYS:HE3	2.01	0.43
1:A:155:ILE:CG2	1:A:178:LEU:HD12	2.49	0.43
1:A:320:LYS:HD2	1:A:320:LYS:N	2.32	0.43
1:D:221:LEU:O	1:D:283:MET:HA	2.19	0.43
1:D:308:ILE:HG22	1:D:314:GLU:HG2	2.01	0.43
1:B:156:GLU:HA	1:B:160:ILE:O	2.18	0.43
1:B:242:GLY:HA2	1:B:296:LYS:HE2	2.01	0.43
1:B:85:ASN:O	1:B:86:GLN:HB2	2.18	0.43
1:C:50:ARG:O	1:C:51:ASN:HB2	2.19	0.43
1:D:233:ILE:O	1:D:237:MET:HG2	2.19	0.43
1:D:169:HIS:CE1	1:D:183:GLU:OE2	2.69	0.42
1:D:54:ILE:HG21	1:D:58:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:HA	1:A:118:PHE:CZ	2.54	0.42
1:C:187:LYS:O	1:C:191:GLN:HG3	2.18	0.42
1:C:250:LYS:HE3	1:C:253:GLU:HB3	2.00	0.42
1:C:106:ASP:HA	1:C:118:PHE:CZ	2.54	0.42
2:A:519:HOH:O	1:D:111:HIS:HD2	2.02	0.42
1:A:351:LEU:HD22	1:B:361:ILE:CD1	2.49	0.42
1:B:183:GLU:HG2	1:B:187:LYS:HE3	2.01	0.42
1:C:200:ILE:H	1:C:200:ILE:HD12	1.85	0.42
1:D:104:HIS:CE1	1:D:299:PRO:HB2	2.55	0.42
1:C:300:SER:HA	1:C:305:GLN:HE22	1.85	0.42
1:D:43:MET:O	1:D:46:ARG:HG2	2.20	0.42
1:B:155:ILE:HG22	1:B:178:LEU:HD12	2.00	0.42
1:B:45:ARG:HH22	1:B:336:GLU:CD	2.23	0.42
1:C:97:LYS:HB2	1:C:97:LYS:HZ3	1.85	0.42
1:D:110:PHE:O	1:D:114:GLY:N	2.50	0.42
1:D:149:VAL:HG11	1:D:211:ILE:HD12	2.01	0.42
1:D:55:THR:O	1:D:58:LYS:HG2	2.19	0.42
1:C:156:GLU:OE1	1:C:161:LYS:HG2	2.20	0.42
1:B:255:SER:OG	1:C:294:HIS:HD2	2.03	0.42
1:B:78:PRO:HB2	1:D:13:PHE:O	2.20	0.42
1:D:156:GLU:HB2	1:D:203:VAL:HB	2.02	0.42
1:B:21:ILE:HD12	1:B:22:GLY:H	1.84	0.41
1:D:172:LYS:O	1:D:172:LYS:HG2	2.19	0.41
1:B:125:SER:O	1:B:127:ARG:N	2.53	0.41
1:C:169:HIS:HA	1:C:172:LYS:HZ2	1.85	0.41
1:B:103:SER:C	1:C:280:LEU:HD11	2.40	0.41
1:B:262:TYR:HD1	1:B:263:ASN:H	1.59	0.41
1:C:320:LYS:CD	1:C:320:LYS:H	2.29	0.41
1:C:343:LEU:O	1:C:347:VAL:HG23	2.20	0.41
1:C:350:ASN:HB3	1:D:362:TYR:OH	2.21	0.41
1:B:101:ARG:NH1	1:B:118:PHE:CE1	2.88	0.41
1:A:235:GLU:HB2	1:D:235:GLU:HB2	2.03	0.41
1:D:105:ALA:N	1:D:123:ARG:HH12	2.06	0.41
1:B:210:SER:HB3	1:B:215:GLN:O	2.20	0.41
1:C:53:PHE:O	1:C:54:ILE:HB	2.20	0.41
1:B:320:LYS:H	1:B:320:LYS:CD	2.31	0.41
1:B:47:GLN:O	1:B:49:GLY:N	2.46	0.41
1:B:70:PHE:CE2	1:B:71:GLU:HG3	2.56	0.41
1:D:115:ILE:CD1	1:D:115:ILE:O	2.63	0.41
1:A:91:LYS:HB2	1:A:92:ASP:H	1.64	0.41
1:B:115:ILE:CD1	1:D:30:SER:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:SER:O	1:B:126:ALA:HB3	2.21	0.41
1:C:267:ASP:HB2	1:C:272:LEU:HD21	2.03	0.41
1:A:123:ARG:CG	1:A:124:SER:H	2.30	0.41
1:A:175:ILE:HG21	1:A:190:ILE:HD12	2.03	0.41
1:D:250:LYS:HB3	1:D:254:SER:OG	2.20	0.41
1:A:151:GLU:OE2	1:A:207:ARG:NH1	2.45	0.40
1:D:267:ASP:C	1:D:267:ASP:OD2	2.58	0.40
1:C:215:GLN:OE1	1:C:215:GLN:HA	2.21	0.40
1:C:302:PHE:HD2	1:C:302:PHE:O	2.04	0.40
1:C:38:LEU:HD23	1:C:38:LEU:O	2.20	0.40
1:D:118:PHE:CD1	1:D:118:PHE:N	2.88	0.40
1:A:235:GLU:OE2	1:D:235:GLU:OE2	2.38	0.40
1:D:277:GLY:O	1:D:289:ILE:HA	2.22	0.40
1:B:250:LYS:HE2	1:B:257:LEU:CD2	2.46	0.40
1:D:21:ILE:HD12	1:D:22:GLY:H	1.86	0.40
1:D:7:PHE:O	1:D:9:ARG:HG3	2.21	0.40
1:A:225:LEU:HD13	1:D:128:GLU:CG	2.50	0.40
1:D:322:ARG:HH11	1:D:322:ARG:H	1.69	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLN:NE2	1:D:89:ARG:NH2[7_545]	1.37	0.83
1:C:316:GLU:OE1	1:C:316:GLU:OE1[2_655]	1.70	0.50
1:C:71:GLU:OE2	1:D:87:ARG:CG[6_555]	1.71	0.49
1:C:71:GLU:OE2	1:D:87:ARG:NE[6_555]	1.92	0.28
1:C:181:GLU:O	1:D:89:ARG:NH1[7_545]	2.05	0.15
1:B:272:LEU:CD2	1:B:272:LEU:CD2[2_655]	2.07	0.13
1:C:71:GLU:OE2	1:D:87:ARG:CD[6_555]	2.14	0.06

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	363/365 (100%)	323 (89%)	30 (8%)	10 (3%)	5	2
1	B	363/365 (100%)	318 (88%)	34 (9%)	11 (3%)	4	2
1	C	363/365 (100%)	323 (89%)	31 (8%)	9 (2%)	5	3
1	D	363/365 (100%)	333 (92%)	17 (5%)	13 (4%)	3	1
All	All	1452/1460 (100%)	1297 (89%)	112 (8%)	43 (3%)	4	2

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	95	ASN
1	A	116	ARG
1	A	123	ARG
1	B	95	ASN
1	B	118	PHE
1	B	125	SER
1	B	262	TYR
1	B	263	ASN
1	B	271	PHE
1	C	61	ASP
1	C	117	ASP
1	C	307	THR
1	D	124	SER
1	A	52	VAL
1	B	50	ARG
1	B	51	ASN
1	B	123	ARG
1	C	124	SER
1	D	56	PRO
1	D	92	ASP
1	A	61	ASP
1	C	54	ILE
1	C	116	ARG
1	C	123	ARG
1	D	59	GLU
1	D	86	GLN
1	D	94	ASP
1	D	96	ILE
1	D	117	ASP
1	D	125	SER

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Mol	Chain	Res	Type
1	A	87	ARG
1	A	97	LYS
1	A	120	GLY
1	D	89	ARG
1	A	92	ASP
1	C	59	GLU
1	D	93	TYR
1	D	118	PHE
1	B	90	SER
1	D	224	GLY
1	B	52	VAL
1	C	96	ILE

5.3.2　Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/300 (100%)	292 (97%)	8 (3%)	44	54
1	B	300/300 (100%)	291 (97%)	9 (3%)	41	50
1	C	300/300 (100%)	290 (97%)	10 (3%)	38	46
1	D	300/300 (100%)	286 (95%)	14 (5%)	26	29
All	All	1200/1200 (100%)	1159 (97%)	41 (3%)	37	45

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE
1	A	89	ARG
1	A	91	LYS
1	A	93	TYR
1	A	168	ASN
1	A	240	LEU
1	A	322	ARG
1	A	330	ARG
1	B	87	ARG

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Mol	Chain	Res	Type
1	B	89	ARG
1	B	172	LYS
1	B	215	GLN
1	B	240	LEU
1	B	241	ASN
1	B	257	LEU
1	B	302	PHE
1	B	322	ARG
1	C	17	HIS
1	C	58	LYS
1	C	87	ARG
1	C	89	ARG
1	C	91	LYS
1	C	172	LYS
1	C	200	ILE
1	C	302	PHE
1	C	322	ARG
1	C	343	LEU
1	D	38	LEU
1	D	87	ARG
1	D	91	LYS
1	D	93	TYR
1	D	95	ASN
1	D	118	PHE
1	D	123	ARG
1	D	172	LYS
1	D	240	LEU
1	D	241	ASN
1	D	302	PHE
1	D	318	LEU
1	D	322	ARG
1	D	343	LEU

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

Mol	Chain	Res	Type
1	A	47	GLN
1	A	85	ASN
1	A	104	HIS
1	A	168	ASN
1	A	169	HIS
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	186	GLN
1	A	215	GLN
1	A	223	GLN
1	A	241	ASN
1	A	294	HIS
1	A	313	ASN
1	B	47	GLN
1	B	51	ASN
1	B	168	ASN
1	B	169	HIS
1	B	186	GLN
1	B	191	GLN
1	B	223	GLN
1	B	241	ASN
1	B	263	ASN
1	B	294	HIS
1	B	313	ASN
1	C	47	GLN
1	C	51	ASN
1	C	168	ASN
1	C	186	GLN
1	C	191	GLN
1	C	214	ASN
1	C	223	GLN
1	C	294	HIS
1	C	303	GLN
1	C	305	GLN
1	C	313	ASN
1	C	323	HIS
1	D	47	GLN
1	D	85	ASN
1	D	104	HIS
1	D	111	HIS
1	D	169	HIS
1	D	186	GLN
1	D	191	GLN
1	D	215	GLN
1	D	223	GLN
1	D	294	HIS

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 ⓘ

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	365/365 (100%)	0.71	46 (12%)	3	3	19, 30, 131, 176	9 (2%)
1	B	365/365 (100%)	1.34	82 (22%)	0	0	23, 41, 141, 167	9 (2%)
1	C	365/365 (100%)	1.95	84 (23%)	0	0	22, 39, 168, 183	9 (2%)
1	D	365/365 (100%)	0.53	46 (12%)	3	3	20, 34, 110, 149	9 (2%)
All	All	1460/1460 (100%)	1.13	258 (17%)	1	1	19, 36, 146, 183	36 (2%)

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	302	PHE	34.1
1	B	270	GLY	29.4
1	C	315	CYS	24.8
1	B	272	LEU	23.0
1	C	301	ILE	23.0
1	C	99	LEU	19.4
1	C	306	ARG	17.6
1	C	52	VAL	17.5
1	A	93	TYR	17.5
1	A	53	PHE	17.1
1	A	55	THR	16.6
1	B	51	ASN	15.2
1	C	305	GLN	15.2
1	A	56	PRO	13.5
1	C	96	ILE	13.5
1	D	90	SER	13.3
1	A	51	ASN	13.3
1	C	98	ASN	13.2
1	B	53	PHE	13.1
1	D	89	ARG	12.8
1	B	88	ALA	12.8

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Mol	Chain	Res	Type	RSRZ
1	C	309	ASP	12.8
1	C	307	THR	12.7
1	B	54	ILE	12.7
1	A	88	ALA	12.7
1	C	54	ILE	12.5
1	C	101	ARG	12.4
1	A	52	VAL	12.3
1	A	58	LYS	11.6
1	C	313	ASN	11.5
1	C	310	ILE	11.5
1	B	271	PHE	11.5
1	C	317	CYS	11.4
1	C	56	PRO	11.3
1	C	88	ALA	11.2
1	A	54	ILE	11.2
1	B	266	MET	11.0
1	B	52	VAL	11.0
1	A	91	LYS	10.9
1	C	303	GLN	10.8
1	C	90	SER	10.8
1	C	93	TYR	10.7
1	C	95	ASN	10.7
1	A	92	ASP	10.6
1	C	314	GLU	10.4
1	B	93	TYR	10.3
1	B	56	PRO	10.3
1	B	268	GLN	10.2
1	C	55	THR	10.0
1	C	300	SER	10.0
1	B	90	SER	9.9
1	C	92	ASP	9.9
1	A	95	ASN	9.7
1	C	320	LYS	9.7
1	D	123	ARG	9.7
1	C	58	LYS	9.7
1	C	118	PHE	9.6
1	D	88	ALA	9.5
1	B	92	ASP	9.5
1	B	87	ARG	9.4
1	A	50	ARG	9.4
1	B	57	ARG	9.3
1	C	102	PRO	9.3

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Mol	Chain	Res	Type	RSRZ
1	B	55	THR	9.2
1	C	213	THR	9.2
1	C	308	ILE	9.1
1	D	121	GLY	9.0
1	A	49	GLY	8.8
1	C	94	ASP	8.8
1	C	311	ASN	8.8
1	C	57	ARG	8.6
1	A	90	SER	8.5
1	C	103	SER	8.4
1	C	86	GLN	8.3
1	B	118	PHE	8.2
1	C	214	ASN	8.1
1	C	321	GLY	8.1
1	C	87	ARG	8.0
1	C	121	GLY	7.9
1	A	89	ARG	7.9
1	B	267	ASP	7.9
1	A	119	ARG	7.9
1	C	59	GLU	7.9
1	D	120	GLY	7.8
1	C	123	ARG	7.6
1	A	121	GLY	7.6
1	B	263	ASN	7.6
1	B	119	ARG	7.4
1	B	94	ASP	7.3
1	A	118	PHE	7.3
1	C	319	LEU	7.3
1	A	96	ILE	7.3
1	D	91	LYS	7.2
1	C	89	ARG	7.2
1	A	120	GLY	7.1
1	A	94	ASP	7.1
1	C	365	ASN	7.1
1	A	86	GLN	7.0
1	C	304	PRO	6.9
1	C	91	LYS	6.9
1	D	365	ASN	6.9
1	D	93	TYR	6.9
1	C	51	ASN	6.8
1	B	265	LEU	6.8
1	D	59	GLU	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	53	PHE	6.5
1	B	120	GLY	6.5
1	B	50	ARG	6.4
1	C	104	HIS	6.3
1	D	58	LYS	6.3
1	C	322	ARG	6.3
1	A	59	GLU	6.2
1	B	91	LYS	6.1
1	A	57	ARG	6.0
1	B	58	LYS	6.0
1	B	273	SER	6.0
1	C	318	LEU	6.0
1	D	94	ASP	6.0
1	B	121	GLY	5.9
1	D	49	GLY	5.7
1	C	124	SER	5.7
1	D	92	ASP	5.7
1	D	124	SER	5.5
1	C	119	ARG	5.5
1	B	116	ARG	5.4
1	A	60	ASP	5.3
1	D	56	PRO	5.3
1	B	365	ASN	5.3
1	B	321	GLY	5.2
1	B	214	ASN	5.2
1	D	119	ARG	5.1
1	B	168	ASN	5.1
1	D	364	GLU	5.1
1	B	89	ARG	5.1
1	C	19	ASP	5.1
1	B	264	ASP	5.0
1	C	49	GLY	5.0
1	C	312	GLY	4.9
1	A	365	ASN	4.9
1	C	105	ALA	4.9
1	B	17	HIS	4.9
1	C	122	GLY	4.8
1	B	322	ARG	4.8
1	C	269	LYS	4.8
1	C	85	ASN	4.7
1	C	100	PHE	4.7
1	B	313	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	19	ASP	4.6
1	B	172	LYS	4.6
1	B	60	ASP	4.6
1	C	272	LEU	4.6
1	B	122	GLY	4.5
1	A	17	HIS	4.4
1	D	87	ARG	4.4
1	C	97	LYS	4.4
1	C	116	ARG	4.3
1	D	172	LYS	4.2
1	C	267	ASP	4.2
1	C	17	HIS	4.2
1	B	212	LYS	4.2
1	B	59	GLU	4.1
1	B	306	ARG	4.1
1	C	316	GLU	4.1
1	A	87	ARG	4.0
1	D	55	THR	3.9
1	D	118	PHE	3.9
1	B	301	ILE	3.9
1	A	85	ASN	3.8
1	D	57	ARG	3.7
1	B	49	GLY	3.7
1	B	61	ASP	3.7
1	B	213	THR	3.6
1	A	115	ILE	3.6
1	D	122	GLY	3.6
1	B	323	HIS	3.6
1	B	302	PHE	3.6
1	B	123	ARG	3.6
1	B	269	LYS	3.6
1	D	321	GLY	3.5
1	B	86	GLN	3.5
1	B	275	ARG	3.4
1	C	110	PHE	3.4
1	C	120	GLY	3.4
1	B	300	SER	3.4
1	A	123	ARG	3.4
1	D	116	ARG	3.3
1	D	322	ARG	3.3
1	C	323	HIS	3.3
1	B	124	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	63	VAL	3.2
1	C	211	ILE	3.2
1	D	17	HIS	3.2
1	D	60	ASP	3.2
1	B	312	GLY	3.2
1	D	97	LYS	3.1
1	A	48	GLY	3.1
1	D	95	ASN	3.1
1	D	154	ILE	3.1
1	B	62	LYS	3.1
1	B	97	LYS	3.1
1	B	95	ASN	3.0
1	C	48	GLY	3.0
1	A	322	ARG	3.0
1	A	19	ASP	2.9
1	C	154	ILE	2.8
1	B	125	SER	2.8
1	B	98	ASN	2.8
1	B	318	LEU	2.8
1	A	97	LYS	2.8
1	B	164	ASN	2.8
1	B	307	THR	2.8
1	B	99	LEU	2.7
1	D	320	LYS	2.7
1	D	115	ILE	2.7
1	C	270	GLY	2.7
1	A	269	LYS	2.6
1	D	86	GLN	2.6
1	C	172	LYS	2.6
1	B	364	GLU	2.6
1	D	117	ASP	2.6
1	A	154	ILE	2.5
1	B	191	GLN	2.5
1	D	85	ASN	2.5
1	D	157	ILE	2.5
1	B	319	LEU	2.5
1	B	315	CYS	2.5
1	B	100	PHE	2.4
1	B	85	ASN	2.4
1	A	157	ILE	2.4
1	B	320	LYS	2.4
1	B	304	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	309	ASP	2.3
1	B	157	ILE	2.3
1	A	122	GLY	2.3
1	C	271	PHE	2.3
1	C	273	SER	2.2
1	A	117	ASP	2.2
1	D	54	ILE	2.2
1	A	98	ASN	2.2
1	B	311	ASN	2.2
1	D	102	PRO	2.2
1	C	37	ALA	2.2
1	D	96	ILE	2.2
1	B	163	LYS	2.1
1	B	262	TYR	2.1
1	C	268	GLN	2.1
1	A	116	ARG	2.1
1	C	197	HIS	2.1
1	D	280	LEU	2.1
1	A	364	GLU	2.1
1	A	163	LYS	2.1
1	C	195	LYS	2.1
1	B	197	HIS	2.1
1	C	164	ASN	2.1
1	A	47	GLN	2.1
1	B	195	LYS	2.1
1	D	306	ARG	2.0
1	D	267	ASP	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.