



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:30 AM UTC

PDB ID : 2INF / pdb_00002inf
Title : Crystal Structure of Uroporphyrinogen Decarboxylase from *Bacillus subtilis*
Authors : Fan, J.; Liu, Q.; Hao, Q.; Teng, M.K.; Niu, L.W.
Deposited on : 2006-10-06
Resolution : 2.30 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

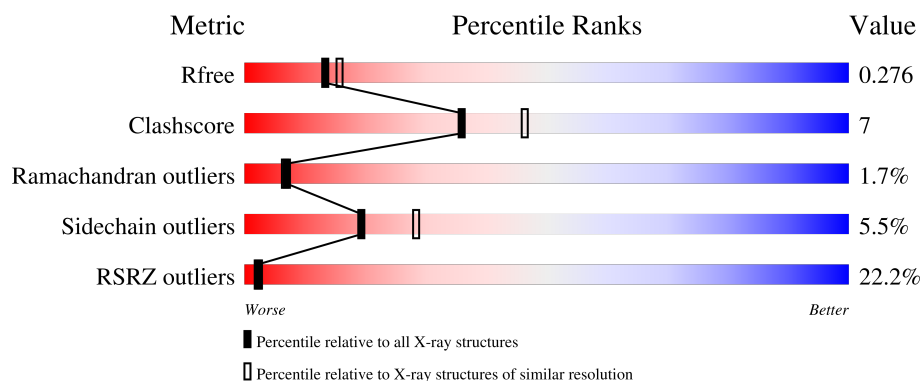
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	359	17% 76% 18% ..
1	B	359	20% 75% 18% .
1	C	359	14% 82% 13% ..
1	D	359	33% 75% 18% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11028 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 Uroporphyrinogen decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2693	1737	444	500	12			
1	B	344	Total	C	N	O	S	0	0	0
			2693	1737	444	500	12			
1	C	344	Total	C	N	O	S	0	0	0
			2693	1737	444	500	12			
1	D	344	Total	C	N	O	S	0	0	0
			2693	1737	444	500	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P32395
A	-4	HIS	-	expression tag	UNP P32395
A	-3	HIS	-	expression tag	UNP P32395
A	-2	HIS	-	expression tag	UNP P32395
A	-1	HIS	-	expression tag	UNP P32395
A	0	HIS	-	expression tag	UNP P32395
A	156	THR	ILE	engineered mutation	UNP P32395
A	198	LYS	GLU	engineered mutation	UNP P32395
B	-5	HIS	-	expression tag	UNP P32395
B	-4	HIS	-	expression tag	UNP P32395
B	-3	HIS	-	expression tag	UNP P32395
B	-2	HIS	-	expression tag	UNP P32395
B	-1	HIS	-	expression tag	UNP P32395
B	0	HIS	-	expression tag	UNP P32395
B	156	THR	ILE	engineered mutation	UNP P32395
B	198	LYS	GLU	engineered mutation	UNP P32395
C	-5	HIS	-	expression tag	UNP P32395
C	-4	HIS	-	expression tag	UNP P32395
C	-3	HIS	-	expression tag	UNP P32395
C	-2	HIS	-	expression tag	UNP P32395
C	-1	HIS	-	expression tag	UNP P32395

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP P32395
C	156	THR	ILE	engineered mutation	UNP P32395
C	198	LYS	GLU	engineered mutation	UNP P32395
D	-5	HIS	-	expression tag	UNP P32395
D	-4	HIS	-	expression tag	UNP P32395
D	-3	HIS	-	expression tag	UNP P32395
D	-2	HIS	-	expression tag	UNP P32395
D	-1	HIS	-	expression tag	UNP P32395
D	0	HIS	-	expression tag	UNP P32395
D	156	THR	ILE	engineered mutation	UNP P32395
D	198	LYS	GLU	engineered mutation	UNP P32395

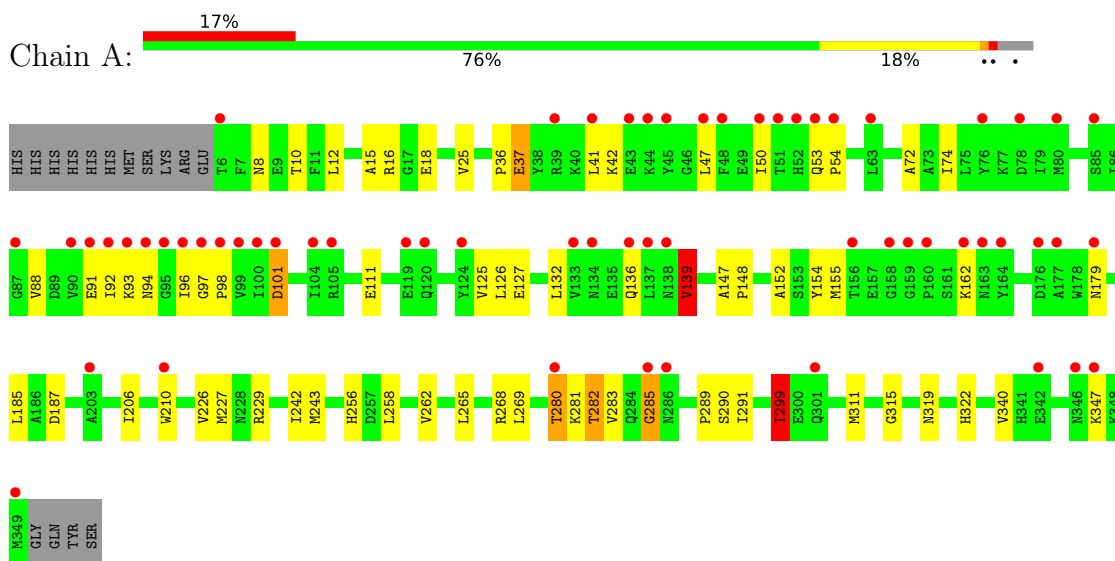
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	73	Total O 73 73	0	0
2	B	63	Total O 63 63	0	0
2	C	66	Total O 66 66	0	0
2	D	54	Total O 54 54	0	0

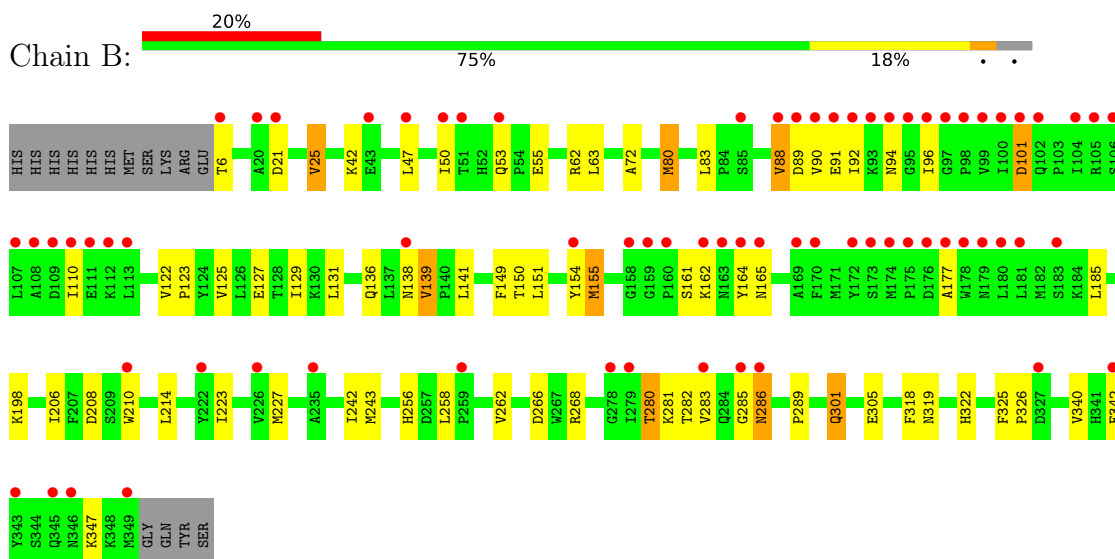
3 Residue-property plots

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.

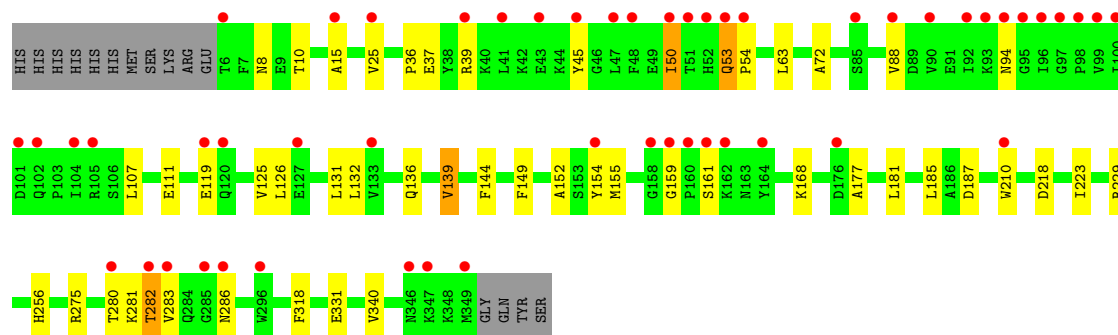
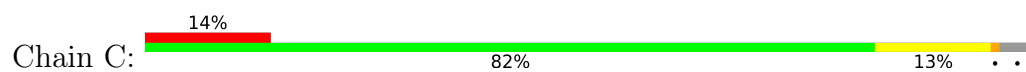
• Molecule 1: Uroporphyrinogen decarboxylase



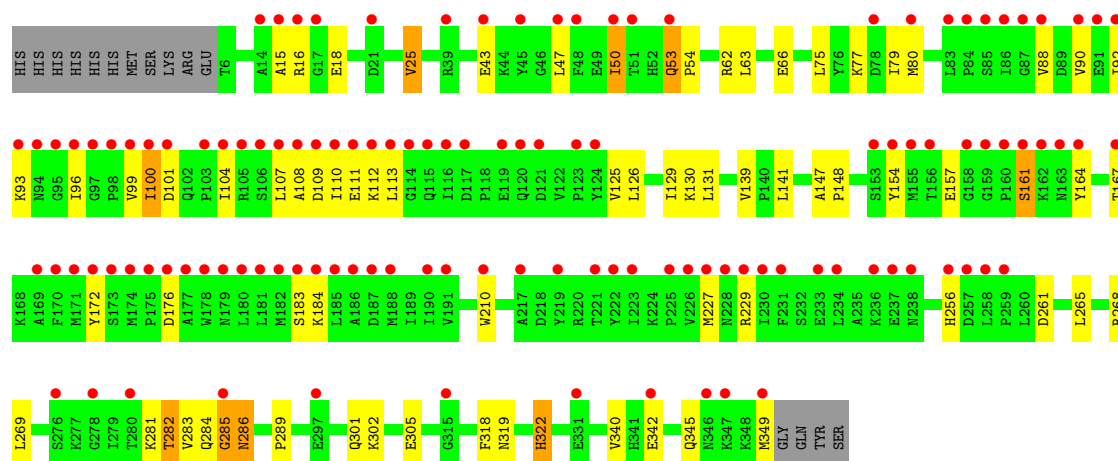
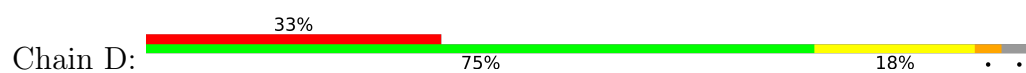
• Molecule 1: Uroporphyrinogen decarboxylase



• Molecule 1: Uroporphyrinogen decarboxylase



• Molecule 1: Uroporphyrinogen decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.61Å 80.41Å 90.94Å 68.68° 89.64° 80.82°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (30.00-2.30) 96.2 (30.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.251 0.234 , 0.276	Depositor DCC
R_{free} test set	3316 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.3	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	0.92	EDS
Total number of atoms	11028	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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

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	0.65	0/2758	0.95	4/3740 (0.1%)
1	B	0.65	1/2758 (0.0%)	0.89	0/3740
1	C	0.66	0/2758	0.95	5/3740 (0.1%)
1	D	0.93	12/2758 (0.4%)	0.96	4/3740 (0.1%)
All	All	0.73	13/11032 (0.1%)	0.93	13/14960 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	176	ASP	CG-OD1	16.20	1.56	1.25
1	D	229	ARG	CD-NE	12.43	1.63	1.46
1	D	108	ALA	C-N	10.06	1.47	1.34
1	D	229	ARG	CZ-NH1	9.17	1.45	1.32
1	D	111	GLU	CD-OE1	6.81	1.38	1.25
1	D	107	LEU	CG-CD1	6.36	1.73	1.52
1	D	172	TYR	C-N	6.01	1.42	1.33
1	B	155	MET	C-N	-5.92	1.25	1.33
1	D	183	SER	C-O	5.68	1.30	1.24
1	D	229	ARG	CZ-NH2	5.46	1.40	1.33
1	D	111	GLU	C-N	5.44	1.41	1.33
1	D	113	LEU	C-N	5.41	1.41	1.33
1	D	184	LYS	CD-CE	5.26	1.68	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	108	ALA	O-C-N	8.78	131.43	122.12
1	A	139	VAL	N-CA-C	-7.88	102.73	109.19
1	A	147	ALA	CA-C-N	6.53	126.03	119.24
1	A	147	ALA	C-N-CA	6.53	126.03	119.24
1	C	159	GLY	CA-C-N	6.27	126.47	119.32
1	C	159	GLY	C-N-CA	6.27	126.47	119.32
1	D	53	GLN	CA-C-N	5.60	125.70	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	53	GLN	C-N-CA	5.60	125.70	119.32
1	C	53	GLN	CA-C-N	5.56	125.66	119.32
1	C	53	GLN	C-N-CA	5.56	125.66	119.32
1	D	161	SER	N-CA-C	5.42	118.06	109.50
1	C	144	PHE	N-CA-C	5.14	116.66	108.79
1	A	299	ILE	CB-CA-C	-5.14	105.30	111.88

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	2693	0	2686	52	0
1	B	2693	0	2686	42	0
1	C	2693	0	2686	31	0
1	D	2693	0	2686	34	0
2	A	73	0	0	0	0
2	B	63	0	0	2	0
2	C	66	0	0	2	0
2	D	54	0	0	0	0
All	All	11028	0	10744	156	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 7.

All (156) 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:148:PRO:HG2	1:A:227:MET:HE1	1.44	0.98
1:A:155:MET:HE1	1:A:185:LEU:HD11	1.47	0.96
1:C:256:HIS:HE1	1:C:281:LYS:H	1.14	0.95
1:D:285:GLY:O	1:D:286:ASN:HB3	1.76	0.83
1:D:285:GLY:HA3	1:D:319:ASN:H	1.46	0.81
1:C:155:MET:HE1	1:C:185:LEU:HD11	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:THR:HG23	1:B:210:TRP:CD1	2.19	0.76
1:B:256:HIS:HE1	1:B:281:LYS:H	1.34	0.76
1:D:345:GLN:HE21	1:D:349:MET:HE2	1.52	0.75
1:D:147:ALA:HB1	1:D:227:MET:HE1	1.68	0.74
1:A:256:HIS:HE1	1:A:281:LYS:H	1.36	0.73
1:A:226:VAL:HG13	1:A:227:MET:CE	2.17	0.73
1:C:256:HIS:CE1	1:C:281:LYS:H	2.04	0.73
1:D:25:VAL:HG13	1:D:318:PHE:HD2	1.53	0.72
1:A:15:ALA:O	1:A:282:THR:HG21	1.89	0.72
1:B:282:THR:HB	2:B:378:HOH:O	1.88	0.72
1:A:148:PRO:CG	1:A:227:MET:HE1	2.18	0.71
1:A:155:MET:CE	1:A:185:LEU:HD11	2.20	0.71
1:D:256:HIS:HE1	1:D:281:LYS:H	1.40	0.70
1:A:256:HIS:CE1	1:A:280:THR:H	2.10	0.69
1:B:285:GLY:O	1:B:286:ASN:HB2	1.93	0.69
1:B:285:GLY:O	1:B:286:ASN:CB	2.40	0.68
1:B:208:ASP:HB2	1:B:243:MET:HE2	1.77	0.66
1:D:154:TYR:CE2	1:D:210:TRP:CH2	2.84	0.66
1:B:285:GLY:HA2	1:B:319:ASN:H	1.62	0.65
1:C:152:ALA:HA	1:C:155:MET:CE	2.27	0.64
1:A:154:TYR:CZ	1:A:210:TRP:CH2	2.85	0.64
1:D:261:ASP:O	1:D:282:THR:HG23	1.99	0.63
1:C:152:ALA:HA	1:C:155:MET:HE2	1.80	0.63
1:A:148:PRO:HG2	1:A:227:MET:CE	2.25	0.62
1:A:16:ARG:HD2	1:A:18:GLU:OE2	2.00	0.61
1:C:36:PRO:HA	1:C:39:ARG:HD3	1.83	0.61
1:C:25:VAL:HG22	1:C:340:VAL:HG11	1.82	0.61
1:A:226:VAL:HG13	1:A:227:MET:HE2	1.83	0.60
1:A:226:VAL:HG13	1:A:227:MET:HE3	1.82	0.60
1:A:206:ILE:CG2	1:A:243:MET:HE3	2.32	0.60
1:A:289:PRO:HG2	1:A:322:HIS:HB3	1.84	0.60
1:B:25:VAL:HG13	1:B:318:PHE:HD2	1.67	0.59
1:B:256:HIS:CE1	1:B:280:THR:H	2.19	0.59
1:B:285:GLY:HA2	1:B:319:ASN:N	2.19	0.58
1:D:154:TYR:CE2	1:D:210:TRP:HH2	2.20	0.58
1:A:101:ASP:N	1:A:101:ASP:OD1	2.37	0.58
1:B:72:ALA:HA	1:B:139:VAL:HG13	1.85	0.58
1:D:148:PRO:HD2	1:D:227:MET:HE1	1.85	0.58
1:A:25:VAL:HG22	1:A:340:VAL:HG11	1.87	0.57
1:A:154:TYR:CZ	1:A:210:TRP:HH2	2.23	0.56
1:A:8:ASN:C	1:A:8:ASN:HD22	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:CG2	1:B:243:MET:HE3	2.35	0.56
1:D:301:GLN:O	1:D:305:GLU:HG3	2.06	0.56
1:D:15:ALA:O	1:D:282:THR:HG21	2.07	0.55
1:D:284:GLN:O	1:D:285:GLY:O	2.25	0.55
1:A:152:ALA:HA	1:A:155:MET:HE3	1.89	0.54
1:C:72:ALA:HA	1:C:139:VAL:HG13	1.89	0.54
1:C:331:GLU:HG2	2:C:378:HOH:O	2.05	0.54
1:A:72:ALA:HA	1:A:139:VAL:HG13	1.90	0.54
1:A:291:ILE:O	1:A:299:ILE:HD13	2.07	0.54
1:D:285:GLY:HA3	1:D:319:ASN:N	2.17	0.54
1:D:99:VAL:HG12	1:D:100:ILE:H	1.73	0.54
1:B:150:THR:HG23	1:B:210:TRP:HD1	1.71	0.54
1:D:265:LEU:HD22	1:D:269:LEU:HD23	1.88	0.53
1:B:256:HIS:CE1	1:B:281:LYS:H	2.20	0.53
1:C:155:MET:CE	1:C:185:LEU:HD11	2.37	0.53
1:A:12:LEU:O	1:A:16:ARG:HG2	2.09	0.52
1:A:152:ALA:HA	1:A:155:MET:CE	2.40	0.51
1:C:107:LEU:HD13	1:C:177:ALA:HA	1.92	0.51
1:D:157:GLU:HG3	1:D:164:TYR:HD2	1.76	0.51
1:A:91:GLU:O	1:A:98:PRO:HA	2.11	0.51
1:B:80:MET:HA	1:B:80:MET:HE2	1.93	0.51
1:A:206:ILE:HG21	1:A:243:MET:HE3	1.93	0.50
1:B:258:LEU:O	1:B:281:LYS:NZ	2.44	0.50
1:D:289:PRO:HG2	1:D:322:HIS:HB3	1.93	0.50
1:C:155:MET:HE1	1:C:181:LEU:HD11	1.93	0.49
1:B:42:LYS:HA	1:B:50:ILE:CD1	2.42	0.49
1:B:262:VAL:HG22	1:B:282:THR:OG1	2.12	0.49
1:C:256:HIS:HE1	1:C:281:LYS:N	1.97	0.49
1:C:154:TYR:CE2	1:C:210:TRP:CH2	3.01	0.49
1:B:80:MET:HE1	1:B:154:TYR:CD1	2.48	0.49
1:C:154:TYR:CE2	1:C:210:TRP:HH2	2.31	0.49
1:A:54:PRO:HB3	1:A:127:GLU:HG2	1.94	0.49
1:B:6:THR:O	1:B:138:ASN:ND2	2.45	0.49
1:B:129:ILE:HG23	1:B:141:LEU:HD23	1.94	0.49
1:D:16:ARG:NH1	1:D:18:GLU:OE1	2.46	0.48
1:C:256:HIS:CE1	1:C:280:THR:H	2.32	0.48
1:A:148:PRO:CD	1:A:227:MET:HE1	2.43	0.48
1:C:25:VAL:HG13	1:C:318:PHE:HD2	1.79	0.48
1:C:218:ASP:OD1	1:D:302:LYS:NZ	2.46	0.47
1:B:62:ARG:HE	1:B:136:GLN:NE2	2.13	0.47
1:C:15:ALA:O	1:C:282:THR:HG21	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ASN:ND2	1:A:10:THR:H	2.11	0.47
1:D:25:VAL:HG22	1:D:340:VAL:HG11	1.97	0.47
1:A:258:LEU:O	1:A:281:LYS:NZ	2.47	0.47
1:B:53:GLN:HE21	1:B:55:GLU:HB2	1.80	0.46
1:C:149:PHE:HB2	1:C:223:ILE:HD12	1.96	0.46
1:A:265:LEU:HD22	1:A:269:LEU:HD23	1.97	0.46
1:A:285:GLY:HA2	1:A:319:ASN:H	1.81	0.46
1:B:161:SER:HB3	1:B:164:TYR:CE2	2.51	0.46
1:D:53:GLN:HA	1:D:54:PRO:HD3	1.84	0.45
1:D:79:ILE:HG23	1:D:80:MET:HG3	1.97	0.45
1:C:132:LEU:HD23	1:C:136:GLN:HE21	1.81	0.45
1:A:154:TYR:CE2	1:A:210:TRP:HH2	2.34	0.45
1:B:266:ASP:C	1:B:266:ASP:OD2	2.60	0.45
1:C:154:TYR:CZ	1:C:210:TRP:CH2	3.05	0.45
1:A:187:ASP:OD1	1:A:229:ARG:NH2	2.50	0.44
1:A:42:LYS:HA	1:A:50:ILE:CD1	2.47	0.44
1:B:83:LEU:HB3	1:B:88:VAL:HG22	2.00	0.44
1:B:206:ILE:HG21	1:B:243:MET:HE3	1.99	0.44
1:D:157:GLU:HG3	1:D:164:TYR:CD2	2.53	0.44
1:A:227:MET:HE2	1:A:227:MET:N	2.32	0.44
1:B:122:VAL:O	1:B:125:VAL:HG22	2.17	0.44
1:D:47:LEU:O	1:D:50:ILE:HG22	2.17	0.44
1:B:282:THR:HG23	2:B:416:HOH:O	2.17	0.44
1:D:109:ASP:HA	1:D:112:LYS:NZ	2.32	0.44
1:D:285:GLY:O	1:D:286:ASN:CB	2.54	0.44
1:C:8:ASN:C	1:C:8:ASN:HD22	2.26	0.44
1:D:62:ARG:HD2	1:D:66:GLU:OE1	2.17	0.44
1:A:16:ARG:HG3	1:A:18:GLU:HG3	2.00	0.43
1:D:99:VAL:HG12	1:D:100:ILE:N	2.32	0.43
1:D:104:ILE:HG21	1:D:110:ILE:HG13	2.01	0.43
1:C:25:VAL:CG2	1:C:340:VAL:HG11	2.47	0.43
1:B:123:PRO:O	1:B:127:GLU:HG3	2.19	0.43
1:B:149:PHE:HB2	1:B:223:ILE:HD12	2.00	0.43
1:A:41:LEU:O	1:A:50:ILE:HD11	2.18	0.43
1:C:53:GLN:HA	1:C:54:PRO:HD3	1.89	0.42
1:A:53:GLN:HA	1:A:54:PRO:HD3	1.90	0.42
1:C:152:ALA:HA	1:C:155:MET:HE3	2.00	0.42
1:A:132:LEU:HA	1:A:136:GLN:HB2	2.01	0.42
1:B:206:ILE:HG22	1:B:243:MET:HE3	2.01	0.42
1:D:75:LEU:HD23	1:D:77:LYS:HE3	2.01	0.42
1:D:161:SER:HB3	1:D:164:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:HIS:CE1	1:A:281:LYS:H	2.27	0.42
1:D:129:ILE:HG23	1:D:141:LEU:HD23	2.01	0.42
1:A:8:ASN:HD22	1:A:10:THR:H	1.67	0.42
1:A:299:ILE:H	1:A:299:ILE:HG12	1.69	0.42
1:B:25:VAL:HG22	1:B:340:VAL:HG11	2.02	0.42
1:A:311:MET:SD	1:A:347:LYS:HG2	2.60	0.42
1:B:151:LEU:O	1:B:155:MET:HG3	2.20	0.41
1:A:8:ASN:C	1:A:8:ASN:ND2	2.76	0.41
1:A:282:THR:HB	1:A:315:GLY:CA	2.50	0.41
1:B:289:PRO:HG2	1:B:322:HIS:HB3	2.02	0.41
1:A:50:ILE:HG22	1:A:50:ILE:O	2.20	0.41
1:A:36:PRO:HD2	1:A:37:GLU:OE1	2.21	0.41
1:B:223:ILE:CG2	1:B:227:MET:HE3	2.50	0.41
1:C:155:MET:CE	1:C:181:LEU:HD11	2.50	0.41
1:A:206:ILE:CG2	1:A:243:MET:CE	2.98	0.41
1:C:187:ASP:OD1	1:C:229:ARG:NH2	2.29	0.41
1:A:242:ILE:HG12	1:A:262:VAL:HB	2.03	0.41
1:B:110:ILE:HD12	1:B:177:ALA:HB1	2.03	0.41
1:B:155:MET:HE1	1:B:185:LEU:HD11	2.03	0.41
1:C:8:ASN:ND2	1:C:10:THR:H	2.19	0.41
1:A:162:LYS:HE2	1:B:162:LYS:HD3	2.03	0.41
1:B:325:PHE:HB2	1:B:326:PRO:HD2	2.03	0.41
1:B:301:GLN:NE2	1:B:305:GLU:OE2	2.48	0.40
1:C:45:TYR:HB2	1:C:50:ILE:HD13	2.01	0.40
1:C:168:LYS:NZ	2:C:372:HOH:O	2.48	0.40
1:A:290:SER:HB3	1:B:165:ASN:OD1	2.22	0.40
1:D:157:GLU:OE2	1:D:167:THR:OG1	2.39	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	342/359 (95%)	323 (94%)	13 (4%)	6 (2%)	6	6
1	B	342/359 (95%)	325 (95%)	10 (3%)	7 (2%)	6	5
1	C	342/359 (95%)	329 (96%)	10 (3%)	3 (1%)	14	17
1	D	342/359 (95%)	323 (94%)	12 (4%)	7 (2%)	6	5
All	All	1368/1436 (95%)	1300 (95%)	45 (3%)	23 (2%)	7	7

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ILE
1	A	93	LYS
1	A	96	ILE
1	B	92	ILE
1	B	96	ILE
1	B	101	ASP
1	B	286	ASN
1	D	92	ILE
1	D	96	ILE
1	D	285	GLY
1	D	286	ASN
1	B	90	VAL
1	C	94	ASN
1	D	90	VAL
1	D	93	LYS
1	C	161	SER
1	C	286	ASN
1	D	101	ASP
1	B	91	GLU
1	A	94	ASN
1	B	94	ASN
1	A	285	GLY
1	A	97	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	288/308 (94%)	273 (95%)	15 (5%)	21	31
1	B	288/308 (94%)	269 (93%)	19 (7%)	15	21
1	C	288/308 (94%)	275 (96%)	13 (4%)	24	37
1	D	288/308 (94%)	272 (94%)	16 (6%)	19	28
All	All	1152/1232 (94%)	1089 (94%)	63 (6%)	19	28

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	47	LEU
1	A	74	ILE
1	A	88	VAL
1	A	101	ASP
1	A	111	GLU
1	A	125	VAL
1	A	126	LEU
1	A	139	VAL
1	A	179	ASN
1	A	268	ARG
1	A	280	THR
1	A	282	THR
1	A	283	VAL
1	A	299	ILE
1	B	21	ASP
1	B	25	VAL
1	B	47	LEU
1	B	63	LEU
1	B	80	MET
1	B	88	VAL
1	B	89	ASP
1	B	101	ASP
1	B	131	LEU
1	B	139	VAL
1	B	198	LYS
1	B	214	LEU
1	B	242	ILE
1	B	268	ARG
1	B	280	THR
1	B	283	VAL
1	B	301	GLN
1	B	342	GLU

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Mol	Chain	Res	Type
1	B	347	LYS
1	C	37	GLU
1	C	50	ILE
1	C	63	LEU
1	C	88	VAL
1	C	111	GLU
1	C	119	GLU
1	C	125	VAL
1	C	126	LEU
1	C	131	LEU
1	C	139	VAL
1	C	275	ARG
1	C	282	THR
1	C	283	VAL
1	D	25	VAL
1	D	43	GLU
1	D	50	ILE
1	D	63	LEU
1	D	88	VAL
1	D	100	ILE
1	D	125	VAL
1	D	126	LEU
1	D	130	LYS
1	D	131	LEU
1	D	139	VAL
1	D	268	ARG
1	D	282	THR
1	D	283	VAL
1	D	322	HIS
1	D	342	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	52	HIS
1	A	228	ASN
1	A	256	HIS
1	A	286	ASN
1	B	8	ASN
1	B	52	HIS
1	B	53	GLN

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Mol	Chain	Res	Type
1	B	120	GLN
1	B	136	GLN
1	B	138	ASN
1	B	256	HIS
1	C	8	ASN
1	C	52	HIS
1	C	102	GLN
1	C	136	GLN
1	C	163	ASN
1	C	228	ASN
1	C	238	ASN
1	C	256	HIS
1	C	322	HIS
1	D	8	ASN
1	D	256	HIS
1	D	345	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](#)

There are no ligands in this entry.

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	344/359 (95%)	1.32	61 (17%) 4 4	46, 52, 69, 83	0
1	B	344/359 (95%)	1.43	72 (20%) 2 3	45, 52, 74, 87	0
1	C	344/359 (95%)	1.23	52 (15%) 5 6	45, 52, 68, 80	0
1	D	344/359 (95%)	1.78	120 (34%) 1 1	45, 53, 70, 82	0
All	All	1376/1436 (95%)	1.44	305 (22%) 2 2	45, 52, 71, 87	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	285	GLY	7.0
1	C	159	GLY	6.5
1	D	285	GLY	5.9
1	B	158	GLY	5.6
1	B	97	GLY	5.4
1	D	177	ALA	5.3
1	D	113	LEU	5.1
1	D	108	ALA	5.1
1	B	285	GLY	5.1
1	D	158	GLY	5.1
1	B	163	ASN	5.0
1	B	159	GLY	5.0
1	C	97	GLY	4.8
1	D	100	ILE	4.8
1	B	108	ALA	4.8
1	A	50	ILE	4.7
1	D	94	ASN	4.7
1	C	96	ILE	4.7
1	B	100	ILE	4.7
1	A	285	GLY	4.6
1	B	164	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	174	MET	4.6
1	D	160	PRO	4.5
1	D	95	GLY	4.5
1	C	95	GLY	4.4
1	C	94	ASN	4.4
1	D	101	ASP	4.4
1	C	158	GLY	4.4
1	C	160	PRO	4.3
1	B	349	MET	4.3
1	D	164	TYR	4.2
1	C	98	PRO	4.2
1	A	159	GLY	4.2
1	D	222	TYR	4.2
1	D	50	ILE	4.2
1	B	95	GLY	4.1
1	D	159	GLY	4.1
1	B	101	ASP	4.1
1	B	92	ILE	4.1
1	C	50	ILE	4.1
1	D	181	LEU	4.0
1	D	225	PRO	4.0
1	D	93	LYS	4.0
1	D	107	LEU	4.0
1	D	259	PRO	4.0
1	A	158	GLY	3.9
1	B	346	ASN	3.9
1	D	179	ASN	3.9
1	D	175	PRO	3.9
1	D	349	MET	3.9
1	A	92	ILE	3.9
1	D	120	GLN	3.9
1	D	110	ILE	3.8
1	D	176	ASP	3.8
1	D	170	PHE	3.8
1	D	169	ALA	3.8
1	B	99	VAL	3.8
1	C	101	ASP	3.7
1	D	182	MET	3.7
1	A	160	PRO	3.7
1	D	98	PRO	3.7
1	A	43	GLU	3.7
1	C	349	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	138	ASN	3.7
1	D	178	TRP	3.6
1	A	90	VAL	3.6
1	D	109	ASP	3.6
1	B	98	PRO	3.6
1	D	172	TYR	3.6
1	D	114	GLY	3.6
1	C	93	LYS	3.6
1	A	164	TYR	3.6
1	B	160	PRO	3.6
1	D	221	THR	3.5
1	A	349	MET	3.5
1	D	180	LEU	3.5
1	D	187	ASP	3.5
1	D	119	GLU	3.4
1	B	88	VAL	3.4
1	A	134	ASN	3.4
1	C	120	GLN	3.4
1	B	6	THR	3.4
1	B	94	ASN	3.4
1	D	173	SER	3.4
1	C	51	THR	3.3
1	D	233	GLU	3.3
1	D	88	VAL	3.3
1	A	286	ASN	3.3
1	D	99	VAL	3.3
1	A	51	THR	3.3
1	D	97	GLY	3.2
1	D	257	ASP	3.2
1	B	110	ILE	3.2
1	D	96	ILE	3.2
1	A	95	GLY	3.2
1	D	17	GLY	3.2
1	A	101	ASP	3.2
1	B	180	LEU	3.2
1	B	174	MET	3.2
1	C	92	ILE	3.2
1	A	94	ASN	3.2
1	D	53	GLN	3.2
1	C	105	ARG	3.1
1	A	93	LYS	3.1
1	B	169	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	286	ASN	3.1
1	A	120	GLN	3.1
1	A	137	LEU	3.1
1	C	48	PHE	3.1
1	D	106	SER	3.1
1	D	90	VAL	3.1
1	B	104	ILE	3.1
1	C	43	GLU	3.1
1	B	85	SER	3.1
1	B	170	PHE	3.1
1	A	97	GLY	3.1
1	B	89	ASP	3.1
1	D	278	GLY	3.1
1	C	99	VAL	3.1
1	B	106	SER	3.1
1	A	163	ASN	3.1
1	D	346	ASN	3.1
1	B	20	ALA	3.1
1	D	154	TYR	3.0
1	B	51	THR	3.0
1	B	107	LEU	3.0
1	B	113	LEU	3.0
1	D	226	VAL	3.0
1	A	100	ILE	3.0
1	D	161	SER	3.0
1	B	210	TRP	3.0
1	B	91	GLU	3.0
1	D	223	ILE	3.0
1	A	6	THR	3.0
1	C	45	TYR	3.0
1	C	280	THR	3.0
1	D	85	SER	3.0
1	B	176	ASP	3.0
1	C	176	ASP	3.0
1	D	48	PHE	2.9
1	C	52	HIS	2.9
1	B	178	TRP	2.9
1	A	133	VAL	2.9
1	D	92	ILE	2.9
1	B	179	ASN	2.9
1	B	175	PRO	2.9
1	D	210	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	258	LEU	2.9
1	D	104	ILE	2.9
1	D	80	MET	2.9
1	D	183	SER	2.9
1	B	90	VAL	2.9
1	D	103	PRO	2.8
1	A	96	ILE	2.8
1	D	116	ILE	2.8
1	C	286	ASN	2.8
1	B	138	ASN	2.8
1	B	173	SER	2.8
1	D	43	GLU	2.8
1	B	112	LYS	2.8
1	B	43	GLU	2.7
1	B	342	GLU	2.7
1	A	41	LEU	2.7
1	A	280	THR	2.7
1	D	91	GLU	2.7
1	B	47	LEU	2.7
1	D	231	PHE	2.7
1	D	191	VAL	2.7
1	B	96	ILE	2.7
1	D	188	MET	2.7
1	A	48	PHE	2.7
1	C	6	THR	2.7
1	C	119	GLU	2.7
1	D	84	PRO	2.7
1	B	181	LEU	2.7
1	A	52	HIS	2.6
1	B	102	GLN	2.6
1	A	45	TYR	2.6
1	B	154	TYR	2.6
1	A	104	ILE	2.6
1	D	155	MET	2.6
1	C	210	TRP	2.6
1	B	111	GLU	2.6
1	B	21	ASP	2.6
1	A	124	TYR	2.6
1	B	222	TYR	2.6
1	D	190	ILE	2.6
1	D	230	ILE	2.6
1	D	111	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	186	ALA	2.6
1	A	98	PRO	2.6
1	B	172	TYR	2.6
1	D	276	SER	2.6
1	A	63	LEU	2.5
1	D	87	GLY	2.5
1	D	315	GLY	2.5
1	A	162	LYS	2.5
1	C	161	SER	2.5
1	B	53	GLN	2.5
1	D	124	TYR	2.5
1	C	127	GLU	2.5
1	D	342	GLU	2.5
1	D	162	LYS	2.5
1	D	236	LYS	2.5
1	D	280	THR	2.5
1	C	85	SER	2.5
1	A	39	ARG	2.5
1	B	105	ARG	2.5
1	D	163	ASN	2.5
1	D	217	ALA	2.5
1	A	136	GLN	2.5
1	A	119	GLU	2.5
1	D	237	GLU	2.5
1	A	105	ARG	2.4
1	C	347	LYS	2.4
1	D	39	ARG	2.4
1	D	45	TYR	2.4
1	A	78	ASP	2.4
1	D	105	ARG	2.4
1	A	53	GLN	2.4
1	A	346	ASN	2.4
1	A	87	GLY	2.4
1	D	14	ALA	2.4
1	A	176	ASP	2.3
1	D	117	ASP	2.3
1	B	343	TYR	2.3
1	D	184	LYS	2.3
1	A	177	ALA	2.3
1	C	283	VAL	2.3
1	C	41	LEU	2.3
1	B	109	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	228	ASN	2.3
1	C	15	ALA	2.3
1	D	156	THR	2.3
1	C	53	GLN	2.3
1	D	331	GLU	2.3
1	B	50	ILE	2.3
1	D	83	LEU	2.3
1	D	51	THR	2.3
1	D	297	GLU	2.3
1	B	279	ILE	2.3
1	C	162	LYS	2.3
1	A	99	VAL	2.3
1	C	133	VAL	2.3
1	D	78	ASP	2.2
1	D	121	ASP	2.2
1	C	164	TYR	2.2
1	B	345	GLN	2.2
1	D	167	THR	2.2
1	B	226	VAL	2.2
1	B	165	ASN	2.2
1	A	301	GLN	2.2
1	D	15	ALA	2.2
1	B	183	SER	2.2
1	A	179	ASN	2.2
1	C	346	ASN	2.2
1	D	16	ARG	2.2
1	A	54	PRO	2.2
1	B	177	ALA	2.2
1	C	154	TYR	2.2
1	D	171	MET	2.2
1	D	238	ASN	2.2
1	B	93	LYS	2.2
1	B	278	GLY	2.2
1	D	256	HIS	2.2
1	A	85	SER	2.2
1	C	282	THR	2.2
1	D	153	SER	2.2
1	D	229	ARG	2.1
1	C	104	ILE	2.1
1	D	21	ASP	2.1
1	C	54	PRO	2.1
1	A	76	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	219	TYR	2.1
1	A	44	LYS	2.1
1	A	156	THR	2.1
1	C	39	ARG	2.1
1	D	47	LEU	2.1
1	B	283	VAL	2.1
1	C	296	TRP	2.1
1	B	162	LYS	2.1
1	B	235	ALA	2.1
1	A	47	LEU	2.1
1	C	47	LEU	2.1
1	C	100	ILE	2.1
1	C	102	GLN	2.1
1	D	185	LEU	2.1
1	B	327	ASP	2.1
1	D	86	ILE	2.1
1	C	25	VAL	2.1
1	C	88	VAL	2.1
1	C	90	VAL	2.1
1	A	210	TRP	2.1
1	A	203	ALA	2.0
1	D	234	LEU	2.0
1	B	259	PRO	2.0
1	A	80	MET	2.0
1	A	91	GLU	2.0
1	A	342	GLU	2.0
1	D	227	MET	2.0
1	D	115	GLN	2.0
1	D	123	PRO	2.0
1	A	347	LYS	2.0
1	D	112	LYS	2.0
1	D	347	LYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.