Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2023 – 07:19 AM EDT

PDB ID	:	2INF
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:

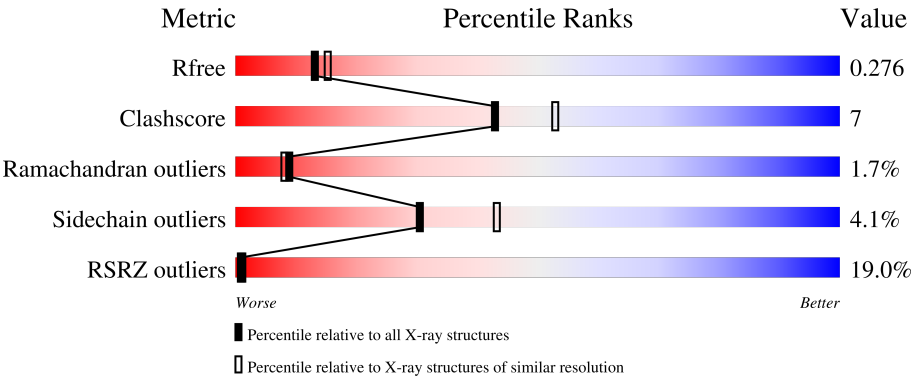
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	14% 77% 17%
1	B	359	20% 78% 16%
1	C	359	15% 83% 12%
1	D	359	24% 76% 18%

2 Entry composition (i)

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.

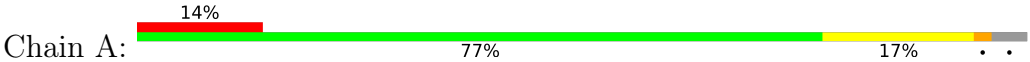
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	73	Total O 73 73	0	0
2	B	63	Total O 63 63	0	0
2	C	66	Total O 66 66	0	0
2	D	54	Total O 54 54	0	0

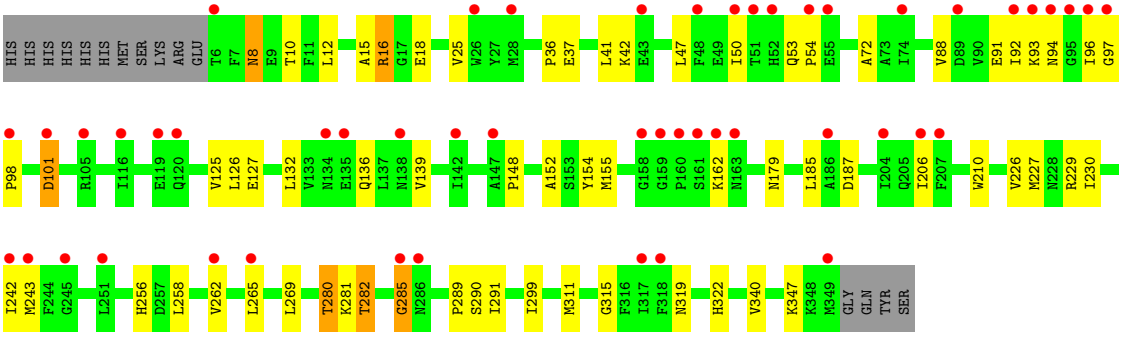
3 Residue-property plots (i)

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

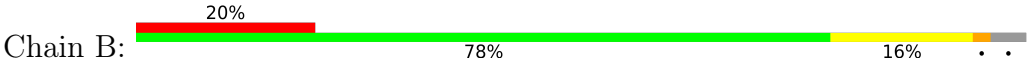
Chain A:

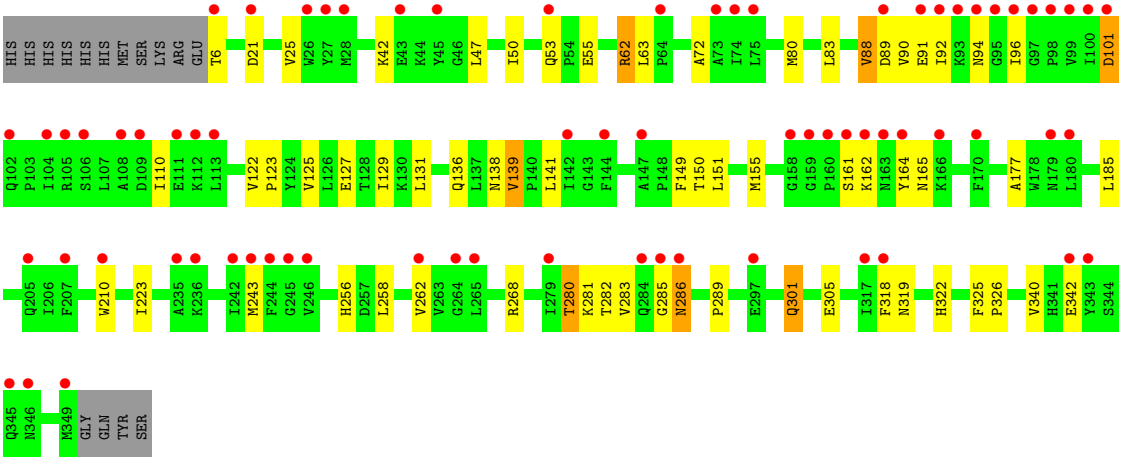




• Molecule 1: Uroporphyrinogen decarboxylase

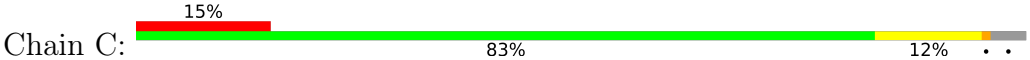
Chain B:

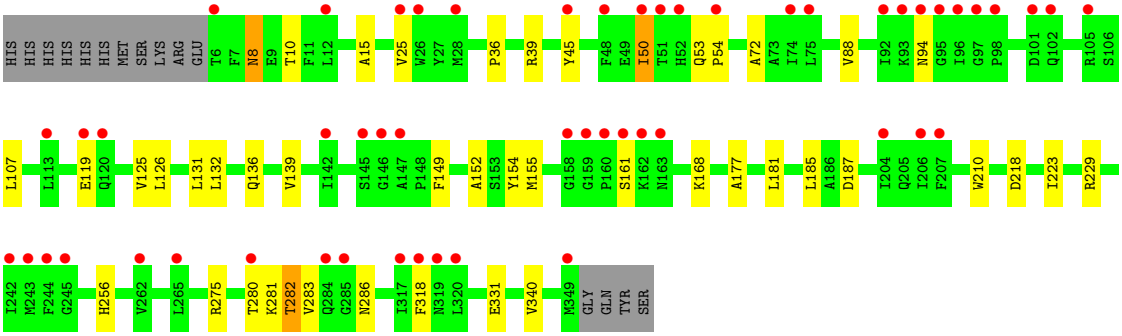




• Molecule 1: Uroporphyrinogen decarboxylase

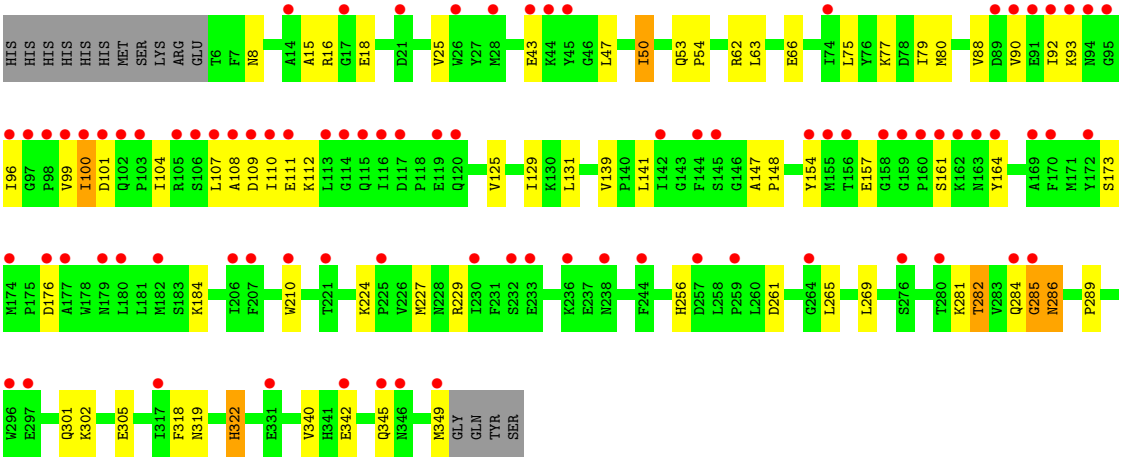
Chain C:





• Molecule 1: Uroporphyrinogen decarboxylase

Chain D:



4 Data and refinement statistics (i)

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 29.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (30.00-2.30) 96.2 (29.46-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.251 0.233 , 0.276	Depositor DCC
R_{free} test set	3316 reflections (5.09%)	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)	0.37 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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

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	0.52	0/2758	0.61	0/3740
1	B	0.51	0/2758	0.59	0/3740
1	C	0.51	0/2758	0.62	0/3740
1	D	0.79	9/2758 (0.3%)	0.69	3/3740 (0.1%)
All	All	0.59	9/11032 (0.1%)	0.63	3/14960 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	176	ASP	CG-OD1	13.39	1.56	1.25
1	D	111	GLU	CD-OE1	11.48	1.38	1.25
1	D	229	ARG	CD-NE	10.12	1.63	1.46
1	D	229	ARG	CZ-NH1	9.65	1.45	1.33
1	D	173	SER	CB-OG	7.51	1.52	1.42
1	D	184	LYS	CD-CE	6.79	1.68	1.51
1	D	107	LEU	CG-CD1	5.86	1.73	1.51
1	D	108	ALA	C-N	5.83	1.47	1.34
1	D	229	ARG	CZ-NH2	5.76	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	229	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	D	176	ASP	CB-CG-OD1	-7.38	111.66	118.30
1	D	108	ALA	O-C-N	5.46	131.43	122.70

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	2693	0	2686	50	0
1	B	2693	0	2686	36	0
1	C	2693	0	2686	30	0
1	D	2693	0	2686	33	0
2	A	73	0	0	0	0
2	B	63	0	0	3	0
2	C	66	0	0	2	0
2	D	54	0	0	0	0
All	All	11028	0	10744	146	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 (146) 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:155:MET:HE1	1:A:185:LEU:HD11	1.48	0.96
1:C:256:HIS:HE1	1:C:281:LYS:H	1.14	0.95
1:A:226:VAL:HG13	1:A:227:MET:HE2	1.60	0.84
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:A:148:PRO:HG2	1:A:227:MET:HE1	1.65	0.77
1:B:150:THR:HG23	1:B:210:TRP:CD1	2.19	0.76
1:C:155:MET:HE1	1:C:185:LEU:HD11	1.68	0.76
1:B:256:HIS:HE1	1:B:281:LYS:H	1.34	0.76
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLY:O	1:B:286:ASN:CB	2.40	0.68
1:A:148:PRO:HG2	1:A:227:MET:CE	2.25	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	1.81	0.61
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: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:80:MET:HA	1:B:80:MET:HE2	1.83	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:A:25:VAL:HG22	1:A:340:VAL:HG11	1.87	0.57
1:A:152:ALA:HA	1:A:155:MET:HE3	1.87	0.57
1:A:154:TYR:CZ	1:A:210:TRP:HH2	2.23	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:227:MET:HE1	1:A:230:ILE:HD12	1.89	0.55
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:A:227:MET:HE2	1:A:227:MET:N	2.23	0.53
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:155:MET:HE1	1:C:181:LEU:HD11	1.92	0.51
1:C:107:LEU:HD13	1:C:177:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLU:HG3	1:D:164:TYR:HD2	1.76	0.51
1:A:8:ASN:C	1:A:8:ASN:HD22	2.13	0.51
1:A:91:GLU:O	1:A:98:PRO:HA	2.11	0.51
1:B:258:LEU:O	1:B:281:LYS:NZ	2.44	0.50
1:D:147:ALA:HB1	1:D:227:MET:HE3	1.94	0.50
1:D:289:PRO:HG2	1:D:322:HIS:HB3	1.93	0.50
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:A:206:ILE:HG21	1:A:243:MET:HE3	1.94	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: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
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:B:243:MET:HE1	2:B:396:HOH:O	2.14	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: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:D:157:GLU:HG3	1:D:164:TYR:CD2	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:CG2	1:A:243:MET:HE3	2.47	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:152:ALA:HA	1:C:155:MET:HE3	1.99	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:A:206:ILE:CG2	1:A:243:MET:CE	2.98	0.42
1:A:132:LEU:HA	1:A:136:GLN:HB2	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
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:148:PRO:CG	1:A:227:MET:HE1	2.44	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: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:D:345:GLN:HE21	1:D:349:MET:CE	2.33	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:C:155:MET:CE	1:C:181:LEU:HD11	2.50	0.41
1:D:148:PRO:HD2	1:D:227:MET:HE1	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:155:MET:HE1	1:B:185:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	342/359 (95%)	323 (94%)	13 (4%)	6 (2%)	8 7
1	B	342/359 (95%)	325 (95%)	10 (3%)	7 (2%)	7 6
1	C	342/359 (95%)	329 (96%)	10 (3%)	3 (1%)	17 20
1	D	342/359 (95%)	323 (94%)	12 (4%)	7 (2%)	7 6
All	All	1368/1436 (95%)	1300 (95%)	45 (3%)	23 (2%)	9 8

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

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Mol	Chain	Res	Type
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 (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	288/308 (94%)	278 (96%)	10 (4%)	36	50
1	B	288/308 (94%)	274 (95%)	14 (5%)	25	35
1	C	288/308 (94%)	278 (96%)	10 (4%)	36	50
1	D	288/308 (94%)	275 (96%)	13 (4%)	27	39
All	All	1152/1232 (94%)	1105 (96%)	47 (4%)	30	43

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	16	ARG
1	A	47	LEU
1	A	88	VAL
1	A	101	ASP
1	A	125	VAL
1	A	126	LEU
1	A	179	ASN
1	A	280	THR

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Mol	Chain	Res	Type
1	A	282	THR
1	B	21	ASP
1	B	47	LEU
1	B	62	ARG
1	B	63	LEU
1	B	88	VAL
1	B	89	ASP
1	B	101	ASP
1	B	131	LEU
1	B	139	VAL
1	B	268	ARG
1	B	280	THR
1	B	283	VAL
1	B	301	GLN
1	B	342	GLU
1	C	8	ASN
1	C	50	ILE
1	C	88	VAL
1	C	119	GLU
1	C	125	VAL
1	C	126	LEU
1	C	131	LEU
1	C	275	ARG
1	C	282	THR
1	C	283	VAL
1	D	8	ASN
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	131	LEU
1	D	139	VAL
1	D	224	LYS
1	D	282	THR
1	D	322	HIS
1	D	342	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	52	HIS
1	A	256	HIS
1	A	286	ASN
1	B	8	ASN
1	B	52	HIS
1	B	53	GLN
1	B	136	GLN
1	B	256	HIS
1	C	8	ASN
1	C	52	HIS
1	C	102	GLN
1	C	136	GLN
1	C	256	HIS
1	D	8	ASN
1	D	136	GLN
1	D	256	HIS
1	D	345	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	344/359 (95%)	1.05	50 (14%)	2 3	46, 52, 69, 83	0
1	B	344/359 (95%)	1.25	72 (20%)	1 1	45, 52, 74, 87	0
1	C	344/359 (95%)	1.00	53 (15%)	2 3	45, 52, 68, 80	0
1	D	344/359 (95%)	1.47	86 (25%)	0 0	45, 53, 70, 82	0
All	All	1376/1436 (95%)	1.19	261 (18%)	1 1	45, 52, 71, 87	0

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	97	GLY	14.0
1	D	94	ASN	9.7
1	B	158	GLY	8.7
1	D	158	GLY	8.3
1	D	159	GLY	7.9
1	C	94	ASN	7.9
1	D	160	PRO	7.8
1	B	95	GLY	7.5
1	A	159	GLY	7.1
1	B	92	ILE	6.9
1	B	108	ALA	6.8
1	B	96	ILE	6.8
1	D	95	GLY	6.7
1	C	160	PRO	6.6
1	A	160	PRO	6.6
1	B	160	PRO	6.6
1	D	93	LYS	6.5
1	D	101	ASP	6.4
1	C	95	GLY	6.2
1	A	97	GLY	6.1
1	D	108	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	159	GLY	6.0
1	B	101	ASP	6.0
1	C	159	GLY	5.9
1	D	180	LEU	5.9
1	A	158	GLY	5.8
1	D	113	LEU	5.8
1	B	346	ASN	5.8
1	D	170	PHE	5.8
1	D	120	GLN	5.6
1	C	158	GLY	5.5
1	D	114	GLY	5.4
1	D	106	SER	5.4
1	C	93	LYS	5.3
1	C	101	ASP	5.1
1	A	96	ILE	5.1
1	B	74	ILE	5.1
1	C	97	GLY	5.1
1	A	92	ILE	5.0
1	D	97	GLY	5.0
1	D	98	PRO	5.0
1	C	242	ILE	4.9
1	D	96	ILE	4.9
1	D	349	MET	4.9
1	B	94	ASN	4.8
1	D	43	GLU	4.6
1	D	162	LYS	4.6
1	D	92	ILE	4.5
1	D	100	ILE	4.5
1	B	43	GLU	4.4
1	D	105	ARG	4.4
1	A	94	ASN	4.4
1	A	119	GLU	4.3
1	B	235	ALA	4.3
1	D	116	ILE	4.3
1	B	26	TRP	4.3
1	D	238	ASN	4.2
1	D	74	ILE	4.2
1	C	163	ASN	4.0
1	B	98	PRO	4.0
1	B	170	PHE	4.0
1	D	225	PRO	3.9
1	D	221	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	99	VAL	3.9
1	C	92	ILE	3.9
1	D	117	ASP	3.9
1	D	107	LEU	3.8
1	B	100	ILE	3.8
1	D	45	TYR	3.8
1	B	105	ARG	3.8
1	B	6	THR	3.8
1	C	120	GLN	3.8
1	C	317	ILE	3.7
1	A	349	MET	3.7
1	B	349	MET	3.7
1	D	161	SER	3.7
1	B	207	PHE	3.7
1	A	242	ILE	3.7
1	B	164	TYR	3.7
1	B	93	LYS	3.7
1	A	95	GLY	3.7
1	B	180	LEU	3.7
1	B	163	ASN	3.7
1	D	179	ASN	3.6
1	C	285	GLY	3.6
1	D	142	ILE	3.6
1	A	50	ILE	3.6
1	C	349	MET	3.6
1	B	142	ILE	3.5
1	D	44	LYS	3.5
1	D	176	ASP	3.5
1	D	169	ALA	3.4
1	D	109	ASP	3.4
1	D	163	ASN	3.4
1	B	28	MET	3.3
1	D	103	PRO	3.3
1	A	93	LYS	3.3
1	C	96	ILE	3.3
1	A	120	GLN	3.2
1	B	106	SER	3.2
1	B	111	GLU	3.2
1	D	297	GLU	3.2
1	C	102	GLN	3.2
1	A	162	LYS	3.2
1	B	285	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	51	THR	3.1
1	D	259	PRO	3.1
1	B	161	SER	3.1
1	A	6	THR	3.1
1	C	206	ILE	3.1
1	B	144	PHE	3.1
1	D	285	GLY	3.1
1	D	164	TYR	3.1
1	C	161	SER	3.0
1	C	207	PHE	3.0
1	B	99	VAL	3.0
1	C	6	THR	3.0
1	D	89	ASP	3.0
1	C	105	ARG	3.0
1	D	264	GLY	2.9
1	B	91	GLU	2.9
1	D	346	ASN	2.9
1	C	142	ILE	2.9
1	B	245	GLY	2.9
1	C	204	ILE	2.9
1	A	101	ASP	2.9
1	D	207	PHE	2.9
1	D	17	GLY	2.9
1	A	142	ILE	2.8
1	C	74	ILE	2.8
1	C	50	ILE	2.8
1	D	296	TRP	2.8
1	B	244	PHE	2.8
1	C	245	GLY	2.8
1	C	26	TRP	2.7
1	D	91	GLU	2.7
1	D	210	TRP	2.7
1	A	74	ILE	2.7
1	A	204	ILE	2.7
1	D	155	MET	2.7
1	D	111	GLU	2.7
1	C	243	MET	2.6
1	B	53	GLN	2.6
1	B	343	TYR	2.6
1	D	342	GLU	2.6
1	B	242	ILE	2.6
1	B	102	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	119	GLU	2.6
1	C	162	LYS	2.6
1	A	186	ALA	2.6
1	D	26	TRP	2.6
1	C	98	PRO	2.6
1	A	285	GLY	2.6
1	D	345	GLN	2.6
1	D	174	MET	2.5
1	D	110	ILE	2.5
1	B	89	ASP	2.5
1	A	28	MET	2.5
1	C	54	PRO	2.5
1	B	109	ASP	2.5
1	A	134	ASN	2.5
1	A	26	TRP	2.5
1	C	145	SER	2.5
1	B	64	PRO	2.5
1	A	163	ASN	2.5
1	A	161	SER	2.4
1	C	28	MET	2.4
1	A	317	ILE	2.4
1	B	317	ILE	2.4
1	A	43	GLU	2.4
1	A	243	MET	2.4
1	D	177	ALA	2.4
1	C	244	PHE	2.4
1	A	51	THR	2.4
1	D	206	ILE	2.4
1	B	284	GLN	2.4
1	C	265	LEU	2.4
1	B	264	GLY	2.4
1	B	342	GLU	2.4
1	B	246	VAL	2.4
1	D	119	GLU	2.4
1	A	147	ALA	2.4
1	A	251	LEU	2.4
1	B	265	LEU	2.4
1	A	48	PHE	2.4
1	B	345	GLN	2.4
1	D	276	SER	2.4
1	A	245	GLY	2.3
1	B	27	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	75	LEU	2.3
1	D	284	GLN	2.3
1	D	232	SER	2.3
1	C	75	LEU	2.3
1	C	262	VAL	2.3
1	A	138	ASN	2.3
1	A	265	LEU	2.3
1	B	210	TRP	2.3
1	C	146	GLY	2.3
1	D	21	ASP	2.3
1	D	280	THR	2.3
1	D	236	LYS	2.3
1	D	257	ASP	2.3
1	C	12	LEU	2.3
1	D	28	MET	2.3
1	D	182	MET	2.3
1	C	48	PHE	2.3
1	D	90	VAL	2.3
1	D	244	PHE	2.3
1	A	54	PRO	2.3
1	D	14	ALA	2.3
1	B	112	LYS	2.2
1	B	45	TYR	2.2
1	B	205	GLN	2.2
1	B	318	PHE	2.2
1	D	317	ILE	2.2
1	A	98	PRO	2.2
1	D	144	PHE	2.2
1	A	89	ASP	2.2
1	A	206	ILE	2.2
1	B	104	ILE	2.2
1	A	55	GLU	2.2
1	C	147	ALA	2.2
1	B	21	ASP	2.2
1	B	262	VAL	2.2
1	C	318	PHE	2.2
1	B	147	ALA	2.2
1	B	279	ILE	2.2
1	D	230	ILE	2.2
1	C	284	GLN	2.2
1	B	162	LYS	2.1
1	B	166	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	236	LYS	2.1
1	A	207	PHE	2.1
1	D	102	GLN	2.1
1	B	179	ASN	2.1
1	B	297	GLU	2.1
1	C	52	HIS	2.1
1	D	154	TYR	2.1
1	B	113	LEU	2.1
1	C	320	LEU	2.1
1	C	25	VAL	2.1
1	A	286	ASN	2.1
1	D	233	GLU	2.1
1	C	45	TYR	2.1
1	A	116	ILE	2.1
1	A	262	VAL	2.1
1	A	52	HIS	2.0
1	C	280	THR	2.0
1	D	156	THR	2.0
1	D	145	SER	2.0
1	D	331	GLU	2.0
1	A	318	PHE	2.0
1	D	172	TYR	2.0
1	B	286	ASN	2.0
1	A	135	GLU	2.0
1	A	105	ARG	2.0
1	C	319	ASN	2.0
1	C	113	LEU	2.0
1	B	243	MET	2.0
1	D	115	GLN	2.0
1	B	73	ALA	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.