



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:19 AM UTC

PDB ID : 4FJS / pdb_00004fjs
Title : Crystal structure of ureidoglycolate dehydrogenase enzyme in apo form
Authors : Kim, M.I.; Shin, I.; Lee, J.; Rhee, S.
Deposited on : 2012-06-12
Resolution : 2.13 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

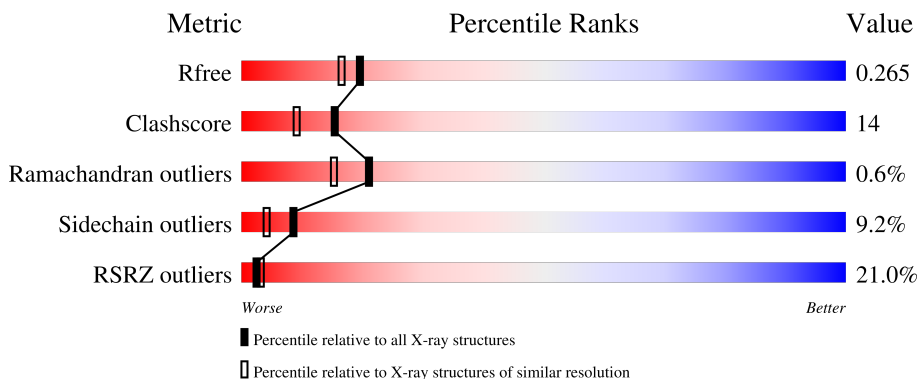
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	351	
1	B	351	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5459 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 Ureidoglycolate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	2570	1621	450	483	16	0	0	0
1	B	315	2389	1502	426	446	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B1XGB5
A	0	HIS	-	expression tag	UNP B1XGB5
B	-1	GLY	-	expression tag	UNP B1XGB5
B	0	HIS	-	expression tag	UNP B1XGB5

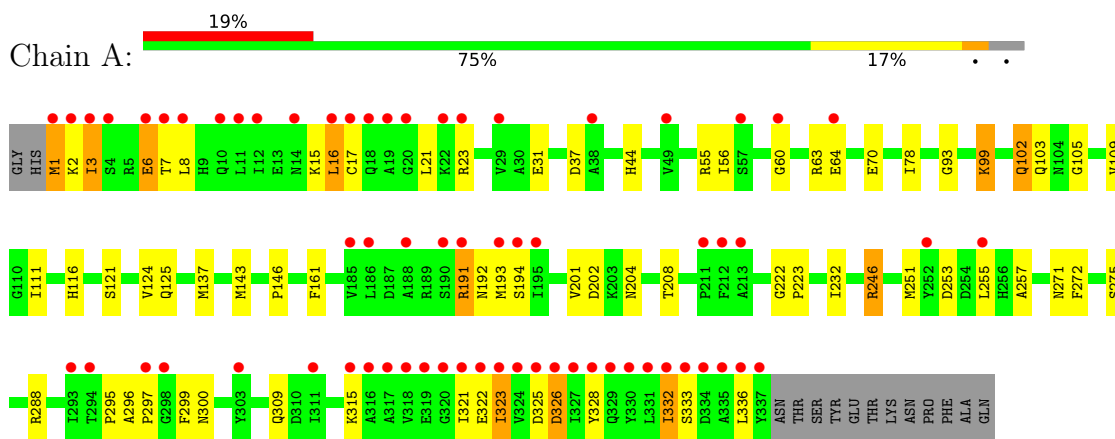
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	232	Total	O	0	0
			232	232		
2	B	268	Total	O	0	0
			268	268		

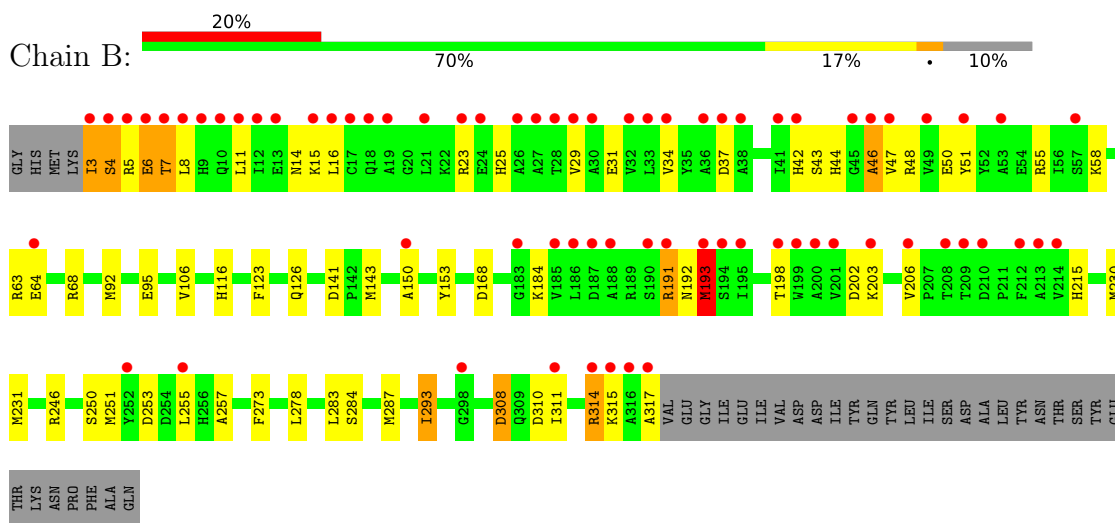
3 Residue-property plots [i](#)

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: Ureidoglycolate dehydrogenase



- Molecule 1: Ureidoglycolate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	162.76Å 162.76Å 61.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.13 49.18 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.18-2.13) 92.7 (49.18-2.13)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.75 (at 2.12Å)	Xtrriage
Refinement program	PHENIX 1.7.2_869, CNS	Depositor
R, R_{free}	0.222 , 0.240 0.247 , 0.265	Depositor DCC
R_{free} test set	2000 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtrriage
Anisotropy	0.006	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5459	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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 [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	0.53	0/2625	0.85	1/3558 (0.0%)
1	B	0.57	2/2441 (0.1%)	0.86	2/3308 (0.1%)
All	All	0.55	2/5066 (0.0%)	0.85	3/6866 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	193	MET	CG-SD	6.64	1.97	1.80
1	B	193	MET	SD-CE	6.62	1.96	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ASP	N-CA-C	9.17	121.28	111.28
1	B	184	LYS	N-CA-C	-6.39	106.07	114.31
1	B	314	ARG	N-CA-C	-6.24	104.64	112.93

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	2570	0	2528	69	2
1	B	2389	0	2347	67	1
2	A	232	0	0	44	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	268	0	0	44	4
All	All	5459	0	4875	133	8

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 14.

All (133) 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:B:42:HIS:HA	2:B:639:HOH:O	1.27	1.24
1:B:231:MET:SD	2:B:565:HOH:O	1.99	1.20
1:A:3:ILE:HG13	2:A:615:HOH:O	1.40	1.17
1:A:271:ASN:ND2	2:A:441:HOH:O	1.81	1.12
1:A:288:ARG:NH1	2:A:596:HOH:O	1.88	1.05
1:A:295:PRO:C	2:A:604:HOH:O	2.00	1.05
1:B:15:LYS:NZ	2:B:587:HOH:O	1.86	0.99
1:A:299:PHE:HA	2:A:602:HOH:O	1.59	0.99
1:B:317:ALA:O	2:B:653:HOH:O	1.80	0.99
1:A:31:GLU:OE1	2:A:606:HOH:O	1.81	0.98
1:A:6:GLU:O	2:A:560:HOH:O	1.80	0.98
1:B:15:LYS:CE	2:B:587:HOH:O	2.09	0.98
1:B:68:ARG:NH1	2:B:603:HOH:O	1.94	0.97
1:A:299:PHE:CA	2:A:602:HOH:O	2.13	0.96
1:B:253:ASP:OD1	2:B:576:HOH:O	1.87	0.92
1:A:202:ASP:OD2	2:A:611:HOH:O	1.88	0.92
1:B:6:GLU:OE1	2:B:579:HOH:O	1.85	0.91
1:B:37:ASP:OD1	2:B:639:HOH:O	1.87	0.91
1:B:68:ARG:NH2	2:B:603:HOH:O	2.00	0.90
1:B:168:ASP:OD1	2:B:656:HOH:O	1.89	0.89
1:A:103:GLN:NE2	2:A:580:HOH:O	2.05	0.88
1:B:141:ASP:OD1	2:B:647:HOH:O	1.91	0.87
1:A:300:ASN:N	2:A:602:HOH:O	1.94	0.86
1:B:37:ASP:OD1	2:B:568:HOH:O	1.94	0.86
2:A:604:HOH:O	1:B:150:ALA:HB2	1.76	0.85
1:B:95:GLU:OE1	2:B:507:HOH:O	1.94	0.83
1:A:1:MET:HG3	1:A:2:LYS:N	1.94	0.81
1:A:64:GLU:OE1	2:A:572:HOH:O	1.99	0.80
2:A:604:HOH:O	1:B:150:ALA:CB	2.30	0.79
1:B:68:ARG:CZ	2:B:603:HOH:O	2.23	0.79
1:B:310:ASP:OD2	2:B:424:HOH:O	2.00	0.78
1:A:70:GLU:OE2	2:A:545:HOH:O	2.01	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PRO:O	2:A:604:HOH:O	1.97	0.78
1:B:37:ASP:CG	2:B:568:HOH:O	2.26	0.77
1:A:3:ILE:CG1	2:A:615:HOH:O	2.13	0.77
1:B:50:GLU:O	2:B:462:HOH:O	2.01	0.77
1:A:103:GLN:OE1	2:A:552:HOH:O	2.03	0.76
1:B:37:ASP:OD2	2:B:568:HOH:O	2.03	0.76
1:B:44:HIS:HD2	1:B:116:HIS:HE1	1.35	0.75
1:A:309:GLN:OE1	2:A:550:HOH:O	2.07	0.73
1:B:314:ARG:O	2:B:578:HOH:O	2.06	0.72
1:B:5:ARG:HA	2:B:426:HOH:O	1.88	0.72
1:B:42:HIS:ND1	2:B:639:HOH:O	1.94	0.72
1:B:50:GLU:C	2:B:462:HOH:O	2.31	0.71
1:B:3:ILE:N	2:B:628:HOH:O	2.23	0.71
1:A:99:LYS:CE	2:A:577:HOH:O	2.35	0.70
1:A:326:ASP:OD2	1:A:326:ASP:N	2.22	0.70
1:B:4:SER:O	2:B:426:HOH:O	2.09	0.70
1:B:44:HIS:CD2	1:B:116:HIS:HE1	2.09	0.69
1:A:204:ASN:HB2	2:A:573:HOH:O	1.93	0.69
1:B:250:SER:HB2	2:B:660:HOH:O	1.94	0.68
1:A:60:GLY:C	2:A:553:HOH:O	2.37	0.66
1:A:253:ASP:OD1	2:A:490:HOH:O	2.13	0.66
1:A:3:ILE:CB	2:A:615:HOH:O	2.41	0.66
1:B:3:ILE:N	2:B:556:HOH:O	2.29	0.65
1:A:99:LYS:NZ	2:A:577:HOH:O	1.91	0.65
1:B:15:LYS:CD	2:B:587:HOH:O	2.39	0.65
1:B:23:ARG:NH1	2:B:573:HOH:O	1.95	0.64
1:A:17:CYS:O	2:A:526:HOH:O	2.15	0.64
1:A:99:LYS:HE3	2:A:577:HOH:O	1.98	0.62
1:A:102:GLN:NE2	2:A:556:HOH:O	1.95	0.62
1:A:78:ILE:HD11	1:B:273:PHE:HA	1.81	0.62
1:A:55:ARG:HD3	2:A:553:HOH:O	2.00	0.61
1:A:44:HIS:HD2	1:A:116:HIS:HE1	1.49	0.60
1:A:288:ARG:NE	2:A:551:HOH:O	2.13	0.58
1:A:336:LEU:HD11	2:A:513:HOH:O	2.05	0.56
1:A:6:GLU:HA	2:A:605:HOH:O	2.06	0.55
1:A:3:ILE:HB	2:A:615:HOH:O	2.06	0.55
1:A:6:GLU:CB	2:A:605:HOH:O	2.56	0.53
1:A:1:MET:HG3	1:A:2:LYS:H	1.74	0.52
1:A:44:HIS:HD2	1:A:116:HIS:CE1	2.28	0.52
1:B:15:LYS:HD3	2:B:587:HOH:O	2.03	0.52
1:A:246:ARG:NH2	2:A:425:HOH:O	2.16	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASN:HA	2:B:573:HOH:O	2.10	0.51
1:A:297:PRO:HA	2:A:563:HOH:O	2.09	0.51
1:B:14:ASN:HB2	2:B:609:HOH:O	2.10	0.51
1:A:37:ASP:HB3	1:A:321:ILE:HG21	1.93	0.51
1:A:6:GLU:HB3	2:A:605:HOH:O	2.11	0.50
1:A:93:GLY:HA3	1:A:111:ILE:HD11	1.93	0.50
1:B:153:TYR:CD1	1:B:246:ARG:HG3	2.47	0.50
1:B:51:TYR:HA	2:B:462:HOH:O	2.10	0.50
1:A:146:PRO:HG3	1:B:293:ILE:HD12	1.92	0.49
1:B:46:ALA:N	2:B:568:HOH:O	2.45	0.49
1:B:8:LEU:HB2	2:B:426:HOH:O	2.11	0.49
1:A:55:ARG:NH1	1:A:257:ALA:O	2.45	0.48
1:A:6:GLU:H	1:A:6:GLU:CD	2.22	0.48
1:A:296:ALA:N	2:A:604:HOH:O	2.33	0.47
1:B:3:ILE:HD11	1:B:8:LEU:HD13	1.96	0.47
1:A:1:MET:HB3	1:A:323:ILE:O	2.15	0.47
1:A:102:GLN:NE2	2:A:580:HOH:O	2.46	0.46
1:A:191:ARG:HH11	1:A:191:ARG:HB3	1.80	0.46
1:A:6:GLU:CA	2:A:605:HOH:O	2.63	0.46
1:B:284:SER:HA	1:B:287:MET:HE3	1.96	0.46
1:A:161:PHE:CD1	1:B:231:MET:HG3	2.50	0.46
1:B:8:LEU:HD12	1:B:8:LEU:HA	1.67	0.46
1:B:50:GLU:N	2:B:641:HOH:O	2.47	0.46
1:B:308:ASP:OD1	1:B:308:ASP:N	2.44	0.46
1:A:328:TYR:CE1	2:A:554:HOH:O	2.68	0.45
1:A:137:MET:HB2	1:A:232:ILE:HG23	1.98	0.45
1:B:3:ILE:CA	2:B:556:HOH:O	2.66	0.44
1:B:191:ARG:HD3	1:B:193:MET:HE3	1.99	0.44
1:A:332:ILE:H	1:A:332:ILE:HG12	1.33	0.44
1:B:68:ARG:NH2	2:B:517:HOH:O	2.49	0.44
1:A:3:ILE:O	1:A:321:ILE:N	2.46	0.44
1:A:2:LYS:HE3	1:A:2:LYS:HB2	1.64	0.44
1:B:198:THR:OG1	2:B:668:HOH:O	2.12	0.43
1:A:1:MET:HE2	1:A:1:MET:HB2	1.76	0.43
1:B:47:VAL:HB	2:B:608:HOH:O	2.18	0.43
1:B:4:SER:O	1:B:7:THR:HB	2.18	0.43
1:A:222:GLY:HA3	1:A:223:PRO:HD3	1.90	0.43
1:B:44:HIS:CD2	1:B:116:HIS:CE1	2.99	0.43
1:B:203:LYS:HD3	1:B:215:HIS:HB2	2.01	0.43
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.88	0.42
1:B:42:HIS:CB	2:B:639:HOH:O	2.56	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASP:OD1	1:B:206:VAL:HB	2.19	0.42
1:B:311:ILE:HA	1:B:314:ARG:HG3	2.02	0.42
1:A:125:GLN:NE2	2:A:567:HOH:O	2.50	0.42
1:B:278:LEU:HA	1:B:278:LEU:HD23	1.84	0.42
1:A:7:THR:OG1	2:A:615:HOH:O	1.97	0.41
1:A:121:SER:HA	1:A:124:VAL:HG22	2.01	0.41
1:B:123:PHE:O	1:B:126:GLN:HB2	2.20	0.41
1:A:1:MET:CG	1:A:2:LYS:N	2.77	0.41
1:B:253:ASP:CB	2:B:576:HOH:O	2.68	0.41
1:B:55:ARG:NH1	1:B:257:ALA:O	2.53	0.41
1:A:44:HIS:CD2	1:A:116:HIS:CE1	3.08	0.41
1:A:21:LEU:HG	1:A:56:ILE:HD13	2.03	0.41
1:A:299:PHE:CB	2:A:602:HOH:O	2.61	0.41
1:B:14:ASN:CB	2:B:609:HOH:O	2.68	0.41
1:B:25:HIS:O	1:B:29:VAL:HG23	2.21	0.41
1:B:230:MET:HE3	1:B:230:MET:HB3	2.00	0.40
1:A:105:GLY:HA2	1:A:272:PHE:CD1	2.57	0.40
1:B:58:LYS:NZ	2:B:410:HOH:O	2.31	0.40
1:A:3:ILE:HD11	1:A:8:LEU:HB2	2.03	0.40

All (8) 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)
2:B:594:HOH:O	2:B:610:HOH:O[7_555]	1.57	0.63
2:B:492:HOH:O	2:B:517:HOH:O[8_554]	1.82	0.38
1:A:1:MET:CE	1:A:204:ASN:ND2[3_544]	1.90	0.30
2:A:552:HOH:O	2:A:600:HOH:O[8_554]	1.96	0.24
2:B:520:HOH:O	2:B:638:HOH:O[7_555]	2.00	0.20
1:B:7:THR:OG1	1:B:7:THR:OG1[7_555]	2.06	0.14
2:B:508:HOH:O	2:B:508:HOH:O[8_555]	2.14	0.06
1:A:271:ASN:O	1:A:275:SER:OG[8_554]	2.18	0.02

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	335/351 (95%)	319 (95%)	15 (4%)	1 (0%)	36	33
1	B	313/351 (89%)	295 (94%)	15 (5%)	3 (1%)	12	7
All	All	648/702 (92%)	614 (95%)	30 (5%)	4 (1%)	21	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER
1	B	192	ASN
1	B	46	ALA
1	B	143	MET

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	266/278 (96%)	241 (91%)	25 (9%)	8	4
1	B	246/278 (88%)	224 (91%)	22 (9%)	9	4
All	All	512/556 (92%)	465 (91%)	47 (9%)	8	4

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ILE
1	A	6	GLU
1	A	15	LYS
1	A	16	LEU
1	A	23	ARG
1	A	63	ARG
1	A	99	LYS
1	A	102	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	109	VAL
1	A	143	MET
1	A	191	ARG
1	A	192	ASN
1	A	193	MET
1	A	194	SER
1	A	201	VAL
1	A	208	THR
1	A	246	ARG
1	A	251	MET
1	A	255	LEU
1	A	315	LYS
1	A	322	GLU
1	A	323	ILE
1	A	326	ASP
1	A	332	ILE
1	B	3	ILE
1	B	4	SER
1	B	6	GLU
1	B	7	THR
1	B	11	LEU
1	B	16	LEU
1	B	31	GLU
1	B	34	VAL
1	B	43	SER
1	B	48	ARG
1	B	63	ARG
1	B	64	GLU
1	B	92	MET
1	B	106	VAL
1	B	191	ARG
1	B	193	MET
1	B	251	MET
1	B	255	LEU
1	B	283	LEU
1	B	293	ILE
1	B	308	ASP
1	B	315	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	14	ASN
1	A	44	HIS
1	A	103	GLN
1	A	104	ASN
1	A	125	GLN
1	A	271	ASN
1	A	300	ASN
1	B	18	GLN
1	B	44	HIS
1	B	116	HIS
1	B	180	GLN
1	B	291	ASN

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 [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, 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	337/351 (96%)	1.05	66 (19%) 3 4	12, 30, 65, 79	0
1	B	315/351 (89%)	1.10	71 (22%) 2 2	11, 30, 61, 92	0
All	All	652/702 (92%)	1.08	137 (21%) 2 3	11, 30, 64, 92	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	ILE	6.0
1	B	3	ILE	5.8
1	A	1	MET	5.7
1	B	193	MET	5.5
1	B	8	LEU	5.5
1	A	335	ALA	5.5
1	B	7	THR	5.4
1	A	324	VAL	5.3
1	B	38	ALA	5.1
1	A	328	TYR	5.0
1	A	318	VAL	4.9
1	A	331	LEU	4.8
1	B	46	ALA	4.8
1	A	336	LEU	4.8
1	A	337	TYR	4.7
1	B	317	ALA	4.6
1	B	47	VAL	4.5
1	B	186	LEU	4.5
1	A	332	ILE	4.4
1	A	325	ASP	4.3
1	B	252	TYR	4.2
1	B	12	ILE	4.2
1	A	330	TYR	4.2
1	A	333	SER	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	4.0
1	B	34	VAL	3.9
1	A	327	ILE	3.8
1	B	21	LEU	3.8
1	B	19	ALA	3.8
1	A	252	TYR	3.7
1	A	329	GLN	3.7
1	B	49	VAL	3.7
1	A	19	ALA	3.6
1	B	6	GLU	3.6
1	B	191	ARG	3.6
1	B	11	LEU	3.6
1	B	190	SER	3.6
1	A	326	ASP	3.6
1	A	8	LEU	3.6
1	A	17	CYS	3.6
1	A	321	ILE	3.5
1	B	9	HIS	3.4
1	B	17	CYS	3.3
1	B	37	ASP	3.3
1	A	298	GLY	3.2
1	B	45	GLY	3.2
1	B	5	ARG	3.2
1	A	12	ILE	3.2
1	B	212	PHE	3.2
1	B	18	GLN	3.2
1	B	41	ILE	3.2
1	B	315	LYS	3.2
1	A	322	GLU	3.1
1	B	30	ALA	3.1
1	B	183	GLY	3.1
1	B	26	ALA	3.1
1	A	188	ALA	3.0
1	B	213	ALA	3.0
1	B	316	ALA	3.0
1	A	4	SER	3.0
1	B	51	TYR	3.0
1	B	214	VAL	3.0
1	A	2	LYS	3.0
1	A	6	GLU	3.0
1	A	195	ILE	3.0
1	A	317	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	194	SER	2.9
1	A	3	ILE	2.9
1	B	255	LEU	2.9
1	B	29	VAL	2.9
1	B	198	THR	2.9
1	B	36	ALA	2.9
1	A	297	PRO	2.9
1	A	193	MET	2.8
1	B	33	LEU	2.8
1	B	16	LEU	2.8
1	A	315	LYS	2.8
1	B	57	SER	2.8
1	A	320	GLY	2.8
1	B	4	SER	2.7
1	B	13	GLU	2.7
1	B	208	THR	2.7
1	A	334	ASP	2.7
1	A	316	ALA	2.6
1	B	314	ARG	2.6
1	B	150	ALA	2.6
1	B	210	ASP	2.5
1	B	27	ALA	2.5
1	A	255	LEU	2.4
1	A	7	THR	2.4
1	A	185	VAL	2.4
1	A	38	ALA	2.4
1	A	186	LEU	2.4
1	A	18	GLN	2.4
1	A	20	GLY	2.4
1	B	187	ASP	2.4
1	B	42	HIS	2.4
1	A	14	ASN	2.3
1	A	319	GLU	2.3
1	B	10	GLN	2.3
1	B	185	VAL	2.3
1	B	188	ALA	2.3
1	B	15	LYS	2.3
1	A	57	SER	2.3
1	B	311	ILE	2.3
1	A	11	LEU	2.3
1	B	23	ARG	2.2
1	A	22	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	53	ALA	2.2
1	A	64	GLU	2.2
1	A	29	VAL	2.2
1	A	16	LEU	2.2
1	A	303	TYR	2.2
1	A	191	ARG	2.2
1	B	203	LYS	2.2
1	A	293	ILE	2.2
1	A	190	SER	2.2
1	B	28	THR	2.2
1	A	311	ILE	2.1
1	B	200	ALA	2.1
1	B	24	GLU	2.1
1	B	64	GLU	2.1
1	B	298	GLY	2.1
1	A	49	VAL	2.1
1	A	60	GLY	2.1
1	B	32	VAL	2.1
1	B	201	VAL	2.1
1	B	206	VAL	2.1
1	A	213	ALA	2.1
1	A	10	GLN	2.0
1	A	23	ARG	2.0
1	A	211	PRO	2.0
1	A	294	THR	2.0
1	B	195	ILE	2.0
1	A	194	SER	2.0
1	B	199	TRP	2.0
1	B	209	THR	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.