



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:30 PM UTC

PDB ID : 9RFA / pdb_00009rfa
Title : Apo structure of glxR
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Deposited on : 2025-06-04
Resolution : 2.07 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

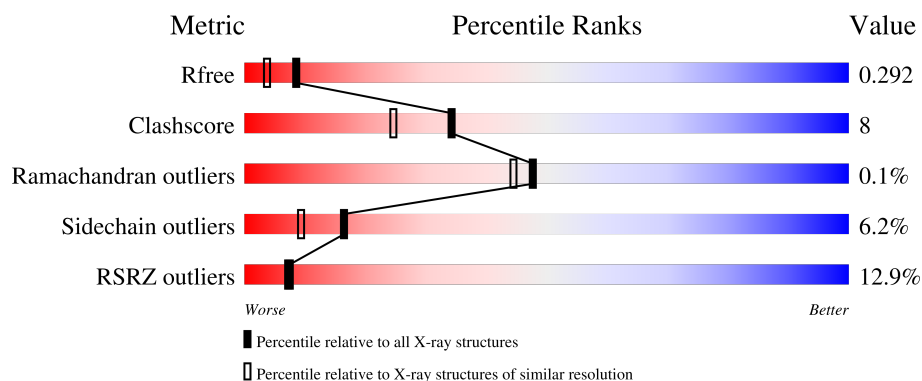
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	312	9% 81% 12% • 5%
1	B	312	23% 70% 21% • 5%
1	C	312	9% 80% 15% 5%
1	D	312	8% 79% 13% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8736 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 Probable oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2171	1364	387	408	12			
1	B	296	Total	C	N	O	S	0	0	0
			2170	1363	385	410	12			
1	C	296	Total	C	N	O	S	0	0	0
			2170	1363	385	410	12			
1	D	297	Total	C	N	O	S	0	0	0
			2180	1369	389	410	12			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9I3L2
A	2	GLY	-	expression tag	UNP Q9I3L2
A	3	HIS	-	expression tag	UNP Q9I3L2
A	4	HIS	-	expression tag	UNP Q9I3L2
A	5	HIS	-	expression tag	UNP Q9I3L2
A	6	HIS	-	expression tag	UNP Q9I3L2
A	7	HIS	-	expression tag	UNP Q9I3L2
A	8	HIS	-	expression tag	UNP Q9I3L2
A	9	ALA	-	expression tag	UNP Q9I3L2
A	10	GLU	-	expression tag	UNP Q9I3L2
A	11	ASN	-	expression tag	UNP Q9I3L2
A	12	LEU	-	expression tag	UNP Q9I3L2
A	13	TYR	-	expression tag	UNP Q9I3L2
A	14	PHE	-	expression tag	UNP Q9I3L2
A	15	GLN	-	expression tag	UNP Q9I3L2
A	16	HIS	-	expression tag	UNP Q9I3L2
B	1	MET	-	initiating methionine	UNP Q9I3L2
B	2	GLY	-	expression tag	UNP Q9I3L2
B	3	HIS	-	expression tag	UNP Q9I3L2
B	4	HIS	-	expression tag	UNP Q9I3L2
B	5	HIS	-	expression tag	UNP Q9I3L2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP Q9I3L2
B	7	HIS	-	expression tag	UNP Q9I3L2
B	8	HIS	-	expression tag	UNP Q9I3L2
B	9	ALA	-	expression tag	UNP Q9I3L2
B	10	GLU	-	expression tag	UNP Q9I3L2
B	11	ASN	-	expression tag	UNP Q9I3L2
B	12	LEU	-	expression tag	UNP Q9I3L2
B	13	TYR	-	expression tag	UNP Q9I3L2
B	14	PHE	-	expression tag	UNP Q9I3L2
B	15	GLN	-	expression tag	UNP Q9I3L2
B	16	HIS	-	expression tag	UNP Q9I3L2
C	1	MET	-	initiating methionine	UNP Q9I3L2
C	2	GLY	-	expression tag	UNP Q9I3L2
C	3	HIS	-	expression tag	UNP Q9I3L2
C	4	HIS	-	expression tag	UNP Q9I3L2
C	5	HIS	-	expression tag	UNP Q9I3L2
C	6	HIS	-	expression tag	UNP Q9I3L2
C	7	HIS	-	expression tag	UNP Q9I3L2
C	8	HIS	-	expression tag	UNP Q9I3L2
C	9	ALA	-	expression tag	UNP Q9I3L2
C	10	GLU	-	expression tag	UNP Q9I3L2
C	11	ASN	-	expression tag	UNP Q9I3L2
C	12	LEU	-	expression tag	UNP Q9I3L2
C	13	TYR	-	expression tag	UNP Q9I3L2
C	14	PHE	-	expression tag	UNP Q9I3L2
C	15	GLN	-	expression tag	UNP Q9I3L2
C	16	HIS	-	expression tag	UNP Q9I3L2
D	1	MET	-	initiating methionine	UNP Q9I3L2
D	2	GLY	-	expression tag	UNP Q9I3L2
D	3	HIS	-	expression tag	UNP Q9I3L2
D	4	HIS	-	expression tag	UNP Q9I3L2
D	5	HIS	-	expression tag	UNP Q9I3L2
D	6	HIS	-	expression tag	UNP Q9I3L2
D	7	HIS	-	expression tag	UNP Q9I3L2
D	8	HIS	-	expression tag	UNP Q9I3L2
D	9	ALA	-	expression tag	UNP Q9I3L2
D	10	GLU	-	expression tag	UNP Q9I3L2
D	11	ASN	-	expression tag	UNP Q9I3L2
D	12	LEU	-	expression tag	UNP Q9I3L2
D	13	TYR	-	expression tag	UNP Q9I3L2
D	14	PHE	-	expression tag	UNP Q9I3L2
D	15	GLN	-	expression tag	UNP Q9I3L2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	16	HIS	-	expression tag	UNP Q9I3L2

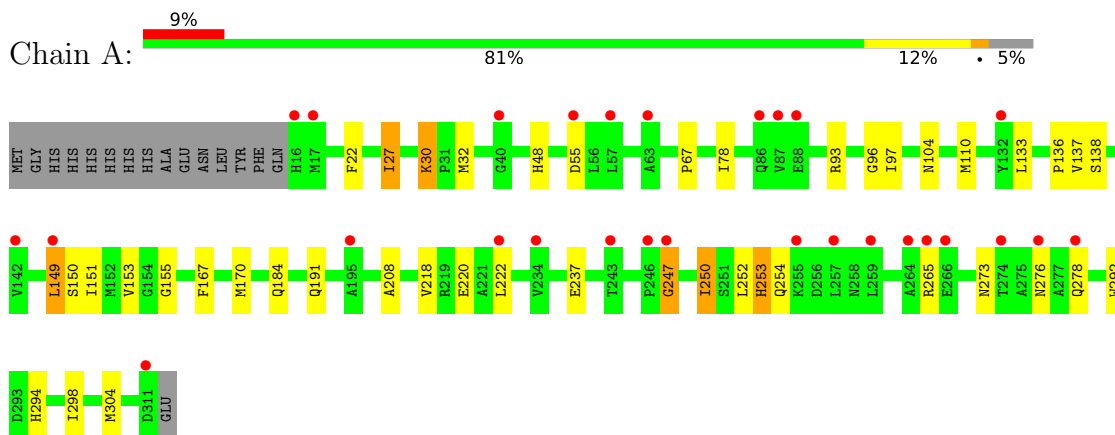
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	O 4	0	0
2	B	10	Total 10	O 10	0	0
2	C	16	Total 16	O 16	0	0
2	D	15	Total 15	O 15	0	0

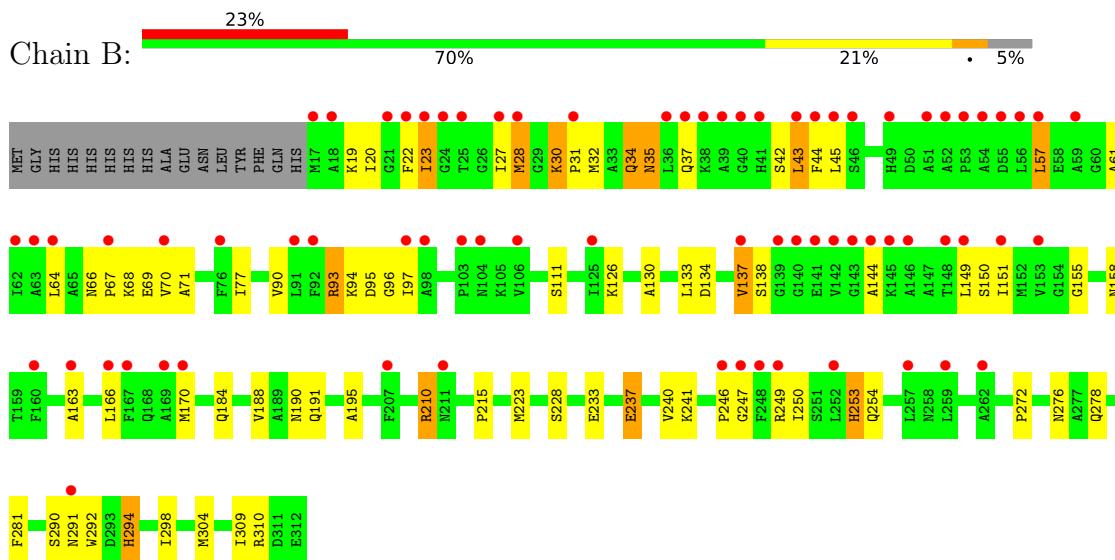
3 Residue-property plots

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.

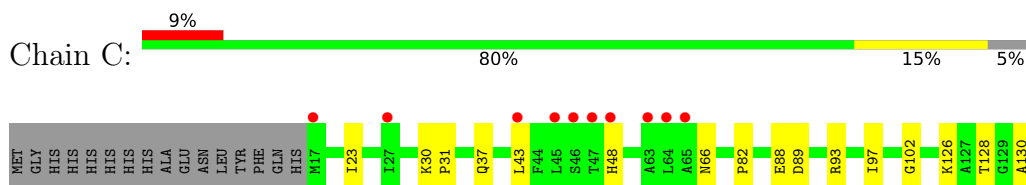
- Molecule 1: Probable oxidoreductase

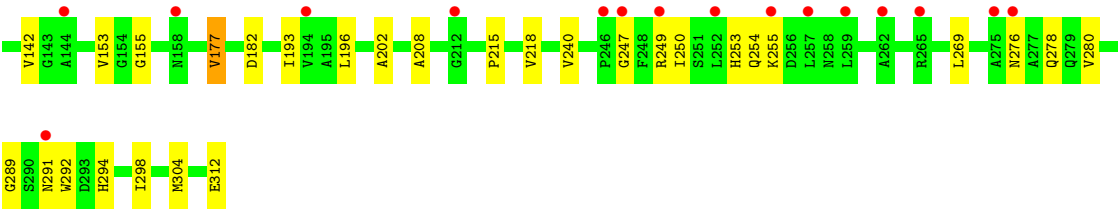


- Molecule 1: Probable oxidoreductase

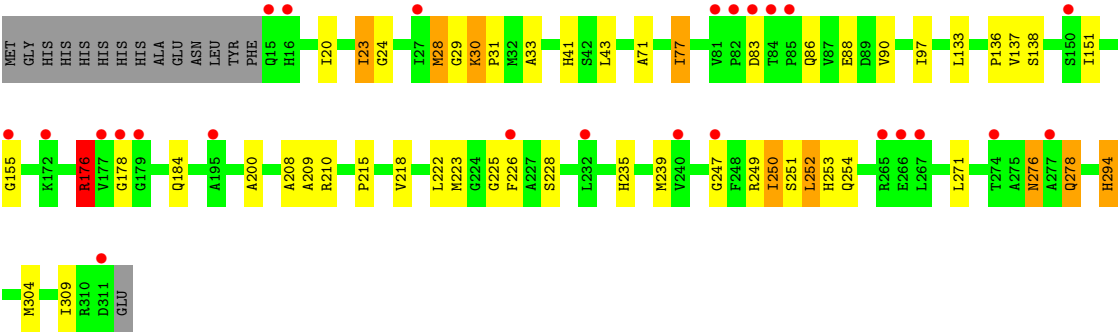
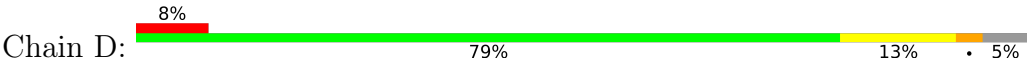


- Molecule 1: Probable oxidoreductase





● Molecule 1: Probable oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.44Å 121.47Å 132.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.73 – 2.07 60.73 – 2.07	Depositor EDS
% Data completeness (in resolution range)	95.5 (60.73-2.07) 95.5 (60.73-2.07)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.07Å)	Xtriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, R_{free}	0.270 , 0.315 0.260 , 0.292	Depositor DCC
R_{free} test set	2070 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8736	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.77% 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	0.78	0/2207	1.14	3/2984 (0.1%)
1	B	0.79	0/2205	1.17	2/2981 (0.1%)
1	C	0.78	0/2205	1.21	3/2981 (0.1%)
1	D	0.80	0/2216	1.13	1/2996 (0.0%)
All	All	0.78	0/8833	1.16	9/11942 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	GLY	N-CA-C	-6.97	96.65	113.18
1	D	247	GLY	N-CA-C	-6.59	97.57	113.18
1	B	246	PRO	N-CA-C	6.29	121.51	111.26
1	C	66	ASN	N-CA-C	6.18	113.79	108.22
1	A	153	VAL	N-CA-C	6.01	116.52	108.11
1	B	247	GLY	N-CA-C	-6.00	98.97	113.18
1	A	55	ASP	CA-CB-CG	5.38	117.97	112.60
1	C	153	VAL	N-CA-C	5.26	115.48	108.11
1	A	247	GLY	N-CA-C	-5.01	101.31	113.18

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ARG	Sidechain
1	B	210	ARG	Sidechain
1	B	310	ARG	Sidechain
1	B	93	ARG	Sidechain
1	D	176	ARG	Sidechain

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	2171	0	2190	29	0
1	B	2170	0	2189	49	0
1	C	2170	0	2189	30	0
1	D	2180	0	2198	37	0
2	A	4	0	0	0	0
2	B	10	0	0	0	0
2	C	16	0	0	0	0
2	D	15	0	0	0	0
All	All	8736	0	8766	133	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 8.

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:22:PHE:HZ	1:B:32:MET:HE3	1.52	0.75
1:A:276:ASN:HD21	1:B:272:PRO:HG2	1.52	0.74
1:B:28:MET:HE3	1:B:144:ALA:HB2	1.68	0.74
1:A:222:LEU:HD22	1:B:190:ASN:HB2	1.71	0.72
1:B:67:PRO:HG2	1:B:96:GLY:HA2	1.71	0.72
1:B:23:ILE:HG21	1:B:90:VAL:HG21	1.72	0.72
1:A:110:MET:HE1	1:A:170:MET:HE1	1.73	0.71
1:D:23:ILE:HG21	1:D:90:VAL:HG11	1.73	0.71
1:A:67:PRO:HG2	1:A:96:GLY:HA2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLY:HA2	1:C:128:THR:O	1.94	0.68
1:B:195:ALA:HB2	1:B:253:HIS:CE1	2.28	0.67
1:D:278:GLN:HA	1:D:278:GLN:HE21	1.61	0.66
1:A:254:GLN:HA	1:A:278:GLN:HE22	1.62	0.64
1:B:138:SER:HB3	1:B:150:SER:HB3	1.79	0.63
1:D:209:ALA:HB2	1:D:215:PRO:HG3	1.82	0.61
1:C:133:LEU:HD23	1:C:155:GLY:HA3	1.82	0.60
1:D:23:ILE:HG13	1:D:97:ILE:HD11	1.83	0.59
1:C:193:ILE:HD12	1:D:222:LEU:HD23	1.85	0.58
1:D:254:GLN:HA	1:D:278:GLN:HE22	1.68	0.58
1:C:215:PRO:HB2	1:C:240:VAL:HG22	1.86	0.58
1:B:64:LEU:HD22	1:B:69:GLU:HB3	1.85	0.58
1:B:163:ALA:HA	1:B:166:LEU:HD13	1.85	0.58
1:A:22:PHE:HZ	1:A:32:MET:HE3	1.67	0.58
1:D:20:ILE:HD12	1:D:41:HIS:HB3	1.84	0.57
1:B:254:GLN:HA	1:B:278:GLN:HE22	1.68	0.57
1:B:250:ILE:HG23	1:B:281:PHE:CD1	2.40	0.56
1:B:137:VAL:HG21	1:B:149:LEU:HD13	1.87	0.56
1:D:133:LEU:HD23	1:D:155:GLY:HA3	1.87	0.56
1:B:278:GLN:HE21	1:B:278:GLN:HA	1.71	0.55
1:C:48:HIS:CE1	1:C:93:ARG:HH12	2.24	0.55
1:C:177:VAL:HG22	1:C:182:ASP:HB3	1.87	0.55
1:B:71:ALA:HA	1:B:77:ILE:HG12	1.88	0.55
1:B:250:ILE:HD13	1:B:294:HIS:HA	1.88	0.55
1:C:276:ASN:HD21	1:D:276:ASN:HD22	1.55	0.54
1:B:137:VAL:CG1	1:B:149:LEU:HD22	2.37	0.54
1:B:37:GLN:HG3	1:B:43:LEU:HD12	1.88	0.54
1:A:250:ILE:O	1:A:254:GLN:HG3	2.09	0.53
1:C:89:ASP:O	1:C:93:ARG:HB2	2.09	0.52
1:C:269:LEU:HD21	1:D:210:ARG:HG2	1.91	0.52
1:B:20:ILE:O	1:B:43:LEU:HA	2.10	0.51
1:D:71:ALA:HA	1:D:77:ILE:HD12	1.93	0.51
1:D:23:ILE:HG21	1:D:90:VAL:CG1	2.40	0.51
1:C:133:LEU:CD2	1:C:155:GLY:HA3	2.40	0.50
1:D:137:VAL:HG12	1:D:151:ILE:HG12	1.93	0.50
1:B:223:MET:HE3	1:B:233:GLU:HG2	1.94	0.50
1:D:24:GLY:O	1:D:29:GLY:HA3	2.12	0.50
1:B:249:ARG:HG2	1:B:291:ASN:HA	1.94	0.49
1:A:278:GLN:HE21	1:A:278:GLN:HA	1.77	0.49
1:B:27:ILE:O	1:B:31:PRO:HG2	2.12	0.49
1:D:133:LEU:CD2	1:D:155:GLY:HA3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LYS:HB3	1:B:31:PRO:HD3	1.93	0.49
1:C:280:VAL:HG13	1:C:304:MET:HE1	1.94	0.48
1:A:78:ILE:HG23	1:A:110:MET:HG3	1.95	0.48
1:D:30:LYS:N	1:D:31:PRO:HD2	2.29	0.48
1:D:33:ALA:HB1	1:D:43:LEU:HD11	1.96	0.48
1:B:34:GLN:HE21	1:B:35:ASN:HD21	1.61	0.48
1:A:208:ALA:HB1	1:A:218:VAL:HG21	1.96	0.48
1:A:273:ASN:HD21	1:B:276:ASN:HB2	1.79	0.47
1:C:48:HIS:ND1	1:C:93:ARG:NH2	2.60	0.47
1:A:137:VAL:HG12	1:A:151:ILE:HG12	1.95	0.47
1:A:138:SER:HB3	1:A:150:SER:HB2	1.97	0.47
1:D:71:ALA:HA	1:D:77:ILE:CD1	2.45	0.47
1:C:196:LEU:HD12	1:D:200:ALA:HA	1.97	0.47
1:D:176:ARG:CZ	1:D:178:GLY:HA2	2.45	0.47
1:B:137:VAL:HG13	1:B:149:LEU:HD22	1.97	0.46
1:B:66:ASN:O	1:B:70:VAL:HG23	2.16	0.46
1:D:176:ARG:NH2	1:D:178:GLY:HA2	2.30	0.46
1:A:30:LYS:HB3	1:A:30:LYS:HE2	1.39	0.46
1:A:304:MET:HG2	1:C:304:MET:HG2	1.98	0.46
1:B:34:GLN:HG2	1:B:35:ASN:N	2.31	0.46
1:A:133:LEU:HD23	1:A:155:GLY:HA3	1.98	0.46
1:B:191:GLN:O	1:B:253:HIS:HE1	1.99	0.46
1:D:28:MET:HE3	1:D:28:MET:HB3	1.74	0.46
1:A:67:PRO:HB2	1:A:97:ILE:HG13	1.98	0.45
1:D:208:ALA:HB1	1:D:218:VAL:HG21	1.98	0.45
1:C:276:ASN:HD21	1:D:276:ASN:ND2	2.13	0.45
1:B:133:LEU:HD23	1:B:155:GLY:HA3	1.98	0.45
1:B:67:PRO:HB2	1:B:97:ILE:HG13	1.98	0.45
1:A:137:VAL:HB	1:A:149:LEU:HG	1.99	0.45
1:C:126:LYS:HA	1:C:130:ALA:O	2.17	0.45
1:D:28:MET:O	1:D:31:PRO:HG2	2.17	0.45
1:D:223:MET:O	1:D:228:SER:HB2	2.15	0.44
1:B:94:LYS:O	1:B:95:ASP:HB2	2.16	0.44
1:B:237:GLU:O	1:B:241:LYS:HG2	2.17	0.44
1:B:19:LYS:HB3	1:B:44:PHE:CE1	2.52	0.44
1:A:276:ASN:ND2	1:B:272:PRO:HG2	2.25	0.44
1:A:27:ILE:H	1:A:27:ILE:HG12	1.61	0.44
1:A:250:ILE:HD12	1:A:292:TRP:HB2	2.00	0.44
1:C:202:ALA:HA	1:C:298:ILE:HD12	2.00	0.43
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.81	0.43
1:C:250:ILE:O	1:C:254:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HA	1:B:61:ALA:HB3	2.00	0.43
1:B:170:MET:HE3	1:B:170:MET:HB2	1.94	0.43
1:C:254:GLN:HA	1:C:278:GLN:HE22	1.83	0.43
1:B:137:VAL:HG11	1:B:149:LEU:HD22	2.00	0.43
1:B:23:ILE:HG21	1:B:90:VAL:CG2	2.44	0.43
1:D:33:ALA:HB1	1:D:43:LEU:CD1	2.49	0.43
1:B:223:MET:HE2	1:B:223:MET:HB3	1.94	0.43
1:D:294:HIS:CD2	1:D:294:HIS:H	2.36	0.43
1:B:37:GLN:HG3	1:B:43:LEU:CD1	2.48	0.42
1:B:137:VAL:CG2	1:B:151:ILE:HG12	2.49	0.42
1:A:78:ILE:HG12	1:A:110:MET:HE3	2.01	0.42
1:B:184:GLN:O	1:B:188:VAL:HG23	2.20	0.42
1:A:48:HIS:HD2	1:A:93:ARG:NH2	2.17	0.42
1:B:215:PRO:HB2	1:B:240:VAL:HG22	2.00	0.42
1:C:30:LYS:HB3	1:C:31:PRO:HD3	2.02	0.42
1:C:280:VAL:HG22	1:C:304:MET:HE1	2.01	0.42
1:D:225:GLY:O	1:D:228:SER:HB3	2.19	0.42
1:B:304:MET:HG2	1:D:304:MET:HG2	2.01	0.42
1:C:82:PRO:O	1:C:255:LYS:HE3	2.20	0.42
1:C:312:GLU:CD	1:C:312:GLU:H	2.28	0.42
1:B:249:ARG:HA	1:B:292:TRP:O	2.20	0.41
1:C:249:ARG:HG2	1:C:291:ASN:HA	2.02	0.41
1:D:136:PRO:HG3	1:D:184:GLN:HA	2.02	0.41
1:A:136:PRO:HG3	1:A:184:GLN:HA	2.02	0.41
1:C:289:GLY:HA3	1:C:292:TRP:CE3	2.56	0.41
1:D:83:ASP:OD1	1:D:86:GLN:HB2	2.21	0.41
1:D:250:ILE:O	1:D:254:GLN:HG3	2.21	0.41
1:D:294:HIS:CD2	1:D:294:HIS:N	2.88	0.41
1:C:23:ILE:HG13	1:C:97:ILE:HD11	2.01	0.41
1:C:37:GLN:HG3	1:C:43:LEU:HG	2.03	0.41
1:C:208:ALA:HB1	1:C:218:VAL:HG21	2.03	0.41
1:D:235:HIS:O	1:D:239:MET:HG3	2.20	0.41
1:A:110:MET:HE2	1:A:167:PHE:HE1	1.85	0.41
1:A:218:VAL:O	1:A:222:LEU:HG	2.20	0.41
1:B:210:ARG:HA	1:B:210:ARG:HD2	1.83	0.41
1:A:191:GLN:O	1:A:253:HIS:HE1	2.04	0.40
1:B:28:MET:O	1:B:32:MET:HE2	2.22	0.40
1:C:48:HIS:CE1	1:C:93:ARG:HH22	2.37	0.40
1:B:126:LYS:HA	1:B:130:ALA:O	2.22	0.40
1:D:249:ARG:HB2	1:D:252:LEU:HD12	2.03	0.40
1:A:278:GLN:HA	1:A:278:GLN:NE2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ASN:ND2	1:D:276:ASN:HD22	2.17	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	294/312 (94%)	281 (96%)	12 (4%)	1 (0%)	36	30
1	B	294/312 (94%)	283 (96%)	11 (4%)	0	100	100
1	C	294/312 (94%)	280 (95%)	14 (5%)	0	100	100
1	D	295/312 (95%)	284 (96%)	11 (4%)	0	100	100
All	All	1177/1248 (94%)	1128 (96%)	48 (4%)	1 (0%)	48	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	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	220/234 (94%)	210 (96%)	10 (4%)	24	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	220/234 (94%)	198 (90%)	22 (10%)	7	3
1	C	220/234 (94%)	214 (97%)	6 (3%)	39	35
1	D	221/234 (94%)	204 (92%)	17 (8%)	12	5
All	All	881/936 (94%)	826 (94%)	55 (6%)	16	9

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	30	LYS
1	A	104	ASN
1	A	149	LEU
1	A	220	GLU
1	A	237	GLU
1	A	250	ILE
1	A	253	HIS
1	A	294	HIS
1	A	298	ILE
1	B	23	ILE
1	B	28	MET
1	B	30	LYS
1	B	34	GLN
1	B	35	ASN
1	B	42	SER
1	B	43	LEU
1	B	45	LEU
1	B	57	LEU
1	B	68	LYS
1	B	93	ARG
1	B	111	SER
1	B	134	ASP
1	B	137	VAL
1	B	158	ASN
1	B	228	SER
1	B	237	GLU
1	B	253	HIS
1	B	290	SER
1	B	294	HIS
1	B	298	ILE
1	B	309	ILE
1	C	88	GLU

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Mol	Chain	Res	Type
1	C	138	SER
1	C	142	VAL
1	C	177	VAL
1	C	253	HIS
1	C	294	HIS
1	D	23	ILE
1	D	28	MET
1	D	30	LYS
1	D	77	ILE
1	D	88	GLU
1	D	138	SER
1	D	176	ARG
1	D	226	PHE
1	D	250	ILE
1	D	251	SER
1	D	252	LEU
1	D	253	HIS
1	D	271	LEU
1	D	276	ASN
1	D	278	GLN
1	D	294	HIS
1	D	309	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	41	HIS
1	A	72	GLN
1	A	253	HIS
1	A	273	ASN
1	A	276	ASN
1	A	278	GLN
1	A	294	HIS
1	B	35	ASN
1	B	49	HIS
1	B	180	ASN
1	B	190	ASN
1	B	253	HIS
1	B	278	GLN
1	B	291	ASN
1	C	37	GLN

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Mol	Chain	Res	Type
1	C	180	ASN
1	C	278	GLN
1	C	291	ASN
1	D	158	ASN
1	D	180	ASN
1	D	273	ASN
1	D	276	ASN
1	D	278	GLN
1	D	303	HIS

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	296/312 (94%)	0.96	28 (9%) 14 14	43, 59, 74, 83	0
1	B	296/312 (94%)	1.38	73 (24%) 2 1	38, 63, 99, 105	0
1	C	296/312 (94%)	0.91	27 (9%) 15 15	40, 53, 74, 91	0
1	D	297/312 (95%)	0.78	25 (8%) 17 17	39, 53, 66, 79	0
All	All	1185/1248 (94%)	1.01	153 (12%) 7 7	38, 56, 86, 105	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	247	GLY	4.6
1	A	86	GLN	4.2
1	A	276	ASN	4.1
1	B	36	LEU	4.0
1	A	55	ASP	3.9
1	B	139	GLY	3.9
1	B	57	LEU	3.9
1	B	247	GLY	3.8
1	B	44	PHE	3.8
1	B	144	ALA	3.7
1	B	142	VAL	3.6
1	B	62	ILE	3.6
1	B	59	ALA	3.6
1	B	166	LEU	3.6
1	A	16	HIS	3.5
1	B	25	THR	3.5
1	B	56	LEU	3.4
1	A	311	ASP	3.4
1	D	265	ARG	3.3
1	B	54	ALA	3.3
1	B	146	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	63	ALA	3.3
1	B	104	ASN	3.3
1	C	47	THR	3.2
1	D	266	GLU	3.2
1	A	247	GLY	3.2
1	B	97	ILE	3.2
1	A	265	ARG	3.2
1	D	178	GLY	3.2
1	C	139	GLY	3.1
1	B	98	ALA	3.0
1	C	144	ALA	3.0
1	B	64	LEU	3.0
1	C	43	LEU	3.0
1	C	27	ILE	3.0
1	A	266	GLU	2.9
1	D	267	LEU	2.9
1	B	53	PRO	2.9
1	B	169	ALA	2.9
1	C	48	HIS	2.9
1	B	148	THR	2.9
1	C	46	SER	2.9
1	C	17	MET	2.8
1	B	262	ALA	2.8
1	D	179	GLY	2.8
1	B	27	ILE	2.8
1	B	43	LEU	2.8
1	B	252	LEU	2.8
1	B	45	LEU	2.8
1	D	311	ASP	2.7
1	B	248	PHE	2.7
1	C	64	LEU	2.7
1	B	137	VAL	2.7
1	B	151	ILE	2.7
1	A	195	ALA	2.7
1	B	207	PHE	2.7
1	A	57	LEU	2.7
1	D	84	THR	2.7
1	B	125	ILE	2.7
1	A	63	ALA	2.7
1	C	262	ALA	2.7
1	A	259	LEU	2.7
1	B	91	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	291	ASN	2.7
1	B	153	VAL	2.7
1	B	52	ALA	2.6
1	B	39	ALA	2.6
1	A	87	VAL	2.6
1	B	140	GLY	2.6
1	B	170	MET	2.6
1	C	291	ASN	2.6
1	B	246	PRO	2.6
1	B	149	LEU	2.6
1	C	276	ASN	2.5
1	C	246	PRO	2.5
1	C	194	VAL	2.5
1	D	27	ILE	2.5
1	B	41	HIS	2.5
1	B	55	ASP	2.5
1	D	83	ASP	2.5
1	B	18	ALA	2.5
1	C	275	ALA	2.5
1	B	257	LEU	2.5
1	C	259	LEU	2.5
1	B	17	MET	2.5
1	B	22	PHE	2.5
1	B	40	GLY	2.5
1	B	51	ALA	2.4
1	C	63	ALA	2.4
1	B	145	LYS	2.4
1	B	259	LEU	2.4
1	C	45	LEU	2.4
1	B	70	VAL	2.4
1	B	163	ALA	2.4
1	D	82	PRO	2.4
1	A	234	VAL	2.4
1	B	103	PRO	2.4
1	B	38	LYS	2.3
1	C	249	ARG	2.3
1	A	243	THR	2.3
1	A	222	LEU	2.3
1	B	143	GLY	2.3
1	D	85	PRO	2.3
1	D	277	ALA	2.3
1	D	226	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	37	GLN	2.3
1	B	31	PRO	2.3
1	B	211	ASN	2.3
1	D	195	ALA	2.3
1	B	49	HIS	2.2
1	B	23	ILE	2.2
1	D	177	VAL	2.2
1	B	141	GLU	2.2
1	A	274	THR	2.2
1	C	158	ASN	2.2
1	D	81	VAL	2.2
1	C	257	LEU	2.2
1	D	150	SER	2.2
1	B	76	PHE	2.2
1	B	92	PHE	2.2
1	D	274	THR	2.2
1	A	142	VAL	2.2
1	B	106	VAL	2.2
1	A	88	GLU	2.2
1	C	212	GLY	2.2
1	A	264	ALA	2.2
1	D	15	GLN	2.2
1	A	17	MET	2.2
1	A	246	PRO	2.1
1	D	240	VAL	2.1
1	B	28	MET	2.1
1	B	67	PRO	2.1
1	B	160	PHE	2.1
1	B	249	ARG	2.1
1	B	24	GLY	2.1
1	B	46	SER	2.1
1	C	265	ARG	2.1
1	D	16	HIS	2.1
1	A	40	GLY	2.1
1	D	247	GLY	2.1
1	C	255	LYS	2.1
1	D	172	LYS	2.1
1	C	65	ALA	2.1
1	A	149	LEU	2.0
1	A	257	LEU	2.0
1	C	252	LEU	2.0
1	D	232	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	255	LYS	2.0
1	B	21	GLY	2.0
1	D	155	GLY	2.0
1	B	167	PHE	2.0
1	A	278	GLN	2.0
1	A	132	TYR	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.