



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:53 PM UTC

PDB ID : 1JQC / pdb_00001jqc
Title : Mn substituted Ribonucleotide reductase R2 from E. Coli oxidized by hydrogen peroxide and hydroxylamine
Authors : Hogbom, M.; Andersson, M.E.; Nordlund, P.
Deposited on : 2001-08-06
Resolution : 1.61 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

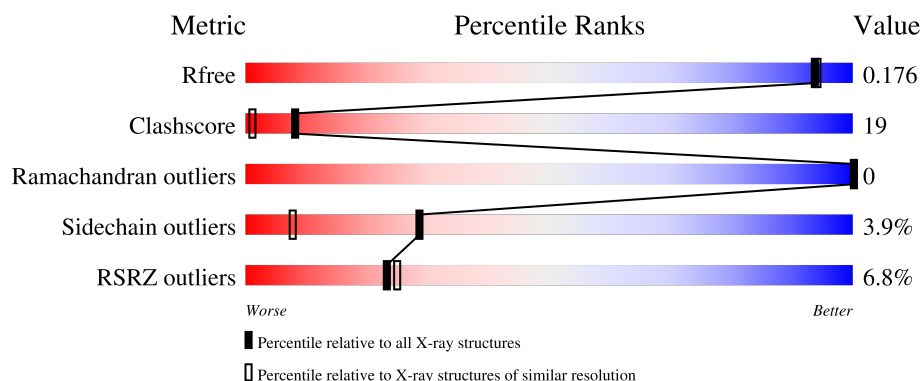
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	375	 3% 71% 17% • 9%
1	B	375	 9% 66% 21% • 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6325 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 Protein R2 of ribonucleotide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2788	1784	464	527	13			
1	B	341	Total	C	N	O	S	0	0	0
			2794	1787	465	529	13			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Hg	0	0
			5	5		
3	B	8	Total	Hg	0	0
			8	8		

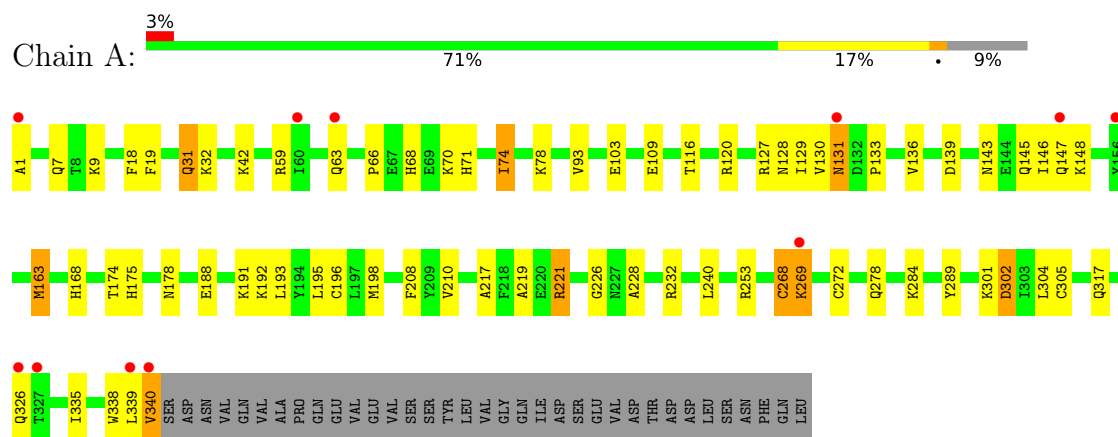
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	376	Total	O	0	0
			376	376		
4	B	350	Total	O	0	0
			350	350		

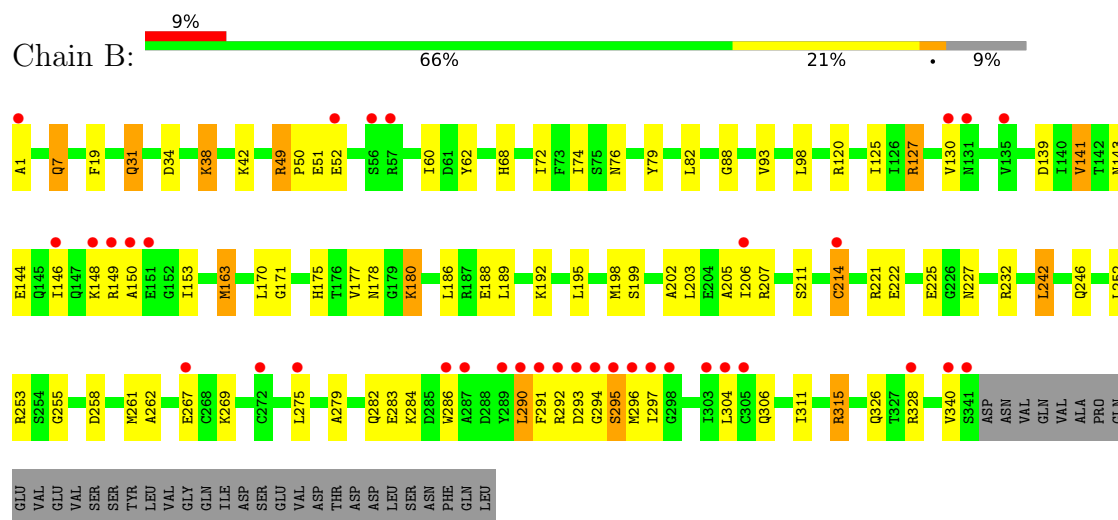
3 Residue-property plots

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: Protein R2 of ribonucleotide reductase



- Molecule 1: Protein R2 of ribonucleotide reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.85Å 84.55Å 114.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 1.61 29.00 – 1.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.00-1.61) 97.9 (29.00-1.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.33 (at 1.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.176 , 0.219 0.178 , 0.176	Depositor DCC
R_{free} test set	4563 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6325	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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

Bond lengths and bond angles in the following residue types are not validated in this section: HG, MN

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	1.05	5/2852 (0.2%)	1.10	8/3869 (0.2%)
1	B	0.98	2/2858 (0.1%)	1.09	5/3877 (0.1%)
All	All	1.01	7/5710 (0.1%)	1.09	13/7746 (0.2%)

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	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	MET	SD-CE	11.58	2.08	1.79
1	B	163	MET	SD-CE	10.13	2.04	1.79
1	A	198	MET	SD-CE	-9.70	1.55	1.79
1	A	268	CYS	CB-SG	9.70	2.13	1.81
1	A	268	CYS	CA-CB	5.79	1.62	1.53
1	B	198	MET	SD-CE	-5.46	1.66	1.79
1	A	268	CYS	CA-C	5.23	1.60	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	GLN	CB-CG-CD	7.16	124.77	112.60
1	B	141	VAL	N-CA-C	6.95	117.70	110.62
1	A	268	CYS	CB-CA-C	6.34	121.28	110.56
1	A	226	GLY	N-CA-C	-6.24	104.94	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	LYS	N-CA-C	-5.69	105.16	111.36
1	B	49	ARG	CA-C-N	5.50	125.59	119.32
1	B	49	ARG	C-N-CA	5.50	125.59	119.32
1	A	66	PRO	N-CA-C	-5.39	102.99	111.34
1	A	196	CYS	N-CA-C	-5.18	105.52	111.07
1	A	70	LYS	N-CA-C	-5.14	105.68	111.28
1	B	267	GLU	CA-C-N	-5.09	114.99	122.83
1	B	267	GLU	C-N-CA	-5.09	114.99	122.83
1	A	217	ALA	N-CA-C	-5.06	105.95	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	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	2788	0	2731	89	0
1	B	2794	0	2735	128	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	0	0
3	B	8	0	0	0	0
4	A	376	0	0	44	0
4	B	350	0	0	40	0
All	All	6325	0	5466	213	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 19.

All (213) 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:163:MET:CE	1:B:163:MET:SD	2.04	1.44
1:A:163:MET:SD	1:A:163:MET:CE	2.08	1.40
1:A:268:CYS:CB	1:A:268:CYS:SG	2.13	1.35
1:A:305:CYS:HB3	4:A:978:HOH:O	1.14	1.30
1:B:199:SER:HB2	4:B:1259:HOH:O	1.01	1.17
1:B:304:LEU:HD11	4:B:968:HOH:O	1.46	1.16
1:B:202:ALA:O	1:B:206:ILE:HG12	1.50	1.10
1:B:72:ILE:HA	1:B:290:LEU:HD11	1.38	1.03
1:A:221:ARG:HD2	4:A:1117:HOH:O	1.58	1.03
1:B:286:TRP:CZ2	1:B:290:LEU:HD13	1.96	0.99
1:A:272:CYS:SG	4:A:997:HOH:O	2.20	0.99
1:B:139:ASP:O	1:B:143:ASN:HB2	1.69	0.94
1:A:302:ASP:HB3	4:A:1286:HOH:O	1.66	0.93
1:B:49:ARG:HD3	4:B:1054:HOH:O	1.72	0.89
1:B:286:TRP:CH2	1:B:290:LEU:HD22	2.08	0.88
1:A:195:LEU:HD21	4:A:997:HOH:O	1.75	0.87
1:B:177:VAL:O	1:B:180:LYS:HG2	1.75	0.86
1:B:252:LEU:HD22	1:B:261:MET:HG2	1.56	0.85
1:B:163:MET:SD	1:B:192:LYS:HE2	2.17	0.84
1:B:150:ALA:HB3	4:B:1148:HOH:O	1.78	0.83
1:A:145:GLN:HG2	1:A:289:TYR:HB2	1.59	0.83
1:B:242:LEU:HD21	1:B:246:GLN:NE2	1.94	0.83
1:B:51:GLU:H	1:B:51:GLU:CD	1.87	0.82
1:B:127:ARG:HH11	1:B:127:ARG:CB	1.92	0.82
1:B:232:ARG:HD2	4:B:1258:HOH:O	1.79	0.82
1:B:207:ARG:HH22	1:B:282:GLN:HE22	1.27	0.81
1:A:284:LYS:HE2	4:A:978:HOH:O	1.81	0.81
1:A:127:ARG:HE	1:A:128:ASN:ND2	1.79	0.80
1:A:74:ILE:HD12	1:A:78:LYS:HE3	1.64	0.79
1:A:147:GLN:HG2	4:A:995:HOH:O	1.83	0.78
1:B:72:ILE:HA	1:B:290:LEU:CD1	2.12	0.78
1:A:210:VAL:HG13	1:A:304:LEU:HD11	1.67	0.77
1:B:72:ILE:HG23	1:B:290:LEU:HD21	1.64	0.77
1:B:205:ALA:HB1	1:B:315:ARG:HD3	1.66	0.77
1:B:31:GLN:HG3	1:B:34:ASP:HA	1.67	0.76
1:B:163:MET:HE1	1:B:188:GLU:HB3	1.69	0.74
1:B:290:LEU:HD12	4:B:1254:HOH:O	1.88	0.74
1:B:286:TRP:CZ3	1:B:290:LEU:HD22	2.22	0.74
1:A:145:GLN:HG2	1:A:289:TYR:CB	2.19	0.73
1:A:188:GLU:OE1	4:A:1089:HOH:O	2.06	0.73
1:A:93:VAL:HG13	4:A:1000:HOH:O	1.87	0.73
1:A:127:ARG:HE	1:A:128:ASN:HD21	1.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HB2	4:A:1144:HOH:O	1.89	0.72
1:A:163:MET:SD	1:A:192:LYS:HG3	2.29	0.72
1:A:7:GLN:HG2	4:A:1041:HOH:O	1.90	0.72
1:B:207:ARG:HH22	1:B:282:GLN:NE2	1.88	0.71
1:B:290:LEU:HD23	1:B:291:PHE:CE1	2.26	0.71
1:B:202:ALA:HB1	1:B:206:ILE:HD11	1.73	0.71
1:A:147:GLN:HG2	4:A:1057:HOH:O	1.92	0.69
1:B:93:VAL:HG13	4:B:1078:HOH:O	1.92	0.69
1:B:211:SER:O	1:B:214:CYS:SG	2.51	0.69
1:B:72:ILE:HG12	1:B:290:LEU:HG	1.75	0.69
1:B:149:ARG:NH1	4:B:1039:HOH:O	2.23	0.69
1:B:242:LEU:HD22	1:B:246:GLN:HG3	1.76	0.68
1:A:191:LYS:HD3	4:A:1058:HOH:O	1.92	0.68
1:A:63:GLN:HG3	4:A:1076:HOH:O	1.93	0.67
1:B:242:LEU:CB	4:B:1043:HOH:O	2.43	0.67
1:B:296:MET:HG2	1:B:297:ILE:H	1.60	0.66
1:A:147:GLN:OE1	4:A:1194:HOH:O	2.12	0.66
1:A:175:HIS:HD2	1:B:178:ASN:HD21	1.42	0.66
1:B:242:LEU:HG	4:B:1043:HOH:O	1.97	0.65
1:A:31:GLN:OE1	4:A:1144:HOH:O	2.14	0.65
1:B:242:LEU:HB3	4:B:1043:HOH:O	1.97	0.64
1:A:317:GLN:HG2	4:A:1107:HOH:O	1.98	0.64
1:B:221:ARG:NH1	1:B:297:ILE:HD12	2.13	0.63
1:A:148:LYS:HD2	4:A:1071:HOH:O	1.98	0.63
1:B:211:SER:HA	1:B:214:CYS:SG	2.39	0.63
1:A:174:THR:HG23	4:A:1256:HOH:O	1.98	0.62
1:B:177:VAL:O	1:B:180:LYS:HE2	2.00	0.62
1:B:291:PHE:HD2	1:B:295:SER:HA	1.62	0.62
1:B:242:LEU:CG	4:B:1043:HOH:O	2.47	0.62
1:B:284:LYS:NZ	4:B:1064:HOH:O	2.31	0.62
1:B:42:LYS:NZ	4:B:1241:HOH:O	2.31	0.61
1:B:50:PRO:HD2	1:B:51:GLU:OE2	2.00	0.61
1:B:62:TYR:OH	1:B:74:ILE:HG13	1.99	0.61
1:B:296:MET:CG	1:B:297:ILE:H	2.13	0.61
1:A:175:HIS:CD2	1:B:178:ASN:HD21	2.18	0.61
1:A:1:ALA:HB3	4:A:1004:HOH:O	2.01	0.61
1:A:269:LYS:NZ	4:A:1263:HOH:O	2.19	0.60
1:B:315:ARG:HA	1:B:315:ARG:HE	1.65	0.60
1:A:1:ALA:N	1:A:168:HIS:O	2.34	0.60
1:B:306:GLN:NE2	4:B:916:HOH:O	2.34	0.59
1:A:335:ILE:HG12	1:A:339:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLU:CD	1:B:222:GLU:O	2.45	0.59
1:B:192:LYS:HE3	4:B:1133:HOH:O	2.01	0.58
1:A:42:LYS:HE2	1:A:240:LEU:HD21	1.85	0.58
1:B:205:ALA:HB2	1:B:242:LEU:HD23	1.85	0.58
1:B:296:MET:HG2	1:B:297:ILE:N	2.19	0.58
1:A:71:HIS:HD2	4:A:1198:HOH:O	1.87	0.57
1:A:221:ARG:NH2	4:A:1092:HOH:O	2.15	0.57
1:A:232:ARG:HH21	1:A:340:VAL:HG21	1.69	0.57
1:B:79:TYR:CE1	1:B:149:ARG:HG2	2.38	0.57
1:A:163:MET:HG3	4:A:1288:HOH:O	2.04	0.57
1:A:253:ARG:NE	4:A:1072:HOH:O	2.37	0.57
1:B:290:LEU:HD23	1:B:291:PHE:CD1	2.41	0.56
1:B:79:TYR:CZ	1:B:149:ARG:HG2	2.40	0.56
1:A:188:GLU:HG2	4:A:1193:HOH:O	2.06	0.56
1:B:180:LYS:HD3	4:B:1223:HOH:O	2.04	0.56
1:B:311:ILE:O	1:B:315:ARG:HG2	2.06	0.55
1:A:232:ARG:NH2	1:A:340:VAL:CG2	2.70	0.55
1:A:74:ILE:HD13	1:A:74:ILE:O	2.07	0.55
1:B:340:VAL:O	1:B:340:VAL:HG23	2.07	0.55
1:B:253:ARG:NE	4:B:1177:HOH:O	2.40	0.54
1:A:42:LYS:HG3	4:A:1111:HOH:O	2.07	0.54
1:B:202:ALA:HB1	1:B:206:ILE:CD1	2.36	0.54
1:A:278:GLN:HG3	4:A:1131:HOH:O	2.06	0.54
1:A:232:ARG:HH21	1:A:340:VAL:CG2	2.21	0.54
1:A:127:ARG:NE	1:A:128:ASN:HD21	2.05	0.54
1:A:42:LYS:HG2	4:A:1200:HOH:O	2.08	0.54
1:B:68:HIS:HB2	1:B:293:ASP:OD1	2.07	0.54
1:B:127:ARG:HH11	1:B:127:ARG:CG	2.21	0.53
1:B:163:MET:SD	1:B:192:LYS:CE	2.95	0.53
1:B:125:ILE:HD13	1:B:227:ASN:HD22	1.73	0.53
1:B:163:MET:CE	1:B:163:MET:CG	2.85	0.53
1:B:149:ARG:HD3	1:B:286:TRP:HB2	1.90	0.53
1:B:286:TRP:CH2	1:B:290:LEU:HD13	2.42	0.53
1:A:139:ASP:O	1:A:143:ASN:HB2	2.09	0.53
1:A:195:LEU:CD2	4:A:997:HOH:O	2.45	0.52
1:B:269:LYS:HG3	4:B:1224:HOH:O	2.10	0.52
1:B:60:ILE:HG23	4:B:1072:HOH:O	2.10	0.52
1:A:335:ILE:HG12	1:A:339:LEU:CD1	2.40	0.52
1:B:49:ARG:HB3	1:B:51:GLU:OE1	2.10	0.52
1:B:127:ARG:HH11	1:B:127:ARG:HB2	1.71	0.52
1:A:148:LYS:HE3	4:A:1129:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PHE:CG	1:A:193:LEU:HD21	2.45	0.51
1:A:129:ILE:HG13	1:A:130:VAL:HG23	1.93	0.51
1:B:188:GLU:HG3	4:B:1015:HOH:O	2.10	0.51
1:A:42:LYS:HE3	4:A:1200:HOH:O	2.10	0.51
1:B:72:ILE:CA	1:B:290:LEU:HD11	2.24	0.51
1:B:296:MET:CG	1:B:297:ILE:N	2.73	0.51
1:B:255:GLY:HA2	1:B:262:ALA:HB2	1.92	0.50
1:A:163:MET:CE	1:A:163:MET:HB3	2.42	0.49
1:A:335:ILE:O	1:A:339:LEU:HD13	2.12	0.49
1:B:279:ALA:HA	1:B:282:GLN:HE21	1.77	0.49
1:B:242:LEU:HD22	1:B:242:LEU:O	2.12	0.49
1:A:19:PHE:CE2	1:A:193:LEU:HD23	2.47	0.49
1:B:139:ASP:OD2	1:B:143:ASN:ND2	2.40	0.49
1:A:228:ALA:O	1:A:232:ARG:HG3	2.12	0.49
1:A:74:ILE:HD11	1:A:136:VAL:HG13	1.94	0.49
1:A:31:GLN:HG3	1:A:103:GLU:HB3	1.94	0.49
1:A:232:ARG:CZ	4:A:1119:HOH:O	2.60	0.49
1:B:149:ARG:NH2	1:B:286:TRP:CE2	2.80	0.49
1:A:19:PHE:HE2	1:A:193:LEU:HD23	1.78	0.49
1:A:163:MET:HB3	1:A:163:MET:HE2	1.94	0.49
1:B:328:ARG:HG2	4:B:1097:HOH:O	2.13	0.48
1:B:328:ARG:CD	4:B:1097:HOH:O	2.62	0.48
1:A:210:VAL:CG1	1:A:304:LEU:HD11	2.40	0.48
1:B:296:MET:HE3	4:B:1181:HOH:O	2.13	0.48
1:A:131:ASN:HD22	1:A:131:ASN:N	2.12	0.48
1:A:133:PRO:HD2	4:A:1112:HOH:O	2.13	0.47
1:B:203:LEU:HD23	1:B:203:LEU:C	2.40	0.47
1:A:163:MET:CE	1:A:163:MET:CG	2.90	0.47
1:B:326:GLN:NE2	4:B:1128:HOH:O	2.48	0.47
1:A:253:ARG:NH1	4:A:1093:HOH:O	2.46	0.47
1:B:141:VAL:HG23	4:B:1096:HOH:O	2.15	0.47
1:B:153:ILE:HA	4:B:1187:HOH:O	2.14	0.47
1:A:219:ALA:HB1	1:A:338:TRP:CH2	2.51	0.46
1:B:1:ALA:HB2	4:B:1216:HOH:O	2.15	0.46
1:B:1:ALA:HB3	4:B:1004:HOH:O	2.15	0.46
1:B:51:GLU:CD	1:B:51:GLU:N	2.65	0.46
1:B:222:GLU:HG2	1:B:225:GLU:OE2	2.16	0.46
1:A:127:ARG:NE	1:A:128:ASN:ND2	2.56	0.46
1:B:49:ARG:NH1	4:B:1230:HOH:O	2.38	0.45
1:A:253:ARG:NH2	4:A:1072:HOH:O	2.49	0.45
1:B:7:GLN:HG2	4:B:1069:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ASN:HD21	1:B:211:SER:HA	1.82	0.45
1:B:221:ARG:HH11	1:B:297:ILE:HD12	1.81	0.45
1:A:326:GLN:HG3	4:A:1080:HOH:O	2.17	0.45
1:A:63:GLN:CG	4:A:1076:HOH:O	2.57	0.45
1:B:221:ARG:NE	4:B:1181:HOH:O	2.48	0.45
1:A:59:ARG:HB2	1:A:128:ASN:O	2.17	0.45
1:B:258:ASP:HB2	4:B:1018:HOH:O	2.17	0.45
1:A:127:ARG:CZ	4:A:1023:HOH:O	2.64	0.44
1:A:178:ASN:HD21	1:B:175:HIS:CD2	2.35	0.44
1:B:144:GLU:O	1:B:148:LYS:HG3	2.17	0.44
1:B:242:LEU:O	1:B:246:GLN:HG3	2.17	0.44
1:B:127:ARG:HH11	1:B:127:ARG:HB3	1.79	0.44
1:A:163:MET:HE1	1:A:188:GLU:HG3	2.00	0.44
1:B:163:MET:CG	4:B:1131:HOH:O	2.65	0.44
1:A:339:LEU:O	1:A:340:VAL:C	2.61	0.43
1:B:38:LYS:N	1:B:38:LYS:CD	2.80	0.43
1:A:71:HIS:HE1	1:A:289:TYR:O	2.00	0.43
1:A:116:THR:O	1:A:120:ARG:HG3	2.18	0.43
1:A:9:LYS:HG3	4:A:1081:HOH:O	2.18	0.43
1:A:232:ARG:NH2	1:A:340:VAL:HG21	2.33	0.43
1:B:49:ARG:HA	1:B:50:PRO:HD3	1.82	0.42
1:B:163:MET:HG3	4:B:1131:HOH:O	2.19	0.42
1:B:150:ALA:CB	4:B:1148:HOH:O	2.50	0.42
1:A:305:CYS:CB	4:A:978:HOH:O	2.04	0.42
1:B:82:LEU:HD22	1:B:146:ILE:CG2	2.50	0.42
1:B:242:LEU:C	1:B:242:LEU:HD13	2.44	0.42
1:B:290:LEU:HA	4:B:1254:HOH:O	2.20	0.42
1:B:149:ARG:HD2	1:B:283:GLU:OE1	2.20	0.42
1:B:163:MET:HB2	1:B:192:LYS:HE3	2.01	0.42
1:B:130:VAL:HG12	4:B:1068:HOH:O	2.19	0.42
1:B:292:ARG:C	1:B:294:GLY:H	2.27	0.42
1:B:304:LEU:HD21	4:B:968:HOH:O	2.20	0.42
1:B:127:ARG:CG	1:B:127:ARG:NH1	2.79	0.41
1:B:242:LEU:HD21	1:B:246:GLN:HE21	1.76	0.41
1:B:130:VAL:CG1	4:B:1068:HOH:O	2.69	0.41
1:A:221:ARG:NH1	4:A:1117:HOH:O	2.21	0.41
1:B:19:PHE:CE1	1:B:98:LEU:HD22	2.56	0.41
1:B:211:SER:C	1:B:214:CYS:SG	3.03	0.41
1:A:18:PHE:CD1	1:A:193:LEU:HD21	2.56	0.41
1:B:38:LYS:N	1:B:38:LYS:HD2	2.35	0.41
1:B:171:GLY:O	1:B:175:HIS:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLY:CA	1:B:262:ALA:HB2	2.51	0.41
1:B:246:GLN:HE22	1:B:315:ARG:NH2	2.19	0.41
1:A:68:HIS:HD2	4:A:1123:HOH:O	2.03	0.40
1:B:284:LYS:HB3	1:B:284:LYS:HE3	1.73	0.40
1:A:269:LYS:HD2	4:A:1278:HOH:O	2.21	0.40
1:B:195:LEU:HD23	1:B:195:LEU:HA	1.76	0.40
1:A:109:GLU:OE2	1:B:88:GLY:O	2.39	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	338/375 (90%)	334 (99%)	4 (1%)	0	100	100
1	B	339/375 (90%)	336 (99%)	3 (1%)	0	100	100
All	All	677/750 (90%)	670 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	307/340 (90%)	298 (97%)	9 (3%)	37	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	308/340 (91%)	293 (95%)	15 (5%)	22	5
All	All	615/680 (90%)	591 (96%)	24 (4%)	28	8

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ILE
1	A	131	ASN
1	A	146	ILE
1	A	208	PHE
1	A	221	ARG
1	A	269	LYS
1	A	301	LYS
1	A	302	ASP
1	A	340	VAL
1	B	7	GLN
1	B	31	GLN
1	B	38	LYS
1	B	52	GLU
1	B	127	ARG
1	B	170	LEU
1	B	180	LYS
1	B	186	LEU
1	B	189	LEU
1	B	214	CYS
1	B	242	LEU
1	B	275	LEU
1	B	290	LEU
1	B	295	SER
1	B	315	ARG

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	68	HIS
1	A	71	HIS
1	A	128	ASN
1	A	131	ASN
1	A	147	GLN
1	A	175	HIS
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	250	ASN
1	A	278	GLN
1	A	306	GLN
1	A	326	GLN
1	B	7	GLN
1	B	12	GLN
1	B	76	ASN
1	B	80	GLN
1	B	131	ASN
1	B	145	GLN
1	B	175	HIS
1	B	227	ASN
1	B	246	GLN
1	B	281	GLN
1	B	282	GLN
1	B	326	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](#)

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	340/375 (90%)	0.17	11 (3%)	50	54	11, 20, 34, 50	0
1	B	341/375 (90%)	0.45	35 (10%)	12	12	12, 22, 40, 61	0
All	All	681/750 (90%)	0.31	46 (6%)	23	25	11, 21, 37, 61	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	LEU	5.2
1	B	275	LEU	5.0
1	B	214	CYS	5.0
1	B	297	ILE	4.9
1	B	340	VAL	4.7
1	B	289	TYR	4.7
1	B	293	ASP	4.1
1	B	286	TRP	4.1
1	B	272	CYS	3.7
1	B	296	MET	3.6
1	B	151	GLU	3.6
1	A	340	VAL	3.6
1	B	328	ARG	3.5
1	A	1	ALA	3.3
1	B	305	CYS	3.2
1	A	156	TYR	3.2
1	B	292	ARG	3.2
1	B	294	GLY	3.2
1	B	291	PHE	3.0
1	A	63	GLN	2.9
1	B	57	ARG	2.9
1	B	130	VAL	2.8
1	B	135	VAL	2.8
1	B	52	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	146	ILE	2.7
1	A	327	THR	2.7
1	B	148	LYS	2.7
1	A	131	ASN	2.6
1	B	303	ILE	2.6
1	B	149	ARG	2.6
1	A	147	GLN	2.6
1	A	339	LEU	2.4
1	B	150	ALA	2.4
1	B	298	GLY	2.4
1	A	60	ILE	2.3
1	A	269	LYS	2.3
1	B	1	ALA	2.3
1	B	267	GLU	2.1
1	A	326	GLN	2.1
1	B	56	SER	2.1
1	B	341	SER	2.1
1	B	131	ASN	2.0
1	B	304	LEU	2.0
1	B	206	ILE	2.0
1	B	287	ALA	2.0
1	B	295	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HG	A	912	1/1	0.97	0.07	25,25,25,25	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HG	B	913	1/1	0.97	0.10	22,22,22,22	1
3	HG	A	908	1/1	0.98	0.06	25,25,25,25	1
3	HG	B	903	1/1	0.98	0.11	34,34,34,34	1
3	HG	B	906	1/1	0.98	0.05	20,20,20,20	1
3	HG	B	911	1/1	0.98	0.07	28,28,28,28	1
3	HG	A	909	1/1	0.98	0.08	17,17,17,17	1
3	HG	B	914	1/1	0.98	0.08	21,21,21,21	1
3	HG	B	915	1/1	0.98	0.06	25,25,25,25	1
3	HG	B	904	1/1	0.99	0.10	14,14,14,14	1
3	HG	B	902	1/1	0.99	0.11	27,27,27,27	1
3	HG	A	907	1/1	0.99	0.11	14,14,14,14	1
2	MN	B	401	1/1	1.00	0.09	17,17,17,17	1
2	MN	B	402	1/1	1.00	0.03	14,14,14,14	0
3	HG	A	901	1/1	1.00	0.06	16,16,16,16	1
2	MN	A	403	1/1	1.00	0.08	16,16,16,16	0
2	MN	A	404	1/1	1.00	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.