



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 11:48 AM EDT

PDB ID : 1MRR
Title : SUBSTITUTION OF MANGANESE FOR IRON IN RIBONUCLEOTIDE REDUCTASE FROM ESCHERICHIA COLI. SPECTROSCOPIC AND CRYSTALLOGRAPHIC CHARACTERIZATION
Authors : Eklund, H.; Nordlund, P.
Deposited on : 1992-07-28
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

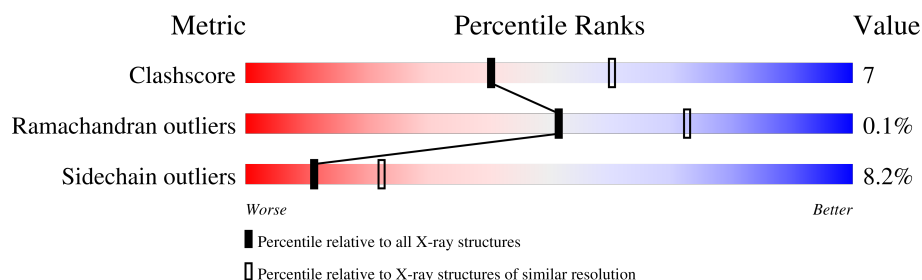
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	375	 70% 17% • • 9%
1	B	375	 65% 19% 6% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5818 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 RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2784	1782	463	526	13			
1	B	340	Total	C	N	O	S	0	0	0
			2784	1782	463	526	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	GLN	CONFLICT	UNP P69924
A	24	GLN	ASN	CONFLICT	UNP P69924
A	326	ASN	GLN	CONFLICT	UNP P69924
B	7	ALA	GLN	CONFLICT	UNP P69924
B	24	GLN	ASN	CONFLICT	UNP P69924
B	326	ASN	GLN	CONFLICT	UNP P69924

- Molecule 2 is MANGANESE (II) ION (three-letter code: 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 (three-letter code: 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	122	Total 122	O 122	0	0
4	B	111	Total 111	O 111	1	0

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.30Å 85.50Å 115.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5818	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.88	4/2848 (0.1%)	1.58	60/3864 (1.6%)
1	B	0.79	0/2848	1.61	59/3864 (1.5%)
All	All	0.84	4/5696 (0.1%)	1.59	119/7728 (1.5%)

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
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	CYS	CA-CB	13.64	1.83	1.53
1	A	268	CYS	CA-CB	-9.29	1.33	1.53
1	A	272	CYS	CB-SG	-9.24	1.66	1.82
1	A	268	CYS	CB-SG	6.79	1.93	1.82

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ARG	NE-CZ-NH1	17.85	129.22	120.30
1	A	272	CYS	CA-CB-SG	16.19	143.14	114.00
1	A	272	CYS	CB-CA-C	12.97	136.34	110.40
1	B	149	ARG	NE-CZ-NH1	-12.93	113.84	120.30
1	B	221	ARG	NE-CZ-NH2	-12.82	113.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	CYS	CA-CB-SG	12.23	136.02	114.00
1	A	272	CYS	N-CA-CB	-11.78	89.40	110.60
1	B	149	ARG	CG-CD-NE	-11.77	87.09	111.80
1	A	328	ARG	NE-CZ-NH1	11.55	126.07	120.30
1	B	221	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	B	70	LYS	CA-CB-CG	11.00	137.60	113.40
1	B	253	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	B	292	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	232	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	B	149	ARG	NE-CZ-NH2	9.51	125.05	120.30
1	A	286	TRP	CD1-CG-CD2	9.34	113.77	106.30
1	B	2	TYR	CB-CG-CD2	-8.58	115.85	121.00
1	B	286	TRP	CE2-CD2-CG	-8.33	100.63	107.30
1	B	328	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	B	107	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	B	286	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	B	338	TRP	CD1-CG-CD2	7.98	112.69	106.30
1	A	315	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	275	LEU	CA-CB-CG	7.90	133.47	115.30
1	B	334	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	A	286	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	A	242	LEU	CA-CB-CG	7.81	133.26	115.30
1	B	296	MET	CA-CB-CG	7.79	126.54	113.30
1	B	48	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	A	107	TRP	CD1-CG-CD2	7.73	112.49	106.30
1	B	107	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	B	334	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	A	268	CYS	CA-CB-SG	-7.63	100.26	114.00
1	A	167	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	A	338	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	A	120	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	B	167	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	B	24	GLN	CA-CB-CG	7.42	129.72	113.40
1	B	253	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	111	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	A	339	LEU	CA-C-N	-7.34	101.05	117.20
1	A	338	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	A	334	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	B	27	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	120	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	111	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	A	334	TRP	CD1-CG-CD2	7.14	112.01	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	B	286	TRP	CG-CD2-CE3	7.09	140.28	133.90
1	B	111	TRP	CD1-CG-CD2	7.08	111.96	106.30
1	B	82	LEU	CA-CB-CG	7.06	131.54	115.30
1	A	48	TRP	CE2-CD2-CG	-6.98	101.71	107.30
1	B	338	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	B	242	LEU	CA-CB-CG	6.90	131.18	115.30
1	A	107	TRP	CE2-CD2-CG	-6.85	101.82	107.30
1	B	286	TRP	CB-CG-CD1	-6.82	118.14	127.00
1	A	48	TRP	CD1-CG-CD2	6.75	111.70	106.30
1	A	111	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	A	82	LEU	CA-CB-CG	6.65	130.60	115.30
1	B	107	TRP	CG-CD2-CE3	6.65	139.89	133.90
1	B	292	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	227	ASN	CB-CG-ND2	6.55	132.43	116.70
1	B	236	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	167	TRP	CG-CD1-NE1	-6.48	103.62	110.10
1	B	334	TRP	CG-CD2-CE3	6.46	139.72	133.90
1	B	203	LEU	CA-CB-CG	6.41	130.05	115.30
1	B	59	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	59	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	207	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	203	LEU	CA-CB-CG	6.14	129.42	115.30
1	B	334	TRP	CB-CG-CD1	-6.09	119.08	127.00
1	B	271	GLU	CA-CB-CG	6.08	126.78	113.40
1	A	267	GLU	C-N-CA	-6.03	106.63	121.70
1	B	70	LYS	CB-CG-CD	-5.99	96.03	111.60
1	A	286	TRP	CG-CD1-NE1	-5.96	104.14	110.10
1	A	69	GLU	CA-CB-CG	5.95	126.49	113.40
1	A	167	TRP	CE2-CD2-CG	-5.95	102.54	107.30
1	A	236	ARG	CB-CG-CD	-5.88	96.30	111.60
1	A	275	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	232	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
1	B	338	TRP	CG-CD1-NE1	-5.83	104.28	110.10
1	A	144	GLU	CA-CB-CG	5.80	126.17	113.40
1	B	187	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	272	CYS	CA-CB-SG	-5.73	103.68	114.00
1	A	149	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	107	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	A	48	TRP	CG-CD2-CE3	5.67	139.01	133.90
1	A	340	VAL	CG1-CB-CG2	-5.66	101.84	110.90
1	A	89	ARG	NE-CZ-NH2	-5.61	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	167	TRP	CE2-CD2-CG	-5.55	102.86	107.30
1	A	167	TRP	CG-CD1-NE1	-5.50	104.59	110.10
1	A	334	TRP	CB-CG-CD1	-5.49	119.87	127.00
1	A	277	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	A	340	VAL	N-CA-C	5.47	125.77	111.00
1	A	339	LEU	O-C-N	5.46	131.43	122.70
1	B	107	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	B	289	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	B	107	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	A	339	LEU	N-CA-C	5.37	125.51	111.00
1	B	79	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	A	338	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	B	328	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	237	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	191	LYS	CB-CA-C	-5.32	99.75	110.40
1	A	107	TRP	CB-CG-CD1	-5.32	120.08	127.00
1	A	334	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	A	268	CYS	N-CA-C	5.29	125.27	111.00
1	A	292	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	122	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	B	315	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	191	LYS	CA-CB-CG	5.23	124.91	113.40
1	A	48	TRP	CB-CG-CD1	-5.22	120.21	127.00
1	A	207	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	334	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	B	149	ARG	CB-CG-CD	5.09	124.85	111.60
1	A	338	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	B	111	TRP	CG-CD2-CE3	5.07	138.47	133.90
1	A	46	PHE	CB-CG-CD2	-5.05	117.27	120.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	ARG	Sidechain
1	B	149	ARG	Sidechain
1	B	157	TYR	Sidechain
1	B	221	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	2784	0	2728	32	0
1	B	2784	0	2729	42	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	122	0	0	4	0
4	B	111	0	0	3	0
All	All	5818	0	5457	74	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 (74) 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:272:CYS:CA	1:A:272:CYS:CB	1.84	1.54
1:A:272:CYS:CB	1:A:272:CYS:N	2.31	0.93
1:A:268:CYS:SG	4:A:509:HOH:O	2.34	0.83
1:A:272:CYS:SG	4:A:509:HOH:O	2.45	0.74
1:B:2:TYR:HB2	1:B:168:HIS:CD2	2.22	0.73
1:A:239:ALA:HB2	1:A:340:VAL:HG13	1.71	0.72
1:B:2:TYR:HB2	1:B:168:HIS:HD2	1.55	0.69
1:B:253:ARG:HH22	1:B:320:GLY:HA3	1.58	0.68
1:A:239:ALA:HB2	1:A:340:VAL:CG1	2.23	0.68
1:B:149:ARG:HH22	1:B:286:TRP:HB2	1.59	0.66
1:A:272:CYS:CB	1:A:272:CYS:H	2.12	0.62
1:A:66:PRO:HG2	1:A:69:GLU:HG2	1.81	0.61
1:A:79:TYR:CE1	1:A:149:ARG:HD3	2.37	0.59
1:B:68:HIS:HB3	1:B:293:ASP:HB2	1.84	0.59
1:B:289:TYR:O	1:B:292:ARG:HB2	2.03	0.59
1:A:35:ILE:HG12	1:A:247:HIS:ND1	2.17	0.58
1:B:59:ARG:HH12	1:B:63:GLN:HE22	1.49	0.58
1:A:268:CYS:O	1:A:272:CYS:SG	2.62	0.58
1:A:195:LEU:HD13	4:A:509:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLU:HG2	1:B:296:MET:HG2	1.86	0.57
1:A:197:LEU:HB3	1:A:249:LEU:HD21	1.88	0.55
1:B:53:VAL:HG13	1:B:229:LYS:HE2	1.90	0.54
1:B:252:LEU:HD22	1:B:261:MET:HG3	1.90	0.53
1:B:19:PHE:HE1	1:B:189:LEU:HD13	1.74	0.53
1:A:205:ALA:HB1	1:A:315:ARG:HG2	1.91	0.52
1:B:6:SER:O	1:B:24:GLN:HG3	2.10	0.51
1:B:42:LYS:HE3	1:B:240:LEU:HD21	1.91	0.51
1:A:79:TYR:CZ	1:A:149:ARG:HD3	2.45	0.51
1:A:235:ALA:HB1	1:A:340:VAL:CG2	2.41	0.51
1:B:59:ARG:HH12	1:B:63:GLN:NE2	2.09	0.51
1:A:268:CYS:C	1:A:272:CYS:SG	2.89	0.51
1:A:209:TYR:OH	1:A:340:VAL:HG11	2.11	0.49
1:B:227:ASN:O	1:B:231:ILE:HG12	2.12	0.49
1:B:198:MET:SD	1:B:276:PHE:HE2	2.35	0.49
1:B:17:MET:HB2	4:B:634:HOH:O	2.13	0.49
1:A:268:CYS:HB2	1:A:271:GLU:HG2	1.95	0.49
1:B:155:SER:O	1:B:159:GLU:HG3	2.12	0.48
1:B:236:ARG:HD2	4:B:572:HOH:O	2.12	0.48
1:B:57:ARG:HG2	1:B:60:ILE:HD12	1.94	0.48
1:B:284:LYS:HZ2	1:B:305:CYS:HB3	1.78	0.48
1:A:205:ALA:HB1	1:A:315:ARG:CG	2.44	0.47
1:B:255:GLY:CA	1:B:262:ALA:HB2	2.45	0.47
1:A:65:LEU:HD22	1:A:69:GLU:HG3	1.97	0.47
1:A:151:GLU:HB3	1:A:282:GLN:NE2	2.29	0.47
1:B:188:GLU:HA	1:B:191:LYS:HD3	1.96	0.47
1:A:287:ALA:HB2	1:A:304:LEU:HD22	1.97	0.46
1:B:19:PHE:CE1	1:B:189:LEU:HD13	2.51	0.45
1:B:68:HIS:CB	1:B:293:ASP:HB2	2.45	0.45
1:A:236:ARG:HD3	4:A:727:HOH:O	2.17	0.45
1:B:79:TYR:CE2	1:B:83:LEU:HD11	2.52	0.45
1:A:19:PHE:CE2	1:A:190:LYS:HG2	2.52	0.45
1:A:53:VAL:HG11	1:A:230:ILE:HG13	1.99	0.45
1:B:253:ARG:HH22	1:B:320:GLY:CA	2.27	0.44
1:B:67:GLU:HA	1:B:70:LYS:HG2	2.00	0.44
1:B:127:ARG:HD3	4:B:713:HOH:O	2.16	0.44
1:A:186:LEU:HG	1:A:190:LYS:HE3	2.00	0.44
1:A:98:LEU:HD21	1:A:164:THR:HG23	1.99	0.43
1:A:255:GLY:HA2	1:A:262:ALA:HB2	2.01	0.43
1:B:113:PHE:CZ	1:B:117:ILE:HD11	2.54	0.43
1:B:171:GLY:O	1:B:175:HIS:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:GLN:HB2	1:B:323:LEU:HD21	2.00	0.43
1:B:328:ARG:HG3	1:B:329:SER:O	2.18	0.42
1:B:59:ARG:HH11	1:B:59:ARG:HG2	1.83	0.42
1:B:301:LYS:O	1:B:305:CYS:SG	2.71	0.42
1:A:133:PRO:HB3	1:A:137:PHE:HE2	1.85	0.42
1:B:330:ASN:HD22	1:B:331:PRO:HD2	1.85	0.42
1:A:59:ARG:O	1:A:63:GLN:HB2	2.20	0.42
1:A:1:ALA:HB2	1:A:168:HIS:O	2.20	0.41
1:B:149:ARG:HD2	1:B:282:GLN:HB3	2.03	0.41
1:B:171:GLY:O	1:B:175:HIS:CE1	2.74	0.41
1:B:129:ILE:HG13	1:B:130:VAL:HG23	2.02	0.41
1:B:187:ARG:NH1	1:B:260:GLU:HG2	2.36	0.41
1:B:49:ARG:HA	1:B:50:PRO:HD3	1.95	0.41
1:B:19:PHE:CE1	1:B:98:LEU:HD22	2.57	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%)	332 (98%)	6 (2%)	0	100	100
1	B	338/375 (90%)	330 (98%)	7 (2%)	1 (0%)	41	61
All	All	676/750 (90%)	662 (98%)	13 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	131	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/339 (90%)	285 (93%)	21 (7%)	15	30
1	B	306/339 (90%)	277 (90%)	29 (10%)	8	17
All	All	612/678 (90%)	562 (92%)	50 (8%)	11	22

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	31	GLN
1	A	38	LYS
1	A	42	LYS
1	A	49	ARG
1	A	133	PRO
1	A	149	ARG
1	A	151	GLU
1	A	155	SER
1	A	187	ARG
1	A	195	LEU
1	A	203	LEU
1	A	242	LEU
1	A	266	GLU
1	A	272	CYS
1	A	278	GLN
1	A	292	ARG
1	A	293	ASP
1	A	296	MET
1	A	315	ARG
1	A	319	VAL
1	B	6	SER
1	B	24	GLN
1	B	31	GLN
1	B	63	GLN
1	B	67	GLU
1	B	100	SER

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Mol	Chain	Res	Type
1	B	134	SER
1	B	142	THR
1	B	145	GLN
1	B	149	ARG
1	B	187	ARG
1	B	189	LEU
1	B	197	LEU
1	B	203	LEU
1	B	208	PHE
1	B	242	LEU
1	B	253	ARG
1	B	270	GLN
1	B	271	GLU
1	B	275	LEU
1	B	281	GLN
1	B	293	ASP
1	B	295	SER
1	B	297	ILE
1	B	317	GLN
1	B	319	VAL
1	B	326	ASN
1	B	330	ASN
1	B	340	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	201	ASN
1	A	306	GLN
1	B	10	ASN
1	B	63	GLN
1	B	168	HIS
1	B	175	HIS
1	B	201	ASN
1	B	326	ASN
1	B	330	ASN

5.3.3 RNA ⓘ

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 monosaccharides 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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.