



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:02 AM UTC

PDB ID : 1MRR / pdb_00001mrr
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

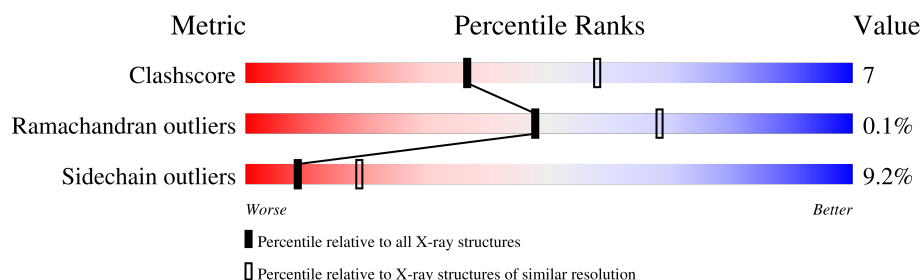
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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	 67% 18% 6% 9%
1	B	375	 60% 22% 8% 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 (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	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	1.09	14/2848 (0.5%)	1.81	57/3864 (1.5%)
1	B	0.96	12/2848 (0.4%)	1.81	72/3864 (1.9%)
All	All	1.03	26/5696 (0.5%)	1.81	129/7728 (1.7%)

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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	CYS	CA-CB	19.29	1.83	1.53
1	A	268	CYS	CA-CB	-14.72	1.33	1.53
1	A	247	HIS	CG-ND1	-9.10	1.28	1.38
1	A	241	HIS	CD2-NE2	-7.98	1.29	1.37
1	A	118	HIS	CD2-NE2	-7.73	1.29	1.37
1	B	168	HIS	CG-ND1	-7.32	1.30	1.38
1	B	241	HIS	CD2-NE2	-7.20	1.29	1.37
1	A	168	HIS	CD2-NE2	-7.17	1.29	1.37
1	B	297	ILE	CA-CB	7.15	1.63	1.54
1	A	268	CYS	CA-C	-7.09	1.44	1.53
1	A	175	HIS	CD2-NE2	-6.95	1.30	1.37
1	A	71	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	118	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	168	HIS	CD2-NE2	-6.30	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	HIS	CD2-NE2	-6.20	1.31	1.37
1	B	319	VAL	CA-CB	6.19	1.61	1.54
1	B	68	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	68	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	247	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	124	HIS	CD2-NE2	-5.95	1.31	1.37
1	B	71	HIS	CD2-NE2	-5.94	1.31	1.37
1	B	124	HIS	CD2-NE2	-5.86	1.31	1.37
1	B	247	HIS	CD2-NE2	-5.73	1.31	1.37
1	A	319	VAL	CA-CB	5.37	1.60	1.54
1	A	272	CYS	CA-C	5.29	1.59	1.52
1	B	241	HIS	CG-ND1	-5.26	1.32	1.38

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	CYS	CB-CA-C	14.99	136.34	110.85
1	A	272	CYS	N-CA-CB	-14.03	89.40	110.16
1	A	272	CYS	CA-CB-SG	12.49	143.14	114.40
1	B	70	LYS	CA-CB-CG	11.75	137.60	114.10
1	B	147	GLN	N-CA-C	11.51	123.83	111.28
1	B	149	ARG	CG-CD-NE	-11.32	87.09	112.00
1	A	293	ASP	CA-CB-CG	11.22	123.82	112.60
1	A	227	ASN	CB-CG-ND2	10.68	132.43	116.40
1	A	227	ASN	OD1-CG-ND2	-10.30	112.30	122.60
1	A	267	GLU	CA-C-N	-9.91	106.63	122.79
1	A	267	GLU	C-N-CA	-9.91	106.63	122.79
1	A	339	LEU	N-CA-C	9.87	125.51	109.72
1	A	268	CYS	N-CA-C	9.51	125.27	111.87
1	B	268	CYS	CA-CB-SG	9.40	136.02	114.40
1	B	145	GLN	OE1-CD-NE2	-8.96	113.64	122.60
1	B	258	ASP	CA-CB-CG	8.88	121.48	112.60
1	B	330	ASN	OD1-CG-ND2	-8.87	113.73	122.60
1	B	326	ASN	CA-CB-CG	8.67	121.27	112.60
1	A	319	VAL	N-CA-CB	-8.57	101.03	112.16
1	A	58	ASP	CA-CB-CG	8.24	120.84	112.60
1	B	330	ASN	CB-CG-ND2	8.02	128.43	116.40
1	B	319	VAL	N-CA-CB	-7.82	101.97	112.22
1	B	24	GLN	CA-CB-CG	7.81	129.72	114.10
1	A	34	ASP	CA-CB-CG	7.75	120.34	112.60
1	A	232	ARG	NE-CZ-NH1	7.72	129.22	121.50
1	A	306	GLN	OE1-CD-NE2	-7.72	114.88	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ARG	NE-CZ-NH1	-7.66	113.84	121.50
1	A	296	MET	CA-C-O	-7.63	112.51	121.44
1	B	12	GLN	OE1-CD-NE2	-7.50	115.10	122.60
1	B	227	ASN	OD1-CG-ND2	-7.43	115.17	122.60
1	B	131	ASN	CA-CB-CG	-7.32	105.28	112.60
1	B	191	LYS	CB-CA-C	-7.09	99.75	110.88
1	B	12	GLN	CG-CD-NE2	7.06	126.98	116.40
1	B	68	HIS	CB-CG-CD2	-6.85	122.30	131.20
1	A	71	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	A	227	ASN	CA-CB-CG	6.81	119.41	112.60
1	A	258	ASP	CA-CB-CG	6.66	119.26	112.60
1	B	70	LYS	CB-CG-CD	-6.64	96.03	111.30
1	B	71	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	B	250	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	A	319	VAL	CB-CA-C	6.55	119.64	111.65
1	A	24	GLN	OE1-CD-NE2	6.54	129.14	122.60
1	A	236	ARG	CB-CG-CD	-6.52	96.30	111.30
1	B	149	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	B	286	TRP	CG-CD2-CE3	6.38	140.28	133.90
1	A	340	VAL	N-CA-CB	-6.35	100.71	111.50
1	A	339	LEU	O-C-N	6.34	131.43	123.19
1	B	271	GLU	CA-CB-CG	6.34	126.78	114.10
1	B	278	GLN	OE1-CD-NE2	-6.27	116.33	122.60
1	B	90	SER	N-CA-C	6.25	123.62	109.81
1	B	296	MET	CA-CB-CG	6.22	126.54	114.10
1	A	272	CYS	N-CA-C	-6.21	104.59	111.36
1	A	69	GLU	CA-CB-CG	6.20	126.49	114.10
1	A	165	SER	CA-C-O	-6.15	114.37	120.70
1	A	268	CYS	CA-CB-SG	-6.15	100.26	114.40
1	B	191	LYS	N-CA-CB	6.09	118.83	110.01
1	A	144	GLU	CA-CB-CG	6.03	126.17	114.10
1	A	168	HIS	CB-CG-CD2	-6.02	123.38	131.20
1	B	227	ASN	CB-CG-ND2	6.02	125.42	116.40
1	B	107	TRP	CG-CD2-CE3	5.99	139.89	133.90
1	B	208	PHE	CA-CB-CG	-5.96	107.84	113.80
1	B	71	HIS	CB-CG-ND1	5.94	131.61	122.70
1	A	63	GLN	OE1-CD-NE2	-5.93	116.67	122.60
1	B	107	TRP	N-CA-C	-5.92	104.91	111.36
1	B	221	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	B	149	ARG	CB-CG-CD	5.89	124.85	111.30
1	A	339	LEU	CA-C-N	5.88	132.28	121.70
1	A	339	LEU	C-N-CA	5.88	132.28	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ASP	CA-CB-CG	-5.88	106.72	112.60
1	B	286	TRP	CB-CG-CD1	-5.84	118.14	126.90
1	A	147	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	B	334	TRP	CG-CD2-CE3	5.82	139.72	133.90
1	B	60	ILE	CB-CG1-CD1	-5.81	101.60	113.80
1	B	36	PHE	CA-CB-CG	-5.80	108.00	113.80
1	A	31	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	B	9	LYS	N-CA-C	-5.76	101.12	109.59
1	B	278	GLN	CG-CD-NE2	5.75	125.02	116.40
1	B	124	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	B	319	VAL	CB-CA-C	5.73	120.08	112.46
1	A	175	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	A	106	THR	CA-CB-OG1	-5.58	101.24	109.60
1	B	289	TYR	N-CA-C	-5.57	105.21	112.23
1	A	118	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	A	246	GLN	CG-CD-NE2	5.53	124.70	116.40
1	B	122	TYR	CA-C-O	-5.47	114.62	120.42
1	B	286	TRP	CE2-CD2-CG	-5.47	100.63	107.20
1	B	214	CYS	O-C-N	-5.46	115.93	122.15
1	B	241	HIS	CA-CB-CG	5.46	119.26	113.80
1	B	247	HIS	CB-CG-CD2	-5.41	124.16	131.20
1	B	205	ALA	N-CA-C	5.41	117.26	111.36
1	B	291	PHE	CA-C-N	5.41	127.79	120.65
1	B	291	PHE	C-N-CA	5.41	127.79	120.65
1	B	191	LYS	CA-CB-CG	5.40	124.91	114.10
1	A	210	VAL	N-CA-C	-5.37	105.49	110.53
1	A	36	PHE	CA-CB-CG	-5.35	108.45	113.80
1	B	131	ASN	N-CA-C	5.35	122.19	110.80
1	B	23	VAL	CA-C-N	-5.33	114.56	122.56
1	B	23	VAL	C-N-CA	-5.33	114.56	122.56
1	A	241	HIS	CA-C-N	5.33	127.36	120.44
1	A	241	HIS	C-N-CA	5.33	127.36	120.44
1	B	336	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	268	CYS	O-C-N	5.32	129.33	122.20
1	A	92	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	340	VAL	N-CA-C	5.27	125.77	111.00
1	A	300	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	B	281	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	B	339	LEU	CA-C-N	5.23	131.11	121.70
1	B	339	LEU	C-N-CA	5.23	131.11	121.70
1	B	334	TRP	CB-CG-CD1	-5.21	119.08	126.90
1	B	76	ASN	OD1-CG-ND2	-5.20	117.40	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	GLU	CB-CG-CD	5.18	121.40	112.60
1	A	80	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	B	53	VAL	N-CA-C	-5.17	100.44	107.99
1	A	68	HIS	CA-CB-CG	5.14	118.94	113.80
1	A	286	TRP	CE2-CD2-CG	-5.13	101.04	107.20
1	B	143	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	143	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	48	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	A	96	LEU	CA-C-O	-5.10	113.17	120.16
1	B	164	THR	CA-CB-OG1	-5.10	101.95	109.60
1	A	68	HIS	CB-CG-CD2	-5.10	124.58	131.20
1	A	297	ILE	O-C-N	-5.07	116.94	121.91
1	B	107	TRP	CE2-CD2-CG	-5.06	101.12	107.20
1	B	167	TRP	CG-CD1-NE1	-5.06	103.62	110.20
1	B	54	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	334	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	B	329	SER	N-CA-CB	-5.04	103.23	110.44
1	B	49	ARG	CA-C-N	5.03	124.63	119.05
1	B	49	ARG	C-N-CA	5.03	124.63	119.05

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
1:B:69:GLU:HG2	1:B:296:MET:HG2	1.86	0.57
1:A:268:CYS:C	1:A:272:CYS:SG	2.89	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:284:LYS:HZ2	1:B:305:CYS:HB3	1.77	0.50
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	55
All	All	676/750 (90%)	662 (98%)	13 (2%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	131	ASN

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	306/339 (90%)	278 (91%)	28 (9%)	8	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	306/339 (90%)	278 (91%)	28 (9%)	8	19
All	All	612/678 (90%)	556 (91%)	56 (9%)	8	19

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	31	GLN
1	A	42	LYS
1	A	49	ARG
1	A	100	SER
1	A	130	VAL
1	A	133	PRO
1	A	144	GLU
1	A	149	ARG
1	A	151	GLU
1	A	155	SER
1	A	193	LEU
1	A	195	LEU
1	A	197	LEU
1	A	199	SER
1	A	203	LEU
1	A	242	LEU
1	A	263	GLU
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	A	328	ARG
1	A	339	LEU
1	B	6	SER
1	B	24	GLN
1	B	31	GLN
1	B	63	GLN
1	B	67	GLU
1	B	82	LEU
1	B	100	SER
1	B	134	SER

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Mol	Chain	Res	Type
1	B	142	THR
1	B	145	GLN
1	B	149	ARG
1	B	189	LEU
1	B	197	LEU
1	B	203	LEU
1	B	208	PHE
1	B	236	ARG
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	290	LEU
1	B	293	ASP
1	B	297	ILE
1	B	319	VAL
1	B	326	ASN
1	B	340	VAL

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	31	GLN
1	A	147	GLN
1	A	201	ASN
1	A	227	ASN
1	B	10	ASN
1	B	63	GLN
1	B	128	ASN
1	B	168	HIS
1	B	175	HIS
1	B	201	ASN
1	B	278	GLN
1	B	282	GLN
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 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

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.