



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 01:17 PM EST

PDB ID : 1A0P
Title : SITE-SPECIFIC RECOMBINASE, XERD
Authors : Subramanya, H.S.; Arciszewska, L.K.; Baker, R.A.; Bird, L.E.; Sherratt, D.J.;
Wigley, D.B.
Deposited on : 1997-12-05
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)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

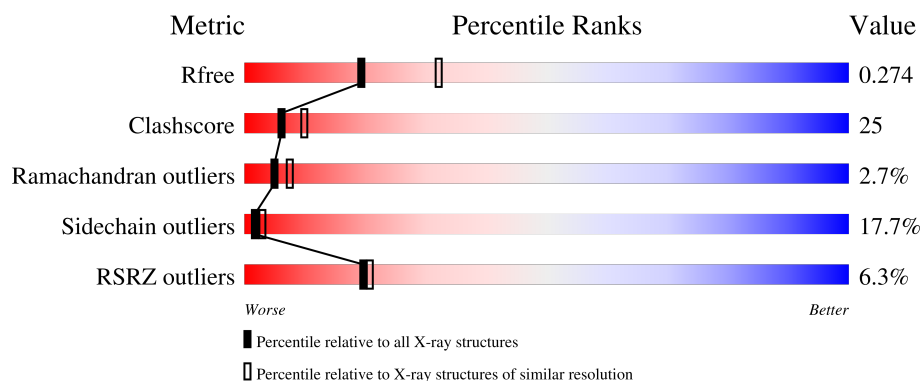
1 Overall quality at a glance

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))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 $\leq 5\%$. 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	290	6% 39% 38% 13% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2310 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 SITE-SPECIFIC RECOMBINASE XERD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2205	1397	403	399	6			

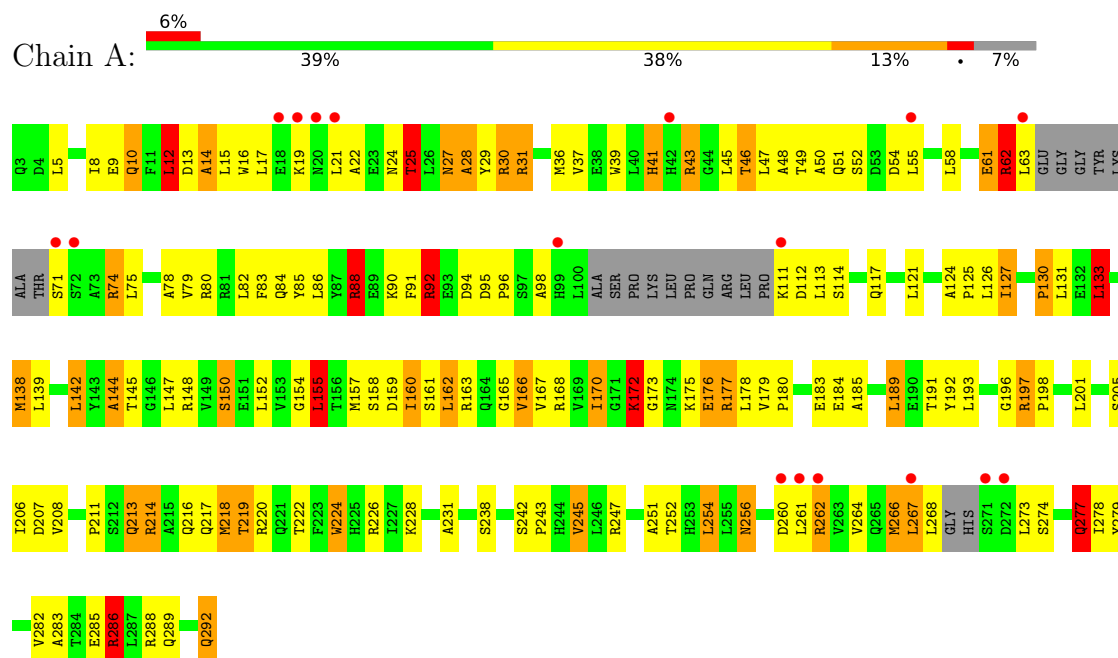
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	105	Total	O	0	0
			105	105		

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: SITE-SPECIFIC RECOMBINASE XERD



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	102.95Å 102.95Å 55.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50 14.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 99.1 (14.88-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.39 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.287 0.210 , 0.274	Depositor DCC
R_{free} test set	930 reflections (7.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 91.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2310	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	0.69	0/2244	1.96	50/3035 (1.6%)

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	27

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	NE-CZ-NH2	-19.75	110.42	120.30
1	A	88	ARG	CD-NE-CZ	15.79	145.71	123.60
1	A	286	ARG	NE-CZ-NH1	15.27	127.94	120.30
1	A	286	ARG	CD-NE-CZ	15.26	144.97	123.60
1	A	288	ARG	CD-NE-CZ	14.37	143.71	123.60
1	A	177	ARG	NE-CZ-NH1	14.07	127.33	120.30
1	A	177	ARG	NE-CZ-NH2	-13.98	113.31	120.30
1	A	148	ARG	NE-CZ-NH2	13.43	127.02	120.30
1	A	168	ARG	CD-NE-CZ	13.11	141.95	123.60
1	A	197	ARG	NE-CZ-NH2	13.10	126.85	120.30
1	A	43	ARG	CD-NE-CZ	12.11	140.55	123.60
1	A	168	ARG	NE-CZ-NH1	12.01	126.31	120.30
1	A	159	ASP	CB-CG-OD2	11.97	129.07	118.30
1	A	92	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	A	197	ARG	CD-NE-CZ	11.23	139.32	123.60
1	A	226	ARG	NE-CZ-NH1	-10.87	114.86	120.30
1	A	148	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	A	74	ARG	NE-CZ-NH1	8.61	124.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	N-CA-CB	-8.56	95.20	110.60
1	A	62	ARG	CG-CD-NE	8.21	129.05	111.80
1	A	286	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	168	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	A	30	ARG	CD-NE-CZ	7.95	134.74	123.60
1	A	88	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	62	ARG	CD-NE-CZ	7.40	133.95	123.60
1	A	288	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	218	MET	CA-CB-CG	7.17	125.49	113.30
1	A	92	ARG	CD-NE-CZ	7.08	133.51	123.60
1	A	88	ARG	CG-CD-NE	6.94	126.37	111.80
1	A	220	ARG	CD-NE-CZ	6.06	132.08	123.60
1	A	177	ARG	CD-NE-CZ	5.95	131.93	123.60
1	A	218	MET	CB-CA-C	5.89	122.17	110.40
1	A	74	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	247	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	159	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	A	12	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	274	SER	N-CA-CB	-5.43	102.36	110.50
1	A	226	ARG	NH1-CZ-NH2	5.42	125.36	119.40
1	A	277	GLN	CB-CG-CD	5.40	125.65	111.60
1	A	266	MET	CA-CB-CG	5.34	122.39	113.30
1	A	224	TRP	CB-CA-C	5.31	121.02	110.40
1	A	192	TYR	CB-CG-CD2	5.29	124.18	121.00
1	A	172	LYS	CA-CB-CG	5.23	124.90	113.40
1	A	288	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	283	ALA	N-CA-CB	5.19	117.36	110.10
1	A	155	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	88	ARG	CB-CG-CD	5.11	124.89	111.60
1	A	112	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	112	ASP	N-CA-CB	-5.02	101.57	110.60
1	A	158	SER	CB-CA-C	-5.01	100.59	110.10

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLN	Mainchain
1	A	113	LEU	Mainchain
1	A	124	ALA	Mainchain
1	A	125	PRO	Mainchain
1	A	127	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	133	LEU	Mainchain
1	A	138	MET	Mainchain
1	A	14	ALA	Mainchain
1	A	142	LEU	Mainchain
1	A	144	ALA	Mainchain
1	A	163	ARG	Mainchain
1	A	173	GLY	Peptide
1	A	175	LYS	Mainchain
1	A	176	GLU	Mainchain
1	A	179	VAL	Mainchain
1	A	213	GLN	Mainchain
1	A	219	THR	Mainchain
1	A	224	TRP	Mainchain
1	A	243	PRO	Mainchain
1	A	245	VAL	Mainchain
1	A	25	THR	Mainchain
1	A	28	ALA	Mainchain
1	A	30	ARG	Mainchain
1	A	41	HIS	Mainchain
1	A	54	ASP	Mainchain
1	A	61	GLU	Peptide
1	A	74	ARG	Mainchain

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	2205	0	2229	109	0
2	A	105	0	0	5	0
All	All	2310	0	2229	109	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 25.

All (109) 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:63:LEU:HD23	1:A:71:SER:HA	1.62	0.81
1:A:85:TYR:HD1	1:A:86:LEU:HD22	1.48	0.78
1:A:273:LEU:HD12	1:A:278:ILE:HG12	1.66	0.77
1:A:36:MET:CE	1:A:79:VAL:HG22	2.16	0.76
1:A:88:ARG:HH11	1:A:88:ARG:HB2	1.51	0.75
1:A:75:LEU:O	1:A:79:VAL:HG23	1.87	0.74
1:A:142:LEU:HD21	1:A:152:LEU:HD22	1.68	0.74
1:A:177:ARG:HD3	2:A:328:HOH:O	1.90	0.72
1:A:36:MET:HE3	1:A:79:VAL:HG22	1.73	0.71
1:A:82:LEU:O	1:A:86:LEU:HD23	1.92	0.70
1:A:114:SER:H	1:A:117:GLN:HE21	1.42	0.66
1:A:242:SER:OG	1:A:245:VAL:HG13	1.95	0.66
1:A:8:ILE:HD11	1:A:37:VAL:HG11	1.77	0.65
1:A:277:GLN:HB2	2:A:371:HOH:O	1.96	0.65
1:A:37:VAL:HG23	1:A:41:HIS:HD2	1.61	0.64
1:A:133:LEU:HD11	1:A:191:THR:HG22	1.80	0.63
1:A:197:ARG:HB3	1:A:198:PRO:HD3	1.79	0.63
1:A:114:SER:H	1:A:117:GLN:NE2	1.97	0.63
1:A:273:LEU:HB3	1:A:278:ILE:HD11	1.80	0.63
1:A:154:GLY:HA2	1:A:217:GLN:OE1	1.99	0.63
1:A:260:ASP:OD2	1:A:286:ARG:HD3	1.99	0.62
1:A:214:ARG:O	1:A:214:ARG:HG3	1.99	0.61
1:A:219:THR:OG1	1:A:222:THR:HG23	2.01	0.60
1:A:85:TYR:CD1	1:A:86:LEU:HD22	2.35	0.60
1:A:29:TYR:CD1	1:A:78:ALA:HB2	2.37	0.60
1:A:80:ARG:HH21	1:A:98:ALA:HA	1.67	0.59
1:A:5:LEU:HA	1:A:8:ILE:HD12	1.84	0.59
1:A:268:LEU:HG	1:A:273:LEU:HD11	1.86	0.58
1:A:138:MET:HB3	1:A:152:LEU:HD21	1.86	0.57
1:A:268:LEU:CG	1:A:273:LEU:HD11	2.35	0.57
1:A:214:ARG:HD3	1:A:216:GLN:HE21	1.68	0.57
1:A:180:PRO:HG2	1:A:286:ARG:HB2	1.87	0.56
1:A:8:ILE:HG22	1:A:12:LEU:HD22	1.87	0.56
1:A:142:LEU:CD2	1:A:152:LEU:HD22	2.36	0.56
1:A:285:GLU:OE2	1:A:289:GLN:NE2	2.38	0.55
1:A:58:LEU:CD2	1:A:75:LEU:HD21	2.37	0.55
1:A:144:ALA:O	1:A:286:ARG:NH2	2.40	0.55
1:A:206:ILE:HD13	1:A:208:VAL:HB	1.89	0.55
1:A:86:LEU:HD12	1:A:91:PHE:CD2	2.41	0.54
1:A:58:LEU:HD23	1:A:75:LEU:HD21	1.89	0.54
1:A:170:ILE:HG13	1:A:176:GLU:HG2	1.88	0.54
1:A:264:VAL:O	1:A:268:LEU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:N	1:A:198:PRO:CD	2.71	0.54
1:A:261:LEU:HD22	1:A:282:VAL:HG22	1.89	0.54
1:A:214:ARG:HD3	1:A:216:GLN:NE2	2.23	0.53
1:A:92:ARG:HD3	1:A:94:ASP:OD1	2.08	0.53
1:A:152:LEU:HA	1:A:155:LEU:HD22	1.90	0.53
1:A:37:VAL:HG23	1:A:41:HIS:CD2	2.43	0.52
1:A:90:LYS:HE2	1:A:111:LYS:HB2	1.92	0.52
1:A:28:ALA:O	1:A:31:ARG:HB3	2.11	0.51
1:A:251:ALA:HB2	1:A:279:TYR:CE2	2.46	0.51
1:A:88:ARG:HH11	1:A:88:ARG:CB	2.22	0.50
1:A:90:LYS:HE2	1:A:111:LYS:HG3	1.94	0.49
1:A:22:ALA:HB3	1:A:25:THR:CG2	2.42	0.49
1:A:22:ALA:HB3	1:A:25:THR:HG23	1.93	0.49
1:A:252:THR:O	1:A:256:ASN:HB2	2.12	0.49
1:A:160:ILE:HD12	1:A:167:VAL:HG23	1.95	0.49
1:A:16:TRP:CD1	1:A:172:LYS:HG3	2.48	0.48
1:A:82:LEU:HD11	1:A:86:LEU:HD21	1.95	0.48
1:A:254:LEU:HD11	1:A:282:VAL:HG21	1.95	0.48
1:A:36:MET:HG3	1:A:58:LEU:CD1	2.43	0.47
1:A:165:GLY:O	2:A:327:HOH:O	2.20	0.47
1:A:50:ALA:O	1:A:92:ARG:NH2	2.44	0.47
1:A:21:LEU:HD23	1:A:25:THR:OG1	2.14	0.47
1:A:63:LEU:HD23	1:A:71:SER:CA	2.40	0.47
1:A:83:PHE:HB3	1:A:95:ASP:OD1	2.15	0.46
1:A:145:THR:OG1	1:A:147:LEU:HG	2.15	0.46
1:A:39:TRP:HE1	1:A:61:GLU:CD	2.20	0.45
1:A:254:LEU:CD1	1:A:282:VAL:HG21	2.47	0.45
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.94	0.45
1:A:39:TRP:CE3	1:A:58:LEU:HD12	2.52	0.44
1:A:185:ALA:O	1:A:189:LEU:HB2	2.16	0.44
1:A:166:VAL:HG21	1:A:178:LEU:HD13	1.98	0.44
1:A:14:ALA:O	1:A:15:LEU:C	2.56	0.44
1:A:121:LEU:HD12	1:A:231:ALA:HA	1.99	0.44
1:A:36:MET:HG3	1:A:58:LEU:HD13	1.99	0.43
1:A:130:PRO:HD2	2:A:378:HOH:O	2.17	0.43
1:A:62:ARG:HG3	1:A:63:LEU:N	2.33	0.43
1:A:17:LEU:HA	1:A:17:LEU:HD23	1.78	0.43
1:A:157:MET:N	1:A:207:ASP:O	2.41	0.43
1:A:170:ILE:HD11	1:A:176:GLU:OE2	2.18	0.43
1:A:138:MET:HB3	1:A:152:LEU:CD2	2.48	0.43
1:A:62:ARG:HH11	1:A:62:ARG:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NH2	1:A:206:ILE:HD12	2.33	0.43
1:A:90:LYS:NZ	1:A:111:LYS:HB2	2.34	0.42
1:A:80:ARG:O	1:A:84:GLN:HG3	2.19	0.42
1:A:172:LYS:HE2	1:A:172:LYS:HB3	1.62	0.42
1:A:80:ARG:NH1	1:A:84:GLN:OE1	2.53	0.42
1:A:197:ARG:NH2	1:A:206:ILE:O	2.53	0.42
1:A:10:GLN:O	1:A:13:ASP:HB2	2.20	0.42
1:A:161:SER:O	1:A:165:GLY:N	2.46	0.42
1:A:46:THR:HG22	1:A:49:THR:OG1	2.20	0.41
1:A:162:LEU:HD21	1:A:193:LEU:CD1	2.50	0.41
1:A:289:GLN:O	1:A:292:GLN:HB3	2.20	0.41
1:A:152:LEU:O	1:A:155:LEU:HB2	2.19	0.41
1:A:51:GLN:NE2	1:A:51:GLN:HA	2.35	0.41
1:A:62:ARG:O	1:A:63:LEU:HB2	2.20	0.41
1:A:83:PHE:CD1	1:A:96:PRO:HG2	2.55	0.41
1:A:201:LEU:HD21	1:A:206:ILE:HD11	2.03	0.41
1:A:94:ASP:OD1	1:A:94:ASP:N	2.54	0.41
1:A:150:SER:HB2	2:A:310:HOH:O	2.21	0.41
1:A:8:ILE:HD11	1:A:37:VAL:CG1	2.45	0.41
1:A:160:ILE:HD12	1:A:167:VAL:CG2	2.51	0.40
1:A:46:THR:HG23	1:A:48:ALA:H	1.87	0.40
1:A:86:LEU:HD12	1:A:91:PHE:CG	2.56	0.40
1:A:27:ASN:O	1:A:31:ARG:HB2	2.21	0.40
1:A:36:MET:CE	1:A:79:VAL:HG13	2.51	0.40
1:A:201:LEU:HD21	1:A:211:PRO:HG3	2.04	0.40
1:A:268:LEU:HD21	1:A:273:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

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	263/290 (91%)	239 (91%)	17 (6%)	7 (3%)	5 7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	62	ARG
1	A	262	ARG
1	A	24	ASN
1	A	267	LEU
1	A	127	ILE
1	A	196	GLY

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	237/251 (94%)	195 (82%)	42 (18%)	2 3

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	12	LEU
1	A	19	LYS
1	A	25	THR
1	A	27	ASN
1	A	31	ARG
1	A	43	ARG
1	A	46	THR
1	A	52	SER
1	A	55	LEU
1	A	62	ARG
1	A	88	ARG
1	A	92	ARG
1	A	126	LEU

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Mol	Chain	Res	Type
1	A	130	PRO
1	A	131	LEU
1	A	133	LEU
1	A	139	LEU
1	A	150	SER
1	A	155	LEU
1	A	160	ILE
1	A	162	LEU
1	A	166	VAL
1	A	170	ILE
1	A	172	LYS
1	A	183	GLU
1	A	184	GLU
1	A	189	LEU
1	A	205	SER
1	A	213	GLN
1	A	214	ARG
1	A	218	MET
1	A	228	LYS
1	A	238	SER
1	A	254	LEU
1	A	256	ASN
1	A	262	ARG
1	A	266	MET
1	A	267	LEU
1	A	277	GLN
1	A	286	ARG
1	A	292	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	51	GLN
1	A	99	HIS
1	A	117	GLN
1	A	123	GLN
1	A	216	GLN
1	A	229	HIS
1	A	256	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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	271/290 (93%)	0.00	17 (6%) 20 21	18, 43, 94, 122	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	LEU	5.7
1	A	19	LYS	5.3
1	A	63	LEU	5.0
1	A	72	SER	3.5
1	A	111	LYS	3.5
1	A	260	ASP	3.4
1	A	271	SER	3.3
1	A	262	ARG	3.2
1	A	99	HIS	3.0
1	A	71	SER	2.9
1	A	261	LEU	2.9
1	A	20	ASN	2.6
1	A	55	LEU	2.5
1	A	21	LEU	2.4
1	A	18	GLU	2.2
1	A	42	HIS	2.2
1	A	272	ASP	2.1

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 monosaccharides 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.