



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:57 PM UTC

PDB ID : 1A0P / pdb_00001a0p
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	:	4-5-2 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

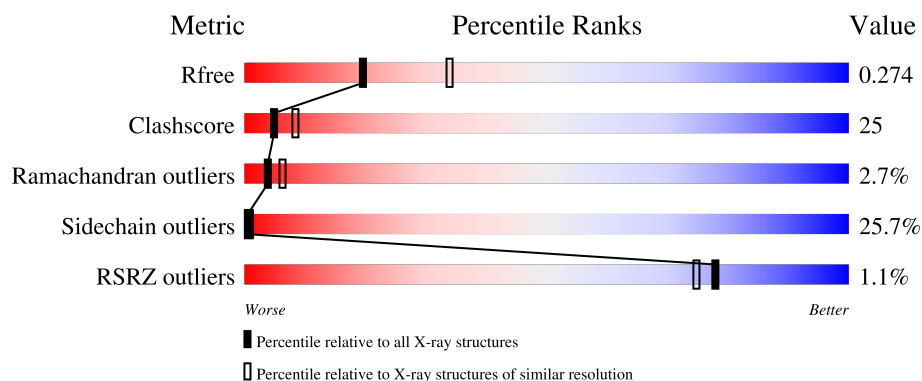
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	31% 35% 19% 8% 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			

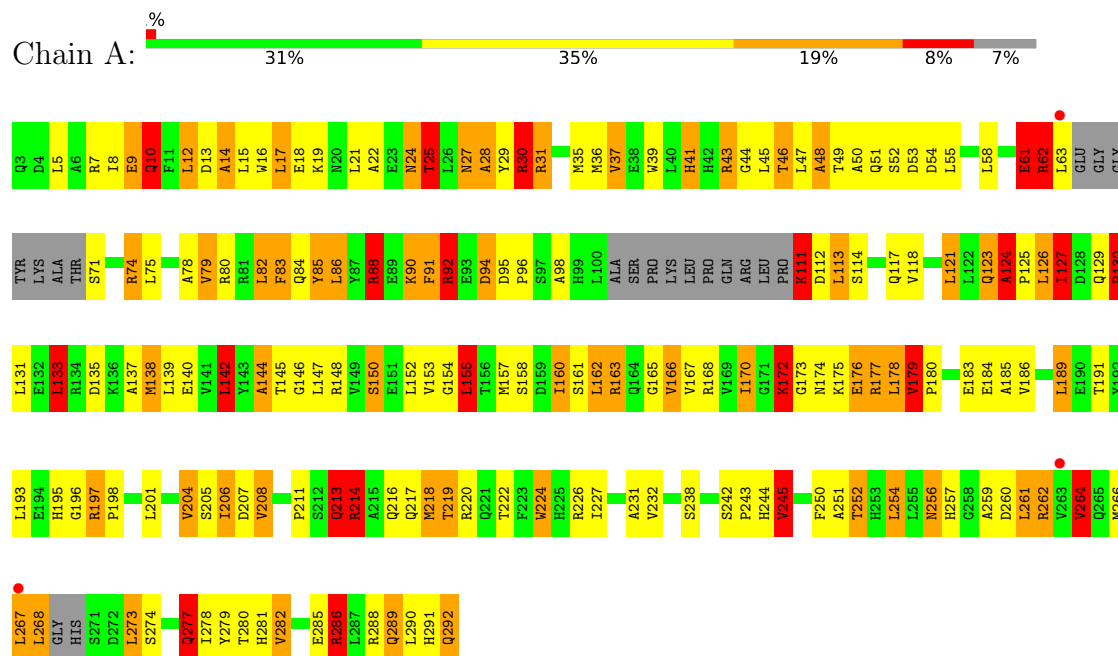
- Molecule 2 is water.

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

3 Residue-property plots

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 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 97.6 (10.00-2.50)	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)	0.42 , 95.4	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	0.91	0/2244	2.25	113/3035 (3.7%)

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	27

There are no bond length outliers.

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	CD-NE-CZ	15.22	145.71	124.40
1	A	286	ARG	CD-NE-CZ	14.69	144.97	124.40
1	A	288	ARG	CD-NE-CZ	13.80	143.71	124.40
1	A	168	ARG	CD-NE-CZ	12.54	141.95	124.40
1	A	43	ARG	CD-NE-CZ	11.54	140.55	124.40
1	A	197	ARG	CD-NE-CZ	10.65	139.32	124.40
1	A	92	ARG	NE-CZ-NH2	-9.75	110.42	119.20
1	A	92	ARG	N-CA-CB	-8.78	95.20	111.53
1	A	148	ARG	NE-CZ-NH2	8.68	127.02	119.20
1	A	53	ASP	CA-CB-CG	-8.67	103.93	112.60
1	A	289	GLN	CA-C-N	8.55	132.43	120.29
1	A	289	GLN	C-N-CA	8.55	132.43	120.29
1	A	197	ARG	NE-CZ-NH2	8.50	126.85	119.20
1	A	179	VAL	CB-CA-C	8.25	119.68	110.52
1	A	135	ASP	CA-CB-CG	8.19	120.79	112.60
1	A	137	ALA	O-C-N	7.88	130.60	122.09
1	A	62	ARG	CG-CD-NE	7.75	129.05	112.00
1	A	137	ALA	CA-C-O	-7.71	112.76	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	GLN	CB-CG-CD	7.67	125.65	112.60
1	A	178	LEU	CA-C-N	-7.61	112.55	123.28
1	A	178	LEU	C-N-CA	-7.61	112.55	123.28
1	A	30	ARG	CD-NE-CZ	7.38	134.74	124.40
1	A	257	HIS	CA-CB-CG	7.36	121.16	113.80
1	A	18	GLU	CA-C-N	7.34	132.57	122.07
1	A	18	GLU	C-N-CA	7.34	132.57	122.07
1	A	127	ILE	CA-C-O	-7.33	111.62	120.78
1	A	204	VAL	CA-C-O	-7.18	112.60	120.71
1	A	218	MET	CB-CA-C	7.05	122.17	109.83
1	A	83	PHE	CA-C-O	-7.00	111.53	119.79
1	A	281	HIS	CA-CB-CG	-6.93	106.87	113.80
1	A	9	GLU	CA-C-O	-6.91	113.10	120.42
1	A	62	ARG	CD-NE-CZ	6.82	133.95	124.40
1	A	226	ARG	NE-CZ-NH1	-6.63	114.86	121.50
1	A	214	ARG	CA-C-O	6.63	128.71	120.15
1	A	130	PRO	CA-C-N	6.58	129.39	120.38
1	A	130	PRO	C-N-CA	6.58	129.39	120.38
1	A	177	ARG	NE-CZ-NH2	-6.54	113.31	119.20
1	A	88	ARG	CG-CD-NE	6.53	126.37	112.00
1	A	92	ARG	CD-NE-CZ	6.51	133.51	124.40
1	A	126	LEU	N-CA-CB	-6.49	100.83	110.24
1	A	91	PHE	N-CA-C	-6.46	104.09	112.23
1	A	282	VAL	CA-C-O	-6.46	114.32	121.17
1	A	232	VAL	CA-C-O	-6.44	114.57	121.27
1	A	286	ARG	NE-CZ-NH1	6.43	127.94	121.50
1	A	24	ASN	CA-CB-CG	6.38	118.98	112.60
1	A	186	VAL	O-C-N	6.35	128.13	121.91
1	A	86	LEU	CA-C-N	6.26	128.96	120.44
1	A	86	LEU	C-N-CA	6.26	128.96	120.44
1	A	124	ALA	CA-C-O	-6.15	112.70	118.73
1	A	118	VAL	N-CA-C	-6.15	104.30	111.00
1	A	48	ALA	CA-C-O	-6.08	113.23	120.10
1	A	86	LEU	CA-C-O	6.03	126.80	119.38
1	A	264	VAL	N-CA-C	-6.03	105.81	113.22
1	A	94	ASP	CA-C-O	-5.95	114.48	121.44
1	A	123	GLN	OE1-CD-NE2	5.92	128.52	122.60
1	A	82	LEU	CA-C-O	5.91	126.69	120.42
1	A	88	ARG	CB-CG-CD	5.91	124.89	111.30
1	A	127	ILE	N-CA-C	5.87	121.54	109.34
1	A	163	ARG	CA-C-O	-5.86	113.23	119.97
1	A	177	ARG	NE-CZ-NH1	5.83	127.33	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	VAL	CB-CA-C	-5.78	104.33	112.14
1	A	259	ALA	CA-C-N	5.78	130.38	120.72
1	A	259	ALA	C-N-CA	5.78	130.38	120.72
1	A	140	GLU	CA-C-N	5.77	127.95	120.56
1	A	140	GLU	C-N-CA	5.77	127.95	120.56
1	A	62	ARG	CA-C-O	5.77	128.76	120.51
1	A	85	TYR	CA-C-O	-5.76	114.45	120.55
1	A	174	ASN	N-CA-C	-5.72	99.03	109.56
1	A	227	ILE	CA-C-O	-5.71	115.01	120.95
1	A	148	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	A	218	MET	CA-CB-CG	5.70	125.49	114.10
1	A	129	GLN	CA-C-N	5.63	125.09	119.24
1	A	129	GLN	C-N-CA	5.63	125.09	119.24
1	A	291	HIS	CA-CB-CG	5.62	119.42	113.80
1	A	168	ARG	O-C-N	5.59	129.86	123.27
1	A	244	HIS	CA-C-N	-5.56	110.72	120.29
1	A	244	HIS	C-N-CA	-5.56	110.72	120.29
1	A	220	ARG	CD-NE-CZ	5.49	132.08	124.40
1	A	213	GLN	CB-CG-CD	5.47	121.90	112.60
1	A	158	SER	CA-C-O	-5.46	111.95	119.05
1	A	155	LEU	O-C-N	-5.46	116.51	123.06
1	A	30	ARG	CA-C-O	5.45	126.54	120.82
1	A	146	GLY	N-CA-C	-5.45	107.80	115.32
1	A	111	LYS	CA-C-N	5.43	131.91	121.54
1	A	111	LYS	C-N-CA	5.43	131.91	121.54
1	A	220	ARG	CA-C-N	5.41	127.97	120.29
1	A	220	ARG	C-N-CA	5.41	127.97	120.29
1	A	172	LYS	CA-CB-CG	5.40	124.90	114.10
1	A	224	TRP	CB-CA-C	5.39	121.02	110.67
1	A	44	GLY	CA-C-N	5.38	131.81	121.54
1	A	44	GLY	C-N-CA	5.38	131.81	121.54
1	A	177	ARG	CD-NE-CZ	5.38	131.93	124.40
1	A	121	LEU	CA-C-N	5.37	128.02	120.28
1	A	121	LEU	C-N-CA	5.37	128.02	120.28
1	A	204	VAL	CA-C-N	-5.36	114.67	122.65
1	A	204	VAL	C-N-CA	-5.36	114.67	122.65
1	A	250	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	112	ASP	N-CA-CB	-5.28	101.57	110.49
1	A	9	GLU	O-C-N	5.28	128.16	122.15
1	A	168	ARG	CA-C-N	-5.23	116.70	123.19
1	A	168	ARG	C-N-CA	-5.23	116.70	123.19
1	A	10	GLN	CA-C-O	-5.19	115.05	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	PHE	CA-C-O	5.15	125.86	119.79
1	A	7	ARG	N-CA-CB	5.14	118.13	110.22
1	A	86	LEU	O-C-N	-5.11	115.59	122.43
1	A	218	MET	O-C-N	-5.10	117.22	122.94
1	A	142	LEU	N-CA-CB	5.09	117.52	109.94
1	A	274	SER	N-CA-CB	-5.08	102.36	110.63
1	A	17	LEU	CA-C-O	-5.05	115.17	120.63
1	A	195	HIS	CA-C-O	-5.04	113.66	119.56
1	A	61	GLU	CA-C-N	5.03	131.16	121.54
1	A	61	GLU	C-N-CA	5.03	131.16	121.54
1	A	135	ASP	CA-C-O	-5.03	115.22	120.55

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
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

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Mol	Chain	Res	Type	Group
1	A	74	ARG	Mainchain

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	2205	0	2229	112	0
2	A	105	0	0	5	0
All	All	2310	0	2229	112	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 (112) 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:82:LEU:O	1:A:86:LEU:HD23	1.92	0.70
1:A:36:MET:HE3	1:A:79:VAL:HG22	1.75	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:39:TRP:HE1	1:A:61:GLU:CD	2.20	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ALA:O	1:A:15:LEU:C	2.56	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: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: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
1:A:197:ARG:NH2	1:A:206:ILE:HD12	2.33	0.43
1:A:36:MET:HE1	1:A:79:VAL:HG13	2.00	0.43
1:A:90:LYS:NZ	1:A:111:LYS:HB2	2.34	0.42
1:A:90:LYS:HZ1	1:A:111:LYS:HB2	1.84	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:83:PHE:CD1	1:A:96:PRO:HG2	2.55	0.41
1:A:123:GLN:O	1:A:124:ALA:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:ARG:O	1:A:63:LEU:HB2	2.20	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%)	4 6

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%)	176 (74%)	61 (26%)	0 1

All (61) 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	30	ARG
1	A	31	ARG
1	A	35	MET
1	A	37	VAL
1	A	43	ARG
1	A	46	THR
1	A	52	SER
1	A	55	LEU
1	A	62	ARG
1	A	74	ARG
1	A	88	ARG
1	A	90	LYS
1	A	92	ARG
1	A	111	LYS
1	A	113	LEU
1	A	126	LEU
1	A	130	PRO
1	A	131	LEU
1	A	133	LEU
1	A	139	LEU
1	A	150	SER
1	A	153	VAL
1	A	155	LEU
1	A	160	ILE
1	A	162	LEU

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Mol	Chain	Res	Type
1	A	166	VAL
1	A	170	ILE
1	A	172	LYS
1	A	179	VAL
1	A	183	GLU
1	A	184	GLU
1	A	189	LEU
1	A	204	VAL
1	A	205	SER
1	A	206	ILE
1	A	208	VAL
1	A	213	GLN
1	A	214	ARG
1	A	218	MET
1	A	238	SER
1	A	245	VAL
1	A	252	THR
1	A	254	LEU
1	A	256	ASN
1	A	261	LEU
1	A	262	ARG
1	A	264	VAL
1	A	266	MET
1	A	267	LEU
1	A	268	LEU
1	A	273	LEU
1	A	277	GLN
1	A	280	THR
1	A	286	ARG
1	A	290	LEU
1	A	292	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	195	HIS
1	A	202	ASN

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Mol	Chain	Res	Type
1	A	213	GLN
1	A	216	GLN
1	A	256	ASN
1	A	289	GLN
1	A	291	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 [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%)	-0.37	3 (1%) 78 75	18, 43, 94, 122	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	LEU	2.8
1	A	263	VAL	2.8
1	A	267	LEU	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 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.