



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:11 PM UTC

PDB ID : 3P0L / pdb_00003p0l
Title : Human steroidogenic acute regulatory protein
Authors : Lehtio, L.; Siponen, M.; Arrowsmith, C.H.; Berglund, H.; Busam, R.D.; Collins, R.; Dahlgren, L.G.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Herman, M.D.; Johansson, A.; Johansson, I.; Kallas, A.; Karlberg, T.; Kotenyova, T.; Moche, M.; Nilsson, M.E.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Sundstrom, M.; Svensson, L.; Thorsell, A.G.; Tresaugues, L.; Van Den Berg, S.; Weigelt, J.; Welin, M.; Schuler, H.; Structural Genomics Consortium (SGC)
Deposited on : 2010-09-29
Resolution : 3.40 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)

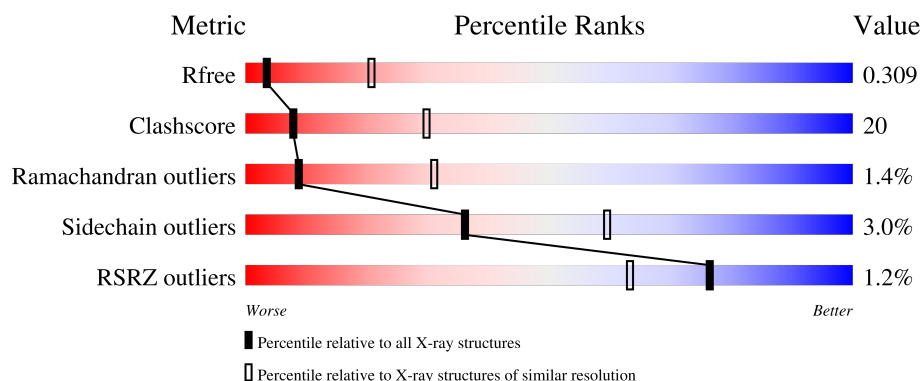
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	221	2% 57% 38% • 5%
1	B	221	% 56% 38% • 6%
1	C	221	55% 36% • 7%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	221	% 51% 32% • 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6373 atoms, of which 0 are hydrogens and 0 are deuteriums.

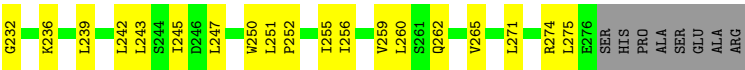
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Steroidogenic acute regulatory protein, mitochondrial.

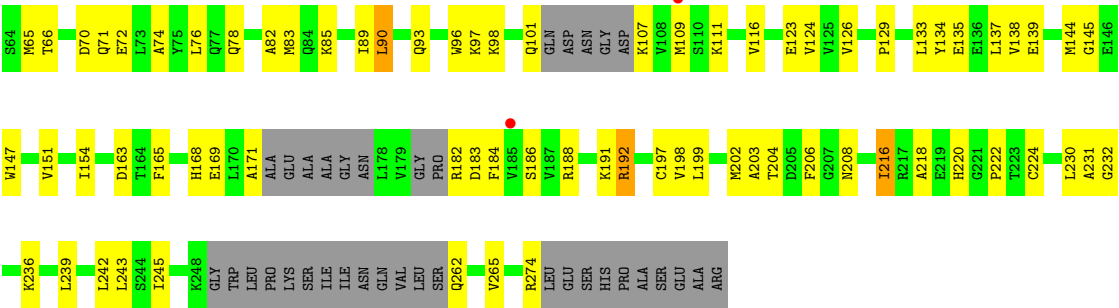
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1654	1041	290	311	12			
1	B	208	Total	C	N	O	S	0	0	0
			1637	1032	287	306	12			
1	C	205	Total	C	N	O	S	0	0	0
			1617	1020	283	302	12			
1	D	185	Total	C	N	O	S	0	0	0
			1465	924	258	271	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	SER	-	expression tag	UNP P49675
A	65	MET	-	expression tag	UNP P49675
B	64	SER	-	expression tag	UNP P49675
B	65	MET	-	expression tag	UNP P49675
C	64	SER	-	expression tag	UNP P49675
C	65	MET	-	expression tag	UNP P49675
D	64	SER	-	expression tag	UNP P49675
D	65	MET	-	expression tag	UNP P49675



● Molecule 1: Steroidogenic acute regulatory protein, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	144.13Å 144.13Å 101.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.91 – 3.40 14.91 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (14.91-3.40) 98.6 (14.91-3.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.257 , 0.287 0.272 , 0.309	Depositor DCC
R_{free} test set	1639 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	83.7	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 93.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.139 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6373	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	0.25	0/1681	0.70	0/2264
1	B	0.25	0/1664	0.69	0/2241
1	C	0.25	0/1642	0.70	0/2208
1	D	0.24	0/1485	0.67	0/1991
All	All	0.25	0/6472	0.69	0/8704

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1654	0	1677	70	0
1	B	1637	0	1665	69	0
1	C	1617	0	1643	66	0
1	D	1465	0	1495	58	0
All	All	6373	0	6480	255	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 20.

All (255) 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:251:LEU:HB3	1:A:255:ILE:HD11	1.51	0.92
1:D:182:ARG:HG2	1:D:216:ILE:HG23	1.52	0.92
1:C:182:ARG:HG2	1:C:216:ILE:HG23	1.53	0.91
1:C:251:LEU:HB3	1:C:255:ILE:HD11	1.50	0.90
1:B:182:ARG:HG2	1:B:216:ILE:HG23	1.52	0.90
1:C:188:ARG:HH21	1:C:199:LEU:HD11	1.37	0.89
1:A:182:ARG:HG2	1:A:216:ILE:HG23	1.53	0.89
1:B:188:ARG:HH21	1:B:199:LEU:HD11	1.38	0.89
1:B:251:LEU:HB3	1:B:255:ILE:HD11	1.51	0.88
1:A:188:ARG:HH21	1:A:199:LEU:HD11	1.38	0.88
1:D:188:ARG:HH21	1:D:199:LEU:HD11	1.39	0.87
1:B:203:ALA:HB2	1:B:220:HIS:H	1.45	0.81
1:C:203:ALA:HB2	1:C:220:HIS:H	1.46	0.81
1:A:203:ALA:HB2	1:A:220:HIS:H	1.45	0.80
1:D:203:ALA:HB2	1:D:220:HIS:H	1.45	0.79
1:B:96:TRP:HD1	1:B:111:LYS:HB2	1.52	0.74
1:D:96:TRP:HD1	1:D:111:LYS:HB2	1.52	0.74
1:C:96:TRP:HD1	1:C:111:LYS:HB2	1.52	0.74
1:A:96:TRP:HD1	1:A:111:LYS:HB2	1.53	0.73
1:A:251:LEU:HD12	1:A:251:LEU:H	1.57	0.70
1:B:192:ARG:HB3	1:B:197:CYS:HA	1.74	0.69
1:C:192:ARG:HB3	1:C:197:CYS:HA	1.74	0.69
1:A:192:ARG:HB3	1:A:197:CYS:HA	1.73	0.69
1:A:83:MET:HE1	1:A:191:LYS:HB2	1.75	0.68
1:B:83:MET:HE1	1:B:191:LYS:HB2	1.75	0.68
1:D:192:ARG:HB3	1:D:197:CYS:HA	1.74	0.68
1:B:70:ASP:OD2	1:D:66:THR:HG23	1.94	0.68
1:C:83:MET:HE1	1:C:191:LYS:HB2	1.75	0.67
1:A:252:PRO:HD2	1:A:255:ILE:HG12	1.77	0.67
1:D:83:MET:HE1	1:D:191:LYS:HB2	1.76	0.66
1:C:126:VAL:HG11	1:C:133:LEU:HD21	1.78	0.66
1:C:251:LEU:HD12	1:C:251:LEU:H	1.61	0.65
1:B:126:VAL:HG11	1:B:133:LEU:HD21	1.78	0.65
1:C:252:PRO:HD2	1:C:255:ILE:HG12	1.78	0.65
1:A:126:VAL:HG11	1:A:133:LEU:HD21	1.77	0.65
1:B:252:PRO:HD2	1:B:255:ILE:HG12	1.78	0.64
1:D:126:VAL:HG11	1:D:133:LEU:HD21	1.78	0.64
1:C:65:MET:HE2	1:C:67:LEU:HD11	1.80	0.63
1:B:133:LEU:O	1:B:137:LEU:HB2	2.00	0.62
1:D:133:LEU:O	1:D:137:LEU:HB2	1.99	0.62
1:A:128:GLN:HG3	1:A:275:LEU:HD13	1.80	0.62
1:B:70:ASP:OD1	1:D:65:MET:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:HB2	1:B:123:GLU:HB2	1.82	0.62
1:C:133:LEU:O	1:C:137:LEU:HB2	2.00	0.61
1:D:107:LYS:HB2	1:D:123:GLU:HB2	1.81	0.61
1:B:128:GLN:HG3	1:B:275:LEU:HD13	1.81	0.61
1:A:107:LYS:HB2	1:A:123:GLU:HB2	1.82	0.61
1:C:128:GLN:HG3	1:C:275:LEU:HD13	1.81	0.61
1:A:133:LEU:O	1:A:137:LEU:HB2	2.00	0.60
1:C:107:LYS:HB2	1:C:123:GLU:HB2	1.83	0.60
1:B:262:GLN:HA	1:B:265:VAL:HG22	1.84	0.59
1:B:82:ALA:HB2	1:B:202:MET:HG2	1.85	0.59
1:B:102:GLN:HB2	1:B:106:ASP:HB2	1.85	0.59
1:B:206:PHE:CE2	1:B:208:ASN:HB3	2.38	0.58
1:C:262:GLN:HA	1:C:265:VAL:HG22	1.84	0.58
1:B:85:LYS:O	1:B:89:ILE:HG13	2.03	0.58
1:D:206:PHE:CE2	1:D:208:ASN:HB3	2.38	0.58
1:A:85:LYS:O	1:A:89:ILE:HG13	2.03	0.58
1:C:102:GLN:HB2	1:C:106:ASP:HB2	1.85	0.58
1:D:262:GLN:HA	1:D:265:VAL:HG22	1.85	0.58
1:C:206:PHE:CE2	1:C:208:ASN:HB3	2.39	0.58
1:A:262:GLN:HA	1:A:265:VAL:HG22	1.84	0.58
1:B:145:GLY:HA2	1:B:151:VAL:HG23	1.86	0.58
1:C:82:ALA:HB2	1:C:202:MET:HG2	1.86	0.58
1:A:82:ALA:HB2	1:A:202:MET:HG2	1.85	0.58
1:C:147:TRP:CD1	1:C:274:ARG:HE	2.22	0.58
1:D:82:ALA:HB2	1:D:202:MET:HG2	1.86	0.58
1:A:206:PHE:CE2	1:A:208:ASN:HB3	2.38	0.57
1:D:145:GLY:HA2	1:D:151:VAL:HG23	1.86	0.57
1:C:98:LYS:HE2	1:C:101:GLN:HB2	1.86	0.57
1:C:85:LYS:O	1:C:89:ILE:HG13	2.05	0.57
1:C:145:GLY:HA2	1:C:151:VAL:HG23	1.85	0.57
1:D:98:LYS:HE2	1:D:101:GLN:HB2	1.86	0.57
1:A:98:LYS:HE2	1:A:101:GLN:HB2	1.87	0.57
1:B:147:TRP:CD1	1:B:274:ARG:HE	2.23	0.57
1:A:102:GLN:HB2	1:A:106:ASP:HB2	1.85	0.57
1:A:247:LEU:HD11	1:A:260:LEU:HD21	1.87	0.57
1:D:147:TRP:CD1	1:D:274:ARG:HE	2.22	0.57
1:C:271:LEU:O	1:C:275:LEU:HG	2.06	0.56
1:A:147:TRP:CD1	1:A:274:ARG:HE	2.23	0.56
1:C:65:MET:HE2	1:C:67:LEU:CD1	2.35	0.56
1:A:165:PHE:CE2	1:A:188:ARG:HG3	2.41	0.56
1:B:165:PHE:CE2	1:B:188:ARG:HG3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LYS:HE2	1:B:101:GLN:HB2	1.87	0.56
1:D:85:LYS:O	1:D:89:ILE:HG13	2.04	0.56
1:B:271:LEU:O	1:B:275:LEU:HG	2.05	0.56
1:C:165:PHE:CE2	1:C:188:ARG:HG3	2.41	0.56
1:A:145:GLY:HA2	1:A:151:VAL:HG23	1.86	0.55
1:A:271:LEU:O	1:A:275:LEU:HG	2.06	0.55
1:C:247:LEU:HD11	1:C:260:LEU:HD21	1.88	0.55
1:B:144:MET:HA	1:B:147:TRP:NE1	2.22	0.55
1:C:144:MET:HA	1:C:147:TRP:NE1	2.22	0.55
1:D:135:GLU:HA	1:D:139:GLU:HB3	1.88	0.55
1:C:135:GLU:HA	1:C:139:GLU:HB3	1.89	0.55
1:A:144:MET:HA	1:A:147:TRP:NE1	2.22	0.54
1:D:165:PHE:CE2	1:D:188:ARG:HG3	2.41	0.54
1:B:247:LEU:HD11	1:B:260:LEU:HD21	1.87	0.54
1:B:97:LYS:NZ	1:B:111:LYS:HA	2.23	0.54
1:D:134:TYR:O	1:D:138:VAL:HG22	2.08	0.54
1:B:135:GLU:HA	1:B:139:GLU:HB3	1.89	0.53
1:D:144:MET:HA	1:D:147:TRP:NE1	2.22	0.53
1:A:97:LYS:NZ	1:A:111:LYS:HA	2.23	0.53
1:A:135:GLU:HA	1:A:139:GLU:HB3	1.89	0.53
1:D:97:LYS:NZ	1:D:111:LYS:HA	2.23	0.53
1:B:96:TRP:CD1	1:B:111:LYS:HD2	2.44	0.53
1:D:230:LEU:HD13	1:D:231:ALA:N	2.24	0.53
1:A:184:PHE:CE2	1:A:218:ALA:HB3	2.44	0.53
1:C:134:TYR:O	1:C:138:VAL:HG22	2.09	0.53
1:A:96:TRP:CD1	1:A:111:LYS:HD2	2.44	0.53
1:C:97:LYS:NZ	1:C:111:LYS:HA	2.23	0.53
1:B:134:TYR:O	1:B:138:VAL:HG22	2.09	0.52
1:B:230:LEU:HD13	1:B:231:ALA:N	2.24	0.52
1:C:96:TRP:CD1	1:C:111:LYS:HD2	2.45	0.52
1:C:184:PHE:CE2	1:C:218:ALA:HB3	2.44	0.52
1:D:184:PHE:CE2	1:D:218:ALA:HB3	2.44	0.52
1:C:230:LEU:HD13	1:C:231:ALA:N	2.24	0.52
1:D:96:TRP:CD1	1:D:111:LYS:HD2	2.45	0.52
1:D:138:VAL:HG23	1:D:139:GLU:H	1.75	0.52
1:A:107:LYS:HE2	1:A:109:MET:HE2	1.92	0.52
1:A:230:LEU:HD13	1:A:231:ALA:N	2.24	0.51
1:C:107:LYS:HE2	1:C:109:MET:HE2	1.92	0.51
1:A:134:TYR:O	1:A:138:VAL:HG22	2.09	0.51
1:C:74:ALA:O	1:C:78:GLN:HG3	2.10	0.51
1:A:138:VAL:HG23	1:A:139:GLU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASP:CG	1:B:66:THR:HG23	2.36	0.51
1:C:138:VAL:HG23	1:C:139:GLU:N	2.26	0.51
1:B:184:PHE:CE2	1:B:218:ALA:HB3	2.45	0.50
1:D:138:VAL:HG23	1:D:139:GLU:N	2.26	0.50
1:A:138:VAL:HG23	1:A:139:GLU:H	1.76	0.50
1:D:107:LYS:HE2	1:D:109:MET:HE2	1.93	0.50
1:B:138:VAL:HG23	1:B:139:GLU:N	2.26	0.50
1:B:74:ALA:O	1:B:78:GLN:HG3	2.11	0.50
1:B:138:VAL:HG23	1:B:139:GLU:H	1.75	0.50
1:C:138:VAL:HG23	1:C:139:GLU:H	1.75	0.50
1:C:82:ALA:HA	1:C:202:MET:HE3	1.93	0.50
1:D:74:ALA:O	1:D:78:GLN:HG3	2.11	0.50
1:A:65:MET:HA	1:D:70:ASP:OD1	2.11	0.49
1:B:243:LEU:HD11	1:B:245:ILE:HD11	1.94	0.49
1:A:243:LEU:HD11	1:A:245:ILE:HD11	1.94	0.49
1:D:82:ALA:HA	1:D:202:MET:HE3	1.95	0.49
1:A:70:ASP:OD2	1:B:66:THR:CG2	2.60	0.49
1:C:243:LEU:HD11	1:C:245:ILE:HD11	1.94	0.49
1:B:107:LYS:HE2	1:B:109:MET:HE2	1.93	0.49
1:D:243:LEU:HD11	1:D:245:ILE:HD11	1.94	0.49
1:A:90:LEU:HD21	1:A:242:LEU:HB2	1.94	0.49
1:C:72:GLU:O	1:C:76:LEU:HD13	2.12	0.49
1:A:252:PRO:HD3	1:C:101:GLN:NE2	2.28	0.49
1:A:82:ALA:HA	1:A:202:MET:HE3	1.95	0.48
1:B:90:LEU:HD21	1:B:242:LEU:HB2	1.95	0.48
1:A:74:ALA:O	1:A:78:GLN:HG3	2.13	0.48
1:C:90:LEU:HD21	1:C:242:LEU:HB2	1.95	0.48
1:D:72:GLU:O	1:D:76:LEU:HD13	2.14	0.47
1:A:70:ASP:OD2	1:B:66:THR:HG23	2.14	0.47
1:B:72:GLU:O	1:B:76:LEU:HD13	2.13	0.47
1:B:82:ALA:HA	1:B:202:MET:HE3	1.94	0.47
1:B:251:LEU:N	1:B:251:LEU:HD12	2.30	0.47
1:A:64:SER:OG	1:A:65:MET:N	2.48	0.47
1:A:97:LYS:HZ3	1:A:111:LYS:HA	1.80	0.46
1:C:251:LEU:H	1:C:251:LEU:CD1	2.27	0.46
1:A:230:LEU:HB2	1:A:236:LYS:HB2	1.98	0.46
1:A:72:GLU:O	1:A:76:LEU:HD13	2.16	0.46
1:A:251:LEU:H	1:A:251:LEU:CD1	2.25	0.46
1:B:230:LEU:HB2	1:B:236:LYS:HB2	1.98	0.46
1:C:251:LEU:HD12	1:C:251:LEU:N	2.30	0.45
1:D:154:ILE:HD12	1:D:154:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:O	1:A:262:GLN:HG3	2.17	0.45
1:C:154:ILE:N	1:C:154:ILE:HD12	2.32	0.45
1:D:230:LEU:HB2	1:D:236:LYS:HB2	1.99	0.45
1:C:259:VAL:O	1:C:262:GLN:HG3	2.17	0.45
1:D:163:ASP:OD2	1:D:191:LYS:HG2	2.17	0.45
1:A:230:LEU:HD13	1:A:232:GLY:H	1.82	0.44
1:C:230:LEU:HB2	1:C:236:LYS:HB2	1.99	0.44
1:A:154:ILE:HD12	1:A:154:ILE:N	2.32	0.44
1:B:259:VAL:O	1:B:262:GLN:HG3	2.17	0.44
1:B:154:ILE:N	1:B:154:ILE:HD12	2.33	0.44
1:A:199:LEU:O	1:A:224:CYS:HA	2.18	0.44
1:B:129:PRO:O	1:B:133:LEU:HD13	2.18	0.44
1:A:251:LEU:HD12	1:A:251:LEU:N	2.29	0.44
1:C:230:LEU:CD1	1:C:232:GLY:H	2.31	0.44
1:D:129:PRO:O	1:D:133:LEU:HD13	2.18	0.44
1:A:230:LEU:CD1	1:A:232:GLY:H	2.31	0.43
1:A:71:GLN:O	1:A:74:ALA:HB3	2.17	0.43
1:B:163:ASP:OD2	1:B:191:LYS:HG2	2.18	0.43
1:C:230:LEU:HD13	1:C:232:GLY:H	1.82	0.43
1:D:199:LEU:O	1:D:224:CYS:HA	2.18	0.43
1:D:230:LEU:CD1	1:D:232:GLY:H	2.31	0.43
1:A:168:HIS:HE1	1:A:183:ASP:OD2	2.02	0.43
1:A:252:PRO:O	1:A:256:ILE:HG13	2.18	0.43
1:B:98:LYS:CE	1:B:101:GLN:HB2	2.49	0.43
1:C:129:PRO:O	1:C:133:LEU:HD13	2.18	0.43
1:B:199:LEU:O	1:B:224:CYS:HA	2.18	0.43
1:B:230:LEU:HD13	1:B:232:GLY:H	1.83	0.43
1:D:98:LYS:CE	1:D:101:GLN:HB2	2.47	0.43
1:A:239:LEU:HD23	1:A:239:LEU:C	2.44	0.43
1:B:239:LEU:C	1:B:239:LEU:HD23	2.44	0.43
1:C:191:LYS:HE2	1:C:191:LYS:HB3	1.83	0.43
1:C:252:PRO:O	1:C:256:ILE:HG13	2.19	0.43
1:A:129:PRO:O	1:A:133:LEU:HD13	2.19	0.43
1:D:239:LEU:C	1:D:239:LEU:HD23	2.44	0.43
1:A:163:ASP:OD2	1:A:191:LYS:HG2	2.19	0.43
1:C:71:GLN:O	1:C:74:ALA:HB3	2.19	0.43
1:C:186:SER:HA	1:C:204:THR:HG22	2.01	0.43
1:B:147:TRP:HD1	1:B:274:ARG:HH21	1.66	0.42
1:B:251:LEU:HD12	1:B:251:LEU:H	1.84	0.42
1:C:98:LYS:CE	1:C:101:GLN:HB2	2.48	0.42
1:D:230:LEU:HD13	1:D:232:GLY:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:HIS:HA	1:A:184:PHE:O	2.20	0.42
1:C:199:LEU:O	1:C:224:CYS:HA	2.19	0.42
1:D:191:LYS:C	1:D:192:ARG:HG3	2.44	0.42
1:C:147:TRP:HD1	1:C:274:ARG:HH21	1.66	0.42
1:C:163:ASP:OD2	1:C:191:LYS:HG2	2.19	0.42
1:C:262:GLN:O	1:C:265:VAL:HG22	2.19	0.42
1:B:262:GLN:O	1:B:265:VAL:HG22	2.20	0.42
1:D:262:GLN:O	1:D:265:VAL:HG22	2.19	0.42
1:A:147:TRP:HD1	1:A:274:ARG:HH21	1.66	0.42
1:A:191:LYS:C	1:A:192:ARG:HG3	2.44	0.42
1:D:186:SER:HA	1:D:204:THR:HG22	2.02	0.42
1:D:147:TRP:HD1	1:D:274:ARG:HH21	1.66	0.42
1:B:71:GLN:O	1:B:74:ALA:HB3	2.20	0.42
1:B:230:LEU:CD1	1:B:232:GLY:H	2.32	0.42
1:B:252:PRO:O	1:B:256:ILE:HG13	2.19	0.42
1:B:186:SER:HA	1:B:204:THR:HG22	2.02	0.42
1:D:90:LEU:HD13	1:D:242:LEU:HD22	2.01	0.42
1:A:262:GLN:O	1:A:265:VAL:HG22	2.19	0.41
1:D:71:GLN:O	1:D:74:ALA:HB3	2.20	0.41
1:A:259:VAL:HG13	1:A:260:LEU:N	2.35	0.41
1:C:239:LEU:C	1:C:239:LEU:HD23	2.45	0.41
1:D:168:HIS:HA	1:D:184:PHE:O	2.20	0.41
1:D:191:LYS:HB3	1:D:191:LYS:HE2	1.83	0.41
1:C:168:HIS:HA	1:C:184:PHE:O	2.20	0.41
1:C:191:LYS:C	1:C:192:ARG:HG3	2.45	0.41
1:A:65:MET:HA	1:D:70:ASP:CG	2.45	0.41
1:C:168:HIS:HE1	1:C:183:ASP:OD2	2.03	0.41
1:B:151:VAL:HA	1:B:171:ALA:HA	2.03	0.41
1:B:191:LYS:C	1:B:192:ARG:HG3	2.45	0.41
1:C:151:VAL:HA	1:C:171:ALA:HA	2.03	0.41
1:D:82:ALA:CA	1:D:202:MET:HE3	2.51	0.41
1:D:168:HIS:HE1	1:D:183:ASP:OD2	2.02	0.41
1:B:76:LEU:HD11	1:B:160:ILE:CG2	2.51	0.41
1:B:151:VAL:HB	1:B:154:ILE:HD11	2.03	0.41
1:B:259:VAL:HG13	1:B:260:LEU:N	2.36	0.41
1:D:151:VAL:HA	1:D:171:ALA:HA	2.03	0.41
1:A:82:ALA:CA	1:A:202:MET:HE3	2.51	0.41
1:B:123:GLU:HB3	1:B:238:LYS:HZ1	1.86	0.41
1:B:168:HIS:HE1	1:B:183:ASP:OD2	2.04	0.41
1:C:82:ALA:CA	1:C:202:MET:HE3	2.50	0.41
1:D:151:VAL:HB	1:D:154:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:SER:HA	1:A:204:THR:HG22	2.03	0.41
1:A:98:LYS:CE	1:A:101:GLN:HB2	2.49	0.40
1:B:168:HIS:HA	1:B:184:PHE:O	2.21	0.40
1:C:151:VAL:HB	1:C:154:ILE:HD11	2.04	0.40
1:A:138:VAL:HG12	1:A:199:LEU:HD12	2.04	0.40
1:B:82:ALA:CA	1:B:202:MET:HE3	2.51	0.40
1:D:90:LEU:HD11	1:D:242:LEU:HB2	2.03	0.40
1:D:154:ILE:HG13	1:D:169:GLU:HG3	2.04	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	206/221 (93%)	186 (90%)	17 (8%)	3 (2%)	8	30
1	B	204/221 (92%)	186 (91%)	15 (7%)	3 (2%)	8	30
1	C	197/221 (89%)	181 (92%)	14 (7%)	2 (1%)	12	40
1	D	175/221 (79%)	157 (90%)	15 (9%)	3 (2%)	7	28
All	All	782/884 (88%)	710 (91%)	61 (8%)	11 (1%)	9	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	B	93	GLN
1	D	93	GLN
1	A	116	VAL
1	B	116	VAL
1	C	116	VAL
1	D	116	VAL

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Mol	Chain	Res	Type
1	A	222	PRO
1	B	222	PRO
1	C	222	PRO
1	D	222	PRO

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	183/189 (97%)	177 (97%)	6 (3%)	33	57
1	B	181/189 (96%)	177 (98%)	4 (2%)	45	63
1	C	179/189 (95%)	173 (97%)	6 (3%)	32	57
1	D	162/189 (86%)	157 (97%)	5 (3%)	35	59
All	All	705/756 (93%)	684 (97%)	21 (3%)	36	59

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	VAL
1	A	173	GLU
1	A	177	ASN
1	A	192	ARG
1	A	198	VAL
1	A	216	ILE
1	B	124	VAL
1	B	192	ARG
1	B	198	VAL
1	B	216	ILE
1	C	67	LEU
1	C	124	VAL
1	C	192	ARG
1	C	198	VAL
1	C	216	ILE
1	C	250	TRP
1	D	90	LEU

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Mol	Chain	Res	Type
1	D	124	VAL
1	D	192	ARG
1	D	198	VAL
1	D	216	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	177	ASN
1	C	220	HIS
1	D	220	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	210/221 (95%)	-0.05	5 (2%) 59 45	15, 107, 183, 255	0
1	B	208/221 (94%)	-0.01	3 (1%) 73 59	36, 122, 197, 326	0
1	C	205/221 (92%)	-0.06	0 100 100	2, 124, 210, 264	0
1	D	185/221 (83%)	0.01	2 (1%) 78 65	12, 143, 222, 299	0
All	All	808/884 (91%)	-0.03	10 (1%) 76 63	2, 125, 205, 326	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	PRO	5.2
1	B	228	HIS	3.6
1	D	109	MET	3.2
1	B	64	SER	3.0
1	A	64	SER	2.8
1	A	144	MET	2.6
1	D	185	VAL	2.1
1	A	82	ALA	2.0
1	A	189	CYS	2.0
1	A	258	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.