



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 PM GMT

PDB ID : 4ALX  
Title : Crystal Structure of Ls-AChBP complexed with the potent nAChR antagonist DHbE  
Authors : Shahsavar, A.; Kastrop, J.S.; Nielsen, E.O.; Kristensen, J.L.; Gajhede, M.; Balle, T.  
Deposited on : 2012-03-06  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

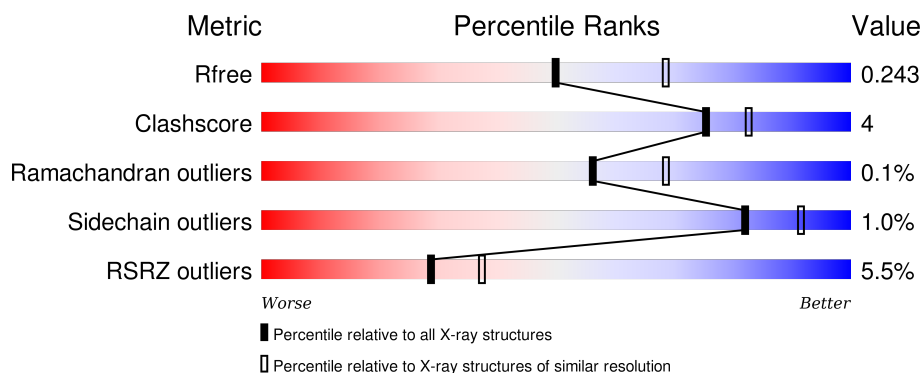
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	229	<div> <div>6%</div> <div>83% 9% 8%</div> </div>
1	B	229	<div> <div>6%</div> <div>80% 7% 12%</div> </div>
1	C	229	<div> <div>6%</div> <div>80% 7% 12%</div> </div>
1	D	229	<div> <div>5%</div> <div>80% 9% 11%</div> </div>
1	E	229	<div> <div>3%</div> <div>80% 7% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	229	
1	G	229	
1	H	229	
1	I	229	
1	J	229	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	B	1206	-	-	X	X
3	1PE	F	1206	-	-	X	-
4	MG	F	1207	-	-	-	X

## 2 Entry composition

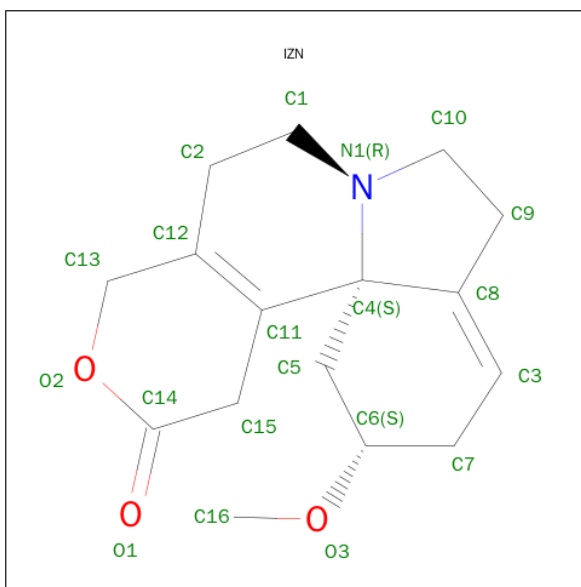
There are 5 unique types of molecules in this entry. The entry contains 17192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINE BINDING PROTEIN.

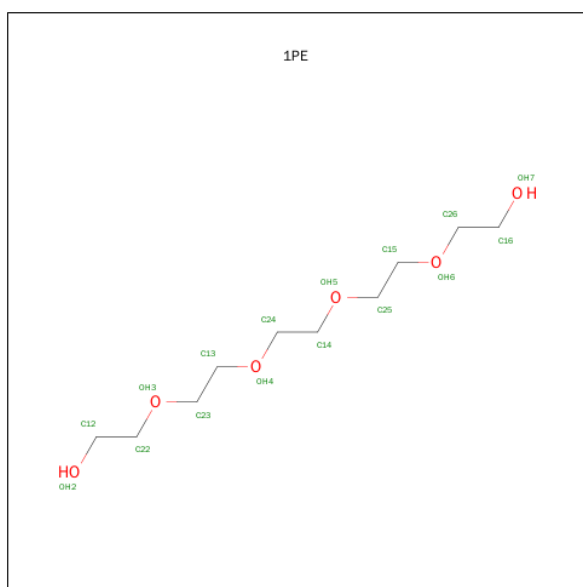
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1679	1049	288	337	5			
1	B	201	Total	C	N	O	S	0	0	0
			1606	1007	275	319	5			
1	C	201	Total	C	N	O	S	0	0	0
			1606	1007	275	319	5			
1	D	204	Total	C	N	O	S	0	1	0
			1640	1026	282	327	5			
1	E	200	Total	C	N	O	S	0	2	0
			1615	1013	280	317	5			
1	F	205	Total	C	N	O	S	0	1	0
			1641	1026	281	329	5			
1	G	201	Total	C	N	O	S	0	1	0
			1611	1010	275	321	5			
1	H	201	Total	C	N	O	S	0	1	0
			1614	1012	278	319	5			
1	I	199	Total	C	N	O	S	0	0	0
			1594	1001	273	315	5			
1	J	201	Total	C	N	O	S	0	0	0
			1606	1007	275	319	5			

- Molecule 2 is (4BS,6S)-6-METHOXY-1,4,6,7,9,10,12,13-OCTAHYDRO-3H,5H-PYRANO[4',3':3,4]PYRIDO[2,1-I]INDOL-3-ONE (three-letter code: IZN) (formula: C<sub>16</sub>H<sub>21</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	16	1	3		
2	B	1	Total	C	N	O	0	0
			20	16	1	3		
2	C	1	Total	C	N	O	0	0
			20	16	1	3		
2	D	1	Total	C	N	O	0	0
			20	16	1	3		
2	E	1	Total	C	N	O	0	0
			20	16	1	3		
2	F	1	Total	C	N	O	0	0
			20	16	1	3		
2	G	1	Total	C	N	O	0	0
			20	16	1	3		
2	H	1	Total	C	N	O	0	0
			20	16	1	3		
2	I	1	Total	C	N	O	0	0
			20	16	1	3		
2	J	1	Total	C	N	O	0	0
			20	16	1	3		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	7	4		
3	B	1	Total	C	O	0	0
			16	10	6		
3	F	1	Total	C	O	0	0
			16	10	6		
3	G	1	Total	C	O	0	0
			16	10	6		
3	H	1	Total	C	O	0	0
			14	9	5		
3	J	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	2	Total	Mg	0	0
			2	2		
4	J	1	Total	Mg	0	0
			1	1		
4	F	2	Total	Mg	0	0
			2	2		

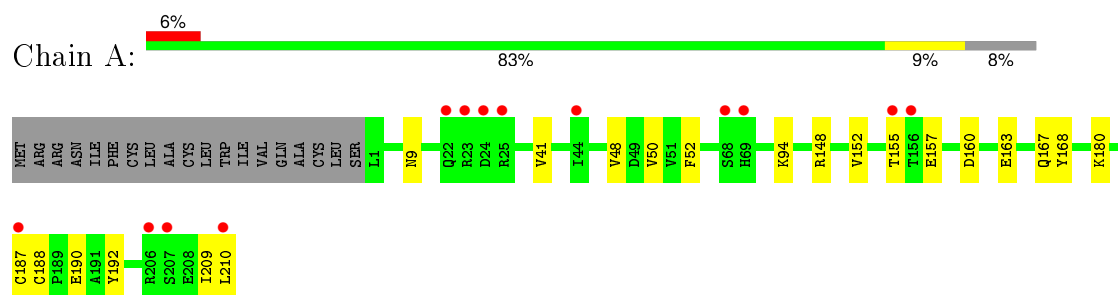
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total 90	O 90	0	0
5	B	58	Total 58	O 58	0	0
5	C	80	Total 80	O 80	0	0
5	D	88	Total 88	O 88	0	0
5	E	76	Total 76	O 76	0	0
5	F	73	Total 73	O 73	0	0
5	G	66	Total 66	O 66	0	0
5	H	65	Total 65	O 65	0	0
5	I	52	Total 52	O 52	0	0
5	J	40	Total 40	O 40	0	0

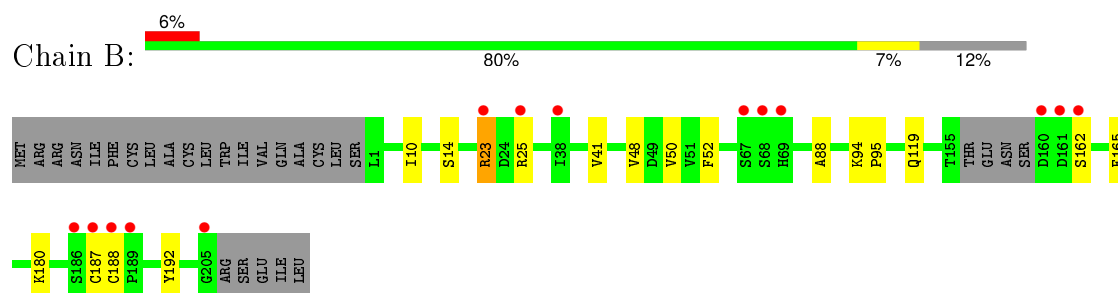
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

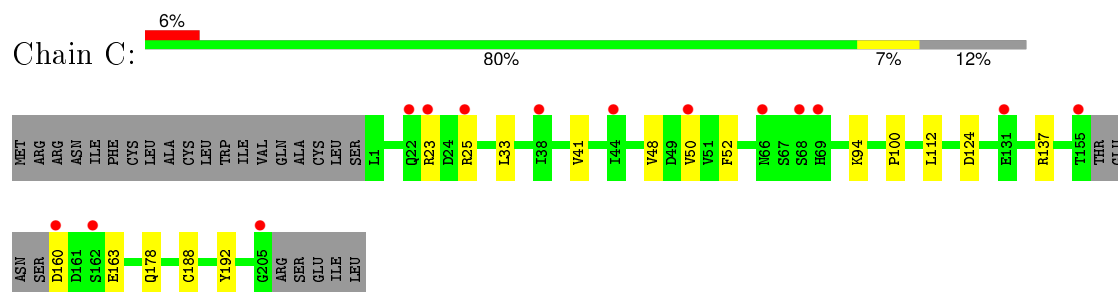
#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN



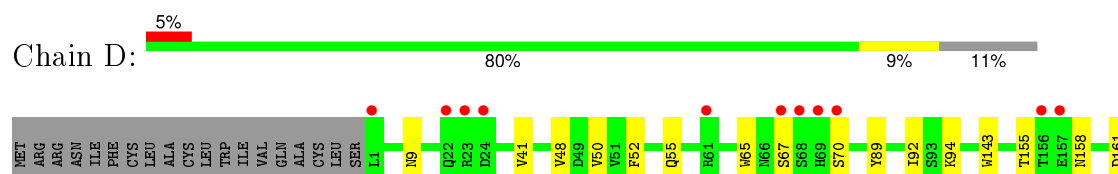
#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN



#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN



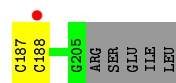
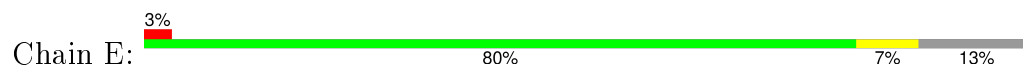
#### • Molecule 1: ACETYLCHOLINE BINDING PROTEIN



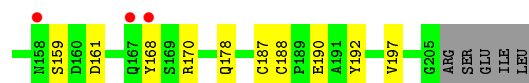
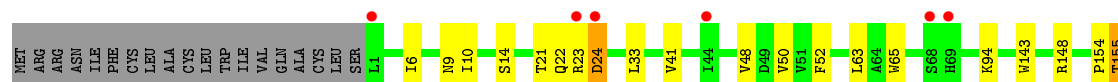
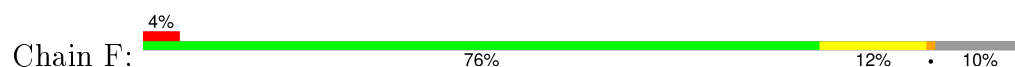




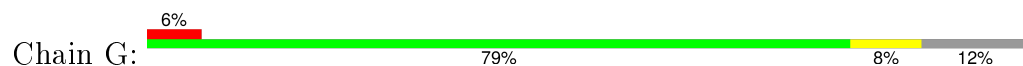
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



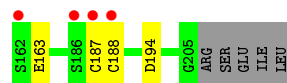
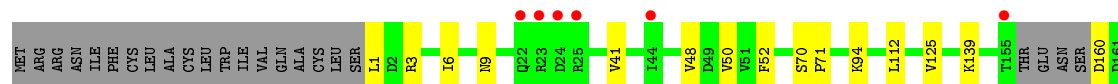
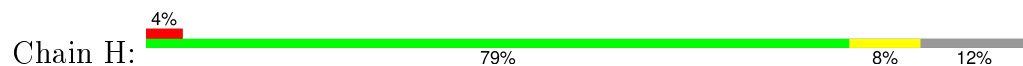
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

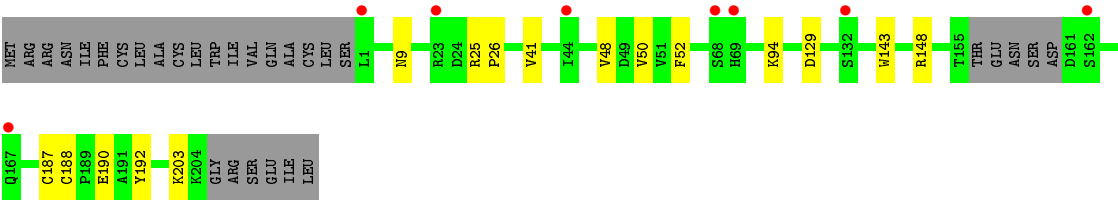


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

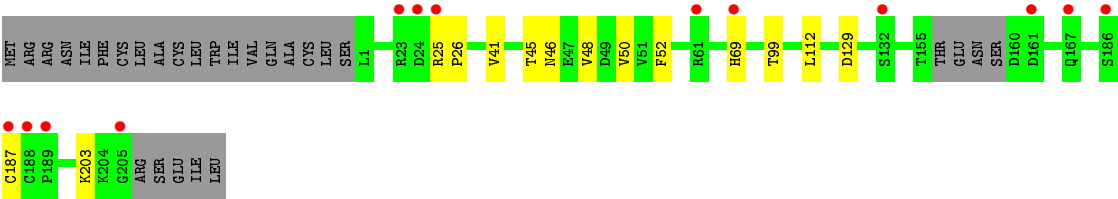
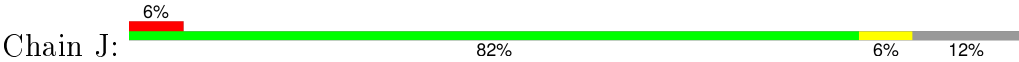


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN





● Molecule 1: ACETYLCHOLINE BINDING PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.25Å 121.31Å 152.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.16 – 2.30 20.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.16-2.30) 98.8 (20.16-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.30Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.203 , 0.250 0.200 , 0.243	Depositor DCC
$R_{free}$ test set	4864 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.0	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 97173 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IZN, 1PE

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	0.45	0/1715	0.56	0/2338
1	B	0.42	0/1641	0.54	0/2238
1	C	0.45	0/1641	0.56	0/2238
1	D	0.45	0/1679	0.56	0/2291
1	E	0.46	0/1656	0.60	1/2256 (0.0%)
1	F	0.46	0/1680	0.58	0/2293
1	G	0.43	0/1649	0.56	0/2249
1	H	0.45	0/1652	0.55	0/2252
1	I	0.44	0/1629	0.56	0/2222
1	J	0.42	0/1641	0.55	0/2238
All	All	0.44	0/16583	0.56	1/22615 (0.0%)

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	F	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	39	LEU	CB-CG-CD1	5.41	120.20	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	21	THR	Peptide

## 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	1679	0	1627	13	0
1	B	1606	0	1556	19	0
1	C	1606	0	1556	10	0
1	D	1640	0	1591	14	0
1	E	1615	0	1575	13	0
1	F	1641	0	1587	21	0
1	G	1611	0	1560	12	0
1	H	1614	0	1569	12	0
1	I	1594	0	1549	10	0
1	J	1606	0	1556	9	0
2	A	20	0	21	2	0
2	B	20	0	21	3	0
2	C	20	0	21	1	0
2	D	20	0	21	3	0
2	E	20	0	21	1	0
2	F	20	0	21	3	0
2	G	20	0	21	2	0
2	H	20	0	21	1	0
2	I	20	0	21	3	0
2	J	20	0	21	0	0
3	A	11	0	13	2	0
3	B	16	0	22	13	0
3	F	16	0	22	7	0
3	G	16	0	22	1	0
3	H	14	0	17	1	0
3	J	13	0	17	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	F	2	0	0	0	0
4	J	1	0	0	0	0
5	A	90	0	0	1	0
5	B	58	0	0	1	0
5	C	80	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	88	0	0	0	0
5	E	76	0	0	0	0
5	F	73	0	0	0	0
5	G	66	0	0	0	0
5	H	65	0	0	0	0
5	I	52	0	0	0	0
5	J	40	0	0	0	0
All	All	17192	0	16049	127	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 4.

All (127) 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:F:65:TRP:HB3	3:F:1206:1PE:H222	1.61	0.82
1:D:9:ASN:HB3	3:F:1206:1PE:H152	1.64	0.78
1:B:23:ARG:HB3	1:B:25:ARG:HH12	1.48	0.77
3:B:1206:1PE:H151	1:C:100:PRO:HD3	1.69	0.75
1:A:9:ASN:HB3	3:A:1211:1PE:H231	1.73	0.71
1:E:160:ASP:HA	1:E:178:GLN:HE21	1.57	0.70
1:B:23:ARG:HB3	1:B:25:ARG:NH1	2.07	0.69
1:C:137:ARG:NH1	5:C:2057:HOH:O	2.21	0.68
1:J:25:ARG:HG2	1:J:26:PRO:HD2	1.76	0.68
1:B:95:PRO:HG3	3:B:1206:1PE:H251	1.76	0.67
1:D:41:VAL:HG22	1:D:48:VAL:HG23	1.77	0.66
1:C:160:ASP:HB3	1:C:163:GLU:HB2	1.79	0.64
1:I:41:VAL:HG22	1:I:48:VAL:HG23	1.80	0.64
1:F:187:CYS:HB3	2:F:400:IZN:O1	1.97	0.63
1:C:41:VAL:HG22	1:C:48:VAL:HG23	1.80	0.62
1:A:41:VAL:HG22	1:A:48:VAL:HG23	1.80	0.62
1:G:41:VAL:HG22	1:G:48:VAL:HG23	1.82	0.62
1:B:187:CYS:HB3	2:B:400:IZN:O1	1.99	0.61
1:J:41:VAL:HG22	1:J:48:VAL:HG23	1.82	0.61
1:B:88:ALA:H	3:B:1206:1PE:H142	1.67	0.60
1:H:41:VAL:HG22	1:H:48:VAL:HG23	1.82	0.60
3:A:1211:1PE:H242	1:I:9:ASN:HB3	1.84	0.60
1:E:32:SER:OG	1:E:160:ASP:HB2	2.00	0.59
1:E:41:VAL:HG22	1:E:48:VAL:HG23	1.83	0.58
1:E:160:ASP:O	1:E:176:VAL:HG11	2.03	0.58
1:E:160:ASP:CG	1:E:161:ASP:H	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:ILE:HD12	1:H:71:PRO:HG2	1.86	0.58
1:B:41:VAL:HG22	1:B:48:VAL:HG23	1.84	0.58
1:E:39:LEU:HD23	1:E:118:ARG:CZ	2.34	0.58
1:F:6:ILE:HG23	3:F:1206:1PE:H221	1.85	0.57
1:D:67:SER:HA	1:D:70:SER:HB2	1.86	0.57
1:G:192:TYR:CZ	2:G:400:IZN:H91C	2.40	0.57
1:E:187:CYS:HB3	2:E:400:IZN:O1	2.06	0.56
1:J:129:ASP:OD1	1:J:203:LYS:HD2	2.05	0.56
1:F:41:VAL:HG22	1:F:48:VAL:HG23	1.88	0.55
1:H:9:ASN:HB3	3:H:1206:1PE:H252	1.89	0.55
1:A:155:THR:HG22	1:A:157:GLU:HG3	1.89	0.55
1:B:119:GLN:HE22	3:B:1206:1PE:H242	1.71	0.55
1:F:63:LEU:O	3:F:1206:1PE:H231	2.07	0.54
1:D:65:TRP:HB3	3:F:1206:1PE:H161	1.90	0.54
1:B:162:SER:HB2	1:B:165:PHE:HB3	1.89	0.54
1:D:187:CYS:HB3	2:D:400:IZN:O1	2.08	0.53
1:D:55:GLN:NE2	1:D:155:THR:HG21	2.24	0.53
1:H:187:CYS:HB3	2:H:400:IZN:O1	2.07	0.53
1:H:1:LEU:HB2	1:H:70:SER:OG	2.10	0.52
1:I:187:CYS:SG	1:I:188:CYS:N	2.83	0.51
1:I:129:ASP:OD1	1:I:203:LYS:HD3	2.11	0.51
1:D:187:CYS:SG	1:D:188:CYS:N	2.84	0.51
1:F:170:ARG:CD	1:J:45:THR:HG22	2.42	0.50
1:A:160:ASP:HB3	1:A:163:GLU:HB2	1.93	0.50
1:G:160:ASP:HB3	1:G:163:GLU:HB2	1.93	0.49
1:C:33:LEU:H	1:C:178:GLN:HE22	1.60	0.49
1:G:9:ASN:HD22	3:G:1206:1PE:H162	1.76	0.49
1:D:50:VAL:HG12	1:D:52:PHE:HD1	1.78	0.49
1:I:143:TRP:CZ2	1:J:99:THR:HG21	2.47	0.49
1:F:155:THR:HB	1:F:159:SER:HB2	1.95	0.49
1:H:160:ASP:HB3	1:H:163:GLU:HB2	1.94	0.49
1:I:25:ARG:HG3	1:I:26:PRO:HD2	1.94	0.49
1:B:192:TYR:CZ	2:B:400:IZN:H91C	2.48	0.48
1:H:50:VAL:HG12	1:H:52:PHE:HD1	1.78	0.48
1:E:160:ASP:HA	1:E:178:GLN:NE2	2.26	0.48
3:B:1206:1PE:H121	3:B:1206:1PE:H241	1.94	0.48
1:B:50:VAL:HG12	1:B:52:PHE:HD2	1.78	0.48
1:F:187:CYS:SG	1:F:188:CYS:N	2.87	0.48
1:H:6:ILE:CD1	1:H:71:PRO:HG2	2.43	0.48
1:J:50:VAL:HG12	1:J:52:PHE:HD1	1.79	0.48
1:F:33:LEU:O	1:F:161:ASP:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:TYR:CZ	2:D:400:IZN:H91C	2.49	0.48
1:G:50:VAL:HG12	1:G:52:PHE:HD1	1.79	0.48
1:G:187:CYS:SG	1:G:188:CYS:N	2.86	0.47
1:F:168:TYR:HB3	1:J:46:ASN:HB3	1.95	0.47
1:A:168:TYR:CE1	1:E:124:ASP:HB2	2.49	0.47
1:F:50:VAL:HG12	1:F:52:PHE:HD1	1.79	0.47
1:B:119:GLN:HE22	3:B:1206:1PE:H141	1.80	0.47
1:H:187:CYS:SG	1:H:188:CYS:N	2.88	0.47
1:G:25:ARG:NH1	1:G:25:ARG:HB2	2.29	0.47
2:G:400:IZN:H162	1:H:112:LEU:HG	1.98	0.46
1:B:187:CYS:SG	1:B:188:CYS:N	2.89	0.46
1:C:50:VAL:HG12	1:C:52:PHE:HD1	1.81	0.46
1:E:50:VAL:HG12	1:E:52:PHE:HD1	1.80	0.46
1:I:50:VAL:HG12	1:I:52:PHE:HD1	1.80	0.46
1:G:178:GLN:HG2	1:G:197:VAL:HG22	1.96	0.46
1:E:187:CYS:SG	1:E:188:CYS:N	2.89	0.46
1:C:124:ASP:HB2	1:D:168:TYR:CE1	2.51	0.45
1:A:50:VAL:HG12	1:A:52:PHE:HD2	1.80	0.45
1:F:9:ASN:HD22	3:F:1206:1PE:H121	1.82	0.45
1:B:88:ALA:H	3:B:1206:1PE:C14	2.28	0.45
3:B:1206:1PE:H241	3:B:1206:1PE:H251	1.70	0.45
1:F:192:TYR:CZ	2:F:400:IZN:H91C	2.52	0.45
1:F:170:ARG:HD2	1:J:45:THR:HG22	1.99	0.45
1:B:180:LYS:NZ	5:B:2051:HOH:O	2.37	0.45
1:B:119:GLN:OE1	3:B:1206:1PE:H242	2.17	0.44
1:D:161:ASP:HB3	1:D:176:VAL:HG23	1.98	0.44
1:F:143:TRP:CZ2	1:G:99:THR:HG21	2.53	0.44
1:A:187:CYS:SG	1:A:188:CYS:N	2.90	0.44
1:B:119:GLN:HE22	3:B:1206:1PE:C14	2.31	0.44
2:B:400:IZN:H162	1:C:112:LEU:HG	2.00	0.43
2:I:400:IZN:H162	1:J:112:LEU:HG	1.99	0.43
1:B:119:GLN:NE2	3:B:1206:1PE:H242	2.33	0.43
1:F:9:ASN:HD22	3:F:1206:1PE:C12	2.31	0.43
1:A:148:ARG:NH2	1:A:190:GLU:OE2	2.48	0.42
1:I:148:ARG:NH2	1:I:190:GLU:OE2	2.47	0.42
1:A:209:ILE:O	1:A:210:LEU:HB2	2.18	0.42
1:B:119:GLN:HE22	3:B:1206:1PE:C24	2.32	0.42
1:I:192:TYR:CZ	2:I:400:IZN:H91C	2.54	0.42
1:C:23:ARG:HB2	1:C:25:ARG:HH11	1.84	0.42
1:A:152:VAL:O	1:A:180:LYS:HG3	2.20	0.42
1:F:178:GLN:HG2	1:F:197:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:PRO:HA	1:F:178:GLN:OE1	2.19	0.42
3:B:1206:1PE:H121	3:B:1206:1PE:H251	2.02	0.42
2:F:400:IZN:H162	1:G:112:LEU:HG	2.01	0.41
1:A:187:CYS:HB3	2:A:400:IZN:O1	2.21	0.41
1:D:89:TYR:OH	2:D:400:IZN:H12C	2.20	0.41
1:A:167:GLN:HG2	5:A:2080:HOH:O	2.21	0.41
1:H:139:LYS:HE3	1:H:194:ASP:OD2	2.20	0.41
1:F:10:ILE:O	1:F:14:SER:HB3	2.21	0.41
1:A:192:TYR:CZ	2:A:400:IZN:H91C	2.56	0.41
1:I:192:TYR:CE1	2:I:400:IZN:H91C	2.56	0.41
1:B:10:ILE:O	1:B:14:SER:HB3	2.21	0.41
1:D:143:TRP:CZ2	1:E:99:THR:HG21	2.56	0.41
1:F:23:ARG:HA	1:F:24:ASP:HA	1.73	0.40
1:D:92:ILE:HB	1:E:39:LEU:HD21	2.03	0.40
1:F:148:ARG:NH2	1:F:190:GLU:OE2	2.47	0.40
1:C:192:TYR:CZ	2:C:400:IZN:H91C	2.56	0.40
1:G:25:ARG:HG3	1:G:26:PRO:HD2	2.04	0.40
1:H:125:VAL:O	1:H:125:VAL:HG12	2.21	0.40
1:G:171:PHE:O	1:G:204:LYS:HE3	2.20	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	208/229 (91%)	207 (100%)	1 (0%)	0	100	100
1	B	197/229 (86%)	196 (100%)	1 (0%)	0	100	100
1	C	197/229 (86%)	194 (98%)	3 (2%)	0	100	100
1	D	203/229 (89%)	202 (100%)	1 (0%)	0	100	100
1	E	198/229 (86%)	195 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	204/229 (89%)	198 (97%)	5 (2%)	1 (0%)	34	41
1	G	198/229 (86%)	196 (99%)	2 (1%)	0	100	100
1	H	198/229 (86%)	197 (100%)	1 (0%)	0	100	100
1	I	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
1	J	197/229 (86%)	196 (100%)	1 (0%)	0	100	100
All	All	1995/2290 (87%)	1975 (99%)	19 (1%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	155	THR

### 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	196/213 (92%)	195 (100%)	1 (0%)	92	97
1	B	187/213 (88%)	185 (99%)	2 (1%)	80	90
1	C	187/213 (88%)	185 (99%)	2 (1%)	80	90
1	D	192/213 (90%)	190 (99%)	2 (1%)	82	91
1	E	188/213 (88%)	186 (99%)	2 (1%)	80	90
1	F	192/213 (90%)	189 (98%)	3 (2%)	70	84
1	G	188/213 (88%)	187 (100%)	1 (0%)	92	97
1	H	188/213 (88%)	186 (99%)	2 (1%)	80	90
1	I	186/213 (87%)	185 (100%)	1 (0%)	92	97
1	J	187/213 (88%)	185 (99%)	2 (1%)	80	90
All	All	1891/2130 (89%)	1873 (99%)	18 (1%)	82	91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LYS
1	B	23	ARG
1	B	94	LYS
1	C	94	LYS
1	C	188	CYS
1	D	94	LYS
1	D	158	ASN
1	E	39	LEU
1	E	94	LYS
1	F	22	GLN
1	F	24	ASP
1	F	94	LYS
1	G	94	LYS
1	H	3	ARG
1	H	94	LYS
1	I	94	LYS
1	J	69	HIS
1	J	187	CYS

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

Mol	Chain	Res	Type
1	D	55	GLN
1	F	9	ASN
1	G	9	ASN
1	G	55	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	1PE	A	1211	-	10,10,15	1.20	0	9,9,14	0.66	0
2	IZN	A	400	-	19,23,23	1.33	3 (15%)	12,35,35	1.35	2 (16%)
3	1PE	B	1206	-	15,15,15	1.07	0	14,14,14	0.93	0
2	IZN	B	400	-	19,23,23	1.02	0	12,35,35	1.19	2 (16%)
2	IZN	C	400	-	19,23,23	1.20	3 (15%)	12,35,35	1.19	2 (16%)
2	IZN	D	400	-	19,23,23	1.11	1 (5%)	12,35,35	1.23	2 (16%)
2	IZN	E	400	-	19,23,23	1.09	1 (5%)	12,35,35	1.02	1 (8%)
3	1PE	F	1206	-	15,15,15	1.07	0	14,14,14	0.82	0
2	IZN	F	400	-	19,23,23	1.21	2 (10%)	12,35,35	1.22	1 (8%)
3	1PE	G	1206	-	15,15,15	1.06	0	14,14,14	0.89	0
2	IZN	G	400	-	19,23,23	1.13	2 (10%)	12,35,35	1.28	1 (8%)
3	1PE	H	1206	-	13,13,15	0.96	0	12,12,14	0.78	0
2	IZN	H	400	-	19,23,23	1.15	2 (10%)	12,35,35	1.38	2 (16%)
2	IZN	I	400	-	19,23,23	1.15	1 (5%)	12,35,35	1.36	2 (16%)
3	1PE	J	1206	-	12,12,15	1.12	0	11,11,14	0.78	0
2	IZN	J	400	-	19,23,23	1.05	0	12,35,35	1.64	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	1211	-	-	0/8/8/13	0/0/0/0
2	IZN	A	400	-	-	0/2/53/53	0/4/4/4
3	1PE	B	1206	-	-	0/13/13/13	0/0/0/0
2	IZN	B	400	-	-	0/2/53/53	0/4/4/4
2	IZN	C	400	-	-	0/2/53/53	0/4/4/4
2	IZN	D	400	-	-	0/2/53/53	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IZN	E	400	-	-	0/2/53/53	0/4/4/4
3	1PE	F	1206	-	-	0/13/13/13	0/0/0/0
2	IZN	F	400	-	-	0/2/53/53	0/4/4/4
3	1PE	G	1206	-	-	0/13/13/13	0/0/0/0
2	IZN	G	400	-	-	0/2/53/53	0/4/4/4
3	1PE	H	1206	-	-	0/11/11/13	0/0/0/0
2	IZN	H	400	-	-	0/2/53/53	0/4/4/4
2	IZN	I	400	-	-	0/2/53/53	0/4/4/4
3	1PE	J	1206	-	-	0/10/10/13	0/0/0/0
2	IZN	J	400	-	-	0/2/53/53	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	IZN	C5-C6	2.01	1.55	1.51
2	E	400	IZN	C5-C6	2.01	1.55	1.51
2	H	400	IZN	C5-C6	2.06	1.55	1.51
2	H	400	IZN	C10-N1	2.11	1.50	1.47
2	G	400	IZN	C5-C6	2.18	1.55	1.51
2	I	400	IZN	C10-N1	2.20	1.50	1.47
2	F	400	IZN	C5-C6	2.20	1.56	1.51
2	D	400	IZN	C4-C11	2.21	1.54	1.52
2	A	400	IZN	C7-C6	2.24	1.55	1.51
2	C	400	IZN	C4-C11	2.24	1.54	1.52
2	A	400	IZN	C4-C11	2.34	1.54	1.52
2	A	400	IZN	C10-N1	2.36	1.50	1.47
2	C	400	IZN	C10-N1	2.36	1.50	1.47
2	G	400	IZN	C4-C11	2.48	1.54	1.52
2	F	400	IZN	C4-C11	2.85	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	400	IZN	C10-C9-C8	-3.99	99.24	103.57
2	F	400	IZN	C10-C9-C8	-3.25	100.05	103.57
2	I	400	IZN	C10-C9-C8	-3.00	100.32	103.57
2	A	400	IZN	C10-C9-C8	-2.84	100.48	103.57
2	H	400	IZN	C10-C9-C8	-2.67	100.67	103.57
2	B	400	IZN	C10-C9-C8	-2.66	100.68	103.57
2	C	400	IZN	C10-C9-C8	-2.16	101.23	103.57
2	D	400	IZN	C10-C9-C8	-2.02	101.38	103.57
2	E	400	IZN	O2-C14-O1	2.13	121.47	118.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	IZN	O2-C14-O1	2.56	122.06	118.56
2	J	400	IZN	O2-C14-O1	2.78	122.36	118.56
2	C	400	IZN	O2-C14-O1	2.80	122.38	118.56
2	H	400	IZN	O2-C14-O1	2.84	122.44	118.56
2	A	400	IZN	O2-C14-O1	3.03	122.70	118.56
2	I	400	IZN	O2-C14-O1	3.17	122.89	118.56
2	D	400	IZN	O2-C14-O1	3.21	122.95	118.56
2	G	400	IZN	O2-C14-O1	3.65	123.56	118.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1211	1PE	2	0
2	A	400	IZN	2	0
3	B	1206	1PE	13	0
2	B	400	IZN	3	0
2	C	400	IZN	1	0
2	D	400	IZN	3	0
2	E	400	IZN	1	0
3	F	1206	1PE	7	0
2	F	400	IZN	3	0
3	G	1206	1PE	1	0
2	G	400	IZN	2	0
3	H	1206	1PE	1	0
2	H	400	IZN	1	0
2	I	400	IZN	3	0

## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	210/229 (91%)	0.16	13 (6%)	24	32	20, 33, 61, 90	4 (1%)
1	B	201/229 (87%)	0.12	14 (6%)	19	27	21, 35, 62, 80	4 (1%)
1	C	201/229 (87%)	0.13	14 (6%)	19	27	20, 33, 63, 92	0
1	D	204/229 (89%)	0.14	12 (5%)	26	34	20, 33, 59, 89	4 (1%)
1	E	200/229 (87%)	-0.00	6 (3%)	54	63	19, 32, 56, 83	0
1	F	205/229 (89%)	0.07	9 (4%)	38	47	22, 36, 61, 89	2 (0%)
1	G	201/229 (87%)	0.21	13 (6%)	22	30	22, 35, 64, 90	3 (1%)
1	H	201/229 (87%)	0.03	10 (4%)	32	41	21, 33, 59, 86	1 (0%)
1	I	199/229 (86%)	0.08	8 (4%)	42	51	22, 35, 61, 85	2 (1%)
1	J	201/229 (87%)	0.09	13 (6%)	22	30	21, 36, 62, 93	4 (1%)
All	All	2023/2290 (88%)	0.10	112 (5%)	29	37	19, 34, 62, 93	24 (1%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	69	HIS	6.8
1	C	23	ARG	5.9
1	J	23	ARG	5.7
1	A	156	THR	5.5
1	I	69	HIS	5.4
1	A	23	ARG	5.3
1	B	23	ARG	5.3
1	H	23	ARG	5.3
1	C	69	HIS	5.0
1	J	69	HIS	5.0
1	G	23	ARG	5.0
1	E	69	HIS	5.0
1	D	23	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	J	205	GLY	4.8
1	B	205	GLY	4.7
1	B	186	SER	4.7
1	B	160	ASP	4.3
1	C	22	GLN	4.3
1	F	44	ILE	4.3
1	H	24	ASP	4.2
1	D	67	SER	4.1
1	D	69	HIS	3.9
1	G	69	HIS	3.9
1	C	205	GLY	3.8
1	B	69	HIS	3.8
1	G	205	GLY	3.8
1	F	23	ARG	3.8
1	H	188	CYS	3.7
1	H	155	THR	3.7
1	D	70	SER	3.6
1	D	157	GLU	3.6
1	A	69	HIS	3.5
1	D	22	GLN	3.4
1	B	188	CYS	3.4
1	F	68	SER	3.4
1	A	25	ARG	3.3
1	E	68	SER	3.3
1	E	160	ASP	3.3
1	H	187	CYS	3.3
1	J	61	ARG	3.3
1	A	24	ASP	3.2
1	E	61	ARG	3.1
1	B	25	ARG	3.1
1	F	24	ASP	3.1
1	I	68	SER	3.1
1	C	155	THR	3.1
1	J	187	CYS	3.1
1	A	206	ARG	3.0
1	C	25	ARG	3.0
1	G	188	CYS	3.0
1	B	68	SER	3.0
1	F	168	TYR	2.9
1	D	24	ASP	2.9
1	D	68	SER	2.9
1	G	24	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	207	SER	2.9
1	F	167	GLN	2.8
1	C	44	ILE	2.8
1	D	61	ARG	2.8
1	G	25	ARG	2.8
1	G	1	LEU	2.8
1	J	189	PRO	2.7
1	H	22	GLN	2.7
1	G	68	SER	2.7
1	E	186	SER	2.7
1	C	38	ILE	2.6
1	B	187	CYS	2.6
1	G	44	ILE	2.6
1	E	188	CYS	2.6
1	G	161	ASP	2.6
1	J	188	CYS	2.6
1	B	161	ASP	2.6
1	A	210	LEU	2.6
1	I	44	ILE	2.6
1	G	155	THR	2.5
1	G	22	GLN	2.5
1	I	132	SER	2.5
1	A	68	SER	2.5
1	C	68	SER	2.5
1	C	160	ASP	2.5
1	J	25	ARG	2.4
1	B	38	ILE	2.4
1	J	24	ASP	2.4
1	J	167	GLN	2.4
1	D	187	CYS	2.4
1	I	23	ARG	2.4
1	C	50	VAL	2.3
1	G	160	ASP	2.3
1	F	1	LEU	2.3
1	H	44	ILE	2.3
1	A	22	GLN	2.3
1	D	1	LEU	2.3
1	J	161	ASP	2.3
1	C	162	SER	2.3
1	D	156	THR	2.3
1	B	67	SER	2.2
1	H	25	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	155	THR	2.2
1	A	44	ILE	2.2
1	C	131	GLU	2.2
1	A	187	CYS	2.2
1	C	66	ASN	2.1
1	H	186	SER	2.1
1	J	132	SER	2.1
1	I	167	GLN	2.1
1	B	162	SER	2.1
1	B	189	PRO	2.1
1	J	186	SER	2.1
1	I	1	LEU	2.1
1	I	162	SER	2.0
1	F	158	ASN	2.0
1	H	162	SER	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	F	1207	1/1	0.79	0.26	5.59	60,60,60,60	0
3	1PE	B	1206	16/16	0.86	0.22	2.77	22,51,69,70	0
3	1PE	A	1211	11/16	0.87	0.17	1.31	28,47,62,67	0
2	IZN	I	400	20/20	0.94	0.16	1.20	20,31,60,67	0
3	1PE	F	1206	16/16	0.86	0.17	0.94	37,50,74,79	0
3	1PE	H	1206	14/16	0.92	0.15	0.72	28,46,57,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1PE	J	1206	13/16	0.90	0.14	0.55	35,43,60,61	0
2	IZN	A	400	20/20	0.93	0.14	0.33	22,28,50,55	0
2	IZN	E	400	20/20	0.93	0.15	0.25	20,26,43,44	0
2	IZN	F	400	20/20	0.95	0.14	0.04	21,32,45,58	0
2	IZN	D	400	20/20	0.94	0.14	-0.03	18,25,36,55	0
2	IZN	G	400	20/20	0.93	0.13	-0.10	23,30,44,51	0
3	1PE	G	1206	16/16	0.91	0.13	-0.15	37,43,57,66	0
2	IZN	J	400	20/20	0.94	0.12	-0.16	23,31,41,42	0
2	IZN	B	400	20/20	0.93	0.15	-0.19	19,26,48,54	0
2	IZN	H	400	20/20	0.94	0.13	-0.24	20,29,41,42	0
2	IZN	C	400	20/20	0.95	0.12	-0.33	15,24,29,42	0
4	MG	B	1207	1/1	0.80	0.09	-	51,51,51,51	0
4	MG	J	1207	1/1	0.90	0.11	-	56,56,56,56	0
4	MG	F	1208	1/1	0.91	0.14	-	57,57,57,57	0
4	MG	D	1205	1/1	0.60	0.24	-	62,62,62,62	0
4	MG	D	1206	1/1	0.87	0.27	-	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.