



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:15 AM UTC

PDB ID : 1JOD / pdb_00001jod
Title : Crystal Structure of Murine Olfactory Marker Protein in Spacegroup P43212
Authors : Smith, P.; Hunt, J.F.
Deposited on : 2001-07-27
Resolution : 3.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

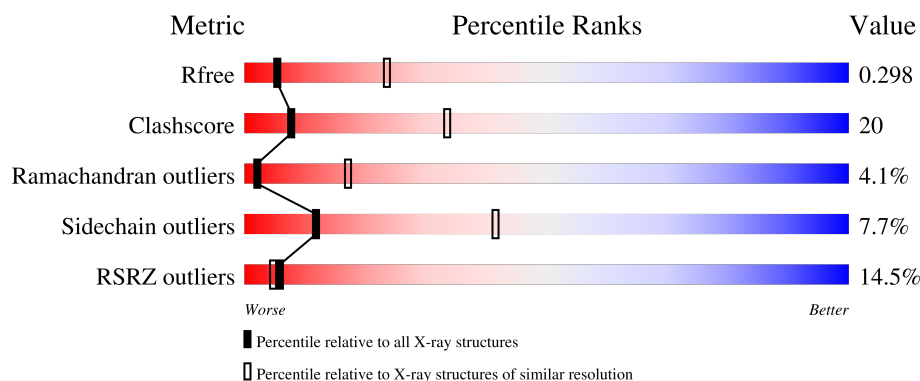
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	162	15% 49% 40% 9% ..
1	B	162	12% 58% 31% 10% .

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	CAC	A	351	-	X	-	-
3	CAC	A	352	-	X	-	-
3	CAC	A	354	-	X	-	-
3	CAC	B	353	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2683 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 Olfactory Marker Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	Se	0	0	0
			1305	826	226	248	5			
1	B	160	Total	C	N	O	Se	0	0	0
			1305	826	226	248	5			

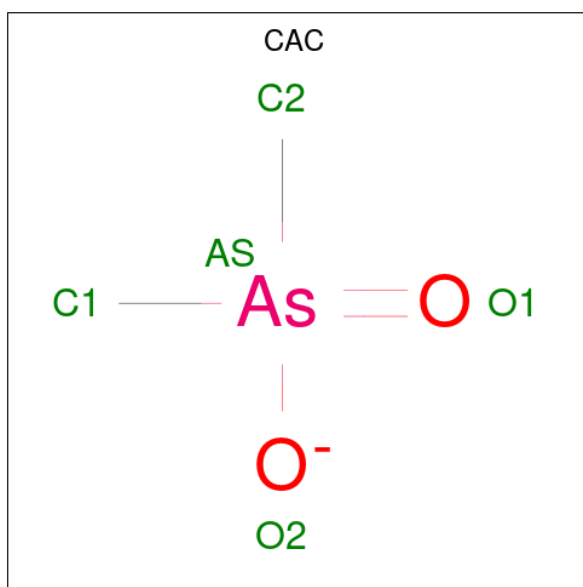
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	MSE	MET	modified residue	UNP Q64288
A	125	MSE	MET	modified residue	UNP Q64288
A	195	MSE	MET	modified residue	UNP Q64288
A	215	MSE	MET	modified residue	UNP Q64288
A	239	MSE	MET	modified residue	UNP Q64288
B	1113	MSE	MET	modified residue	UNP Q64288
B	1125	MSE	MET	modified residue	UNP Q64288
B	1195	MSE	MET	modified residue	UNP Q64288
B	1215	MSE	MET	modified residue	UNP Q64288
B	1239	MSE	MET	modified residue	UNP Q64288

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	Zn	0	0
			14	14		
2	B	8	Total	Zn	0	0
			8	8		

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		

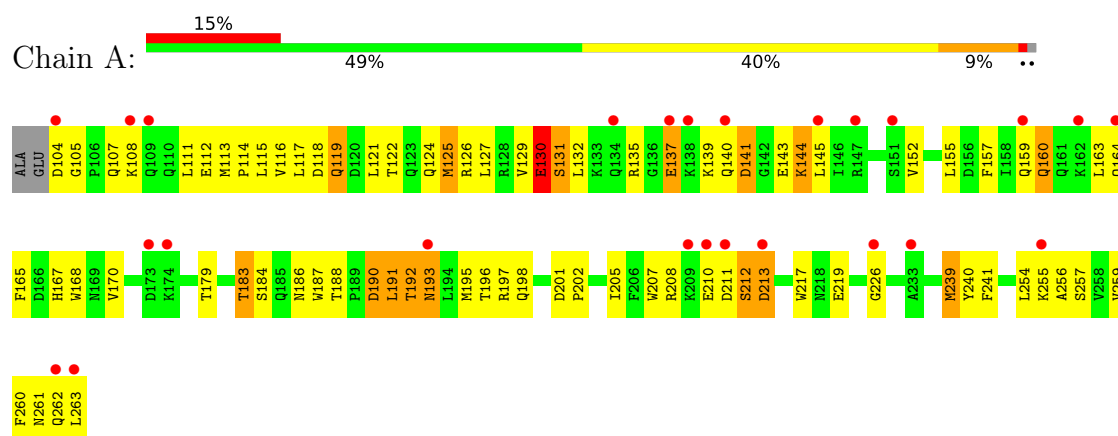
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	14	Total	O	0	0
			14	14		

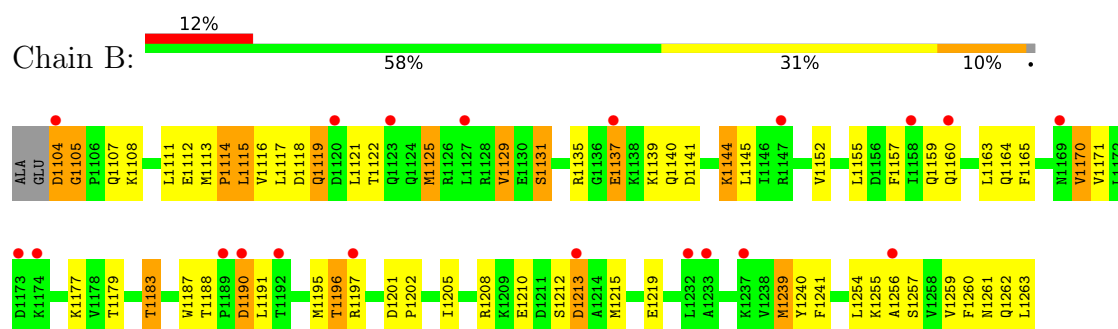
3 Residue-property plots [i](#)

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: Olfactory Marker Protein



• Molecule 1: Olfactory Marker Protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.13Å 89.13Å 158.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	80.5 (40.00-3.20) 94.5 (40.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.06Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.256 , 0.326 (Not available) , 0.298	Depositor DCC
R_{free} test set	1321 reflections (10.31%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	2683	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, ZN

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	0.71	0/1324	1.15	9/1778 (0.5%)
1	B	0.71	1/1324 (0.1%)	1.16	12/1778 (0.7%)
All	All	0.71	1/2648 (0.0%)	1.16	21/3556 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1170	VAL	CA-CB	6.02	1.61	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1255	LYS	N-CA-C	-8.69	95.23	109.40
1	A	255	LYS	N-CA-C	-8.00	96.36	109.40
1	B	1254	LEU	N-CA-C	7.49	121.65	109.59
1	A	254	LEU	N-CA-C	7.21	121.15	109.40
1	A	130	GLU	N-CA-C	-7.08	95.71	110.80
1	B	1213	ASP	N-CA-C	-6.30	104.84	114.16
1	B	1119	GLN	N-CA-C	6.15	118.77	111.33
1	A	114	PRO	N-CA-C	6.11	120.02	110.80
1	B	1114	PRO	N-CA-C	6.08	119.98	110.80
1	A	119	GLN	N-CA-C	5.91	118.48	111.33
1	B	1115	LEU	N-CA-C	-5.81	99.06	108.41
1	B	1131	SER	N-CA-C	-5.80	105.04	111.36
1	A	122	THR	N-CA-C	-5.72	104.24	111.11
1	B	1212	SER	CA-C-O	5.69	121.24	117.94
1	A	190	ASP	N-CA-C	-5.68	105.07	112.23
1	B	1105	GLY	CA-C-N	5.56	126.30	120.12
1	B	1105	GLY	C-N-CA	5.56	126.30	120.12
1	B	1122	THR	N-CA-C	-5.35	104.69	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASN	N-CA-C	-5.30	100.53	109.07
1	A	191	LEU	N-CA-C	5.23	119.30	112.13
1	B	1191	LEU	N-CA-C	5.17	119.05	111.04

There are no chirality outliers.

There are no planarity outliers.

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	1305	0	1303	61	0
1	B	1305	0	1303	45	0
2	A	14	0	0	0	0
2	B	8	0	0	0	0
3	A	15	0	0	1	0
3	B	5	0	0	1	0
4	A	17	0	0	0	0
4	B	14	0	0	0	0
All	All	2683	0	2606	104	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 (104) 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:B:1115:LEU:HG	1:B:1256:ALA:O	1.75	0.86
1:A:113:MSE:HE1	1:A:157:PHE:HD2	1.39	0.86
1:A:115:LEU:HG	1:A:256:ALA:O	1.75	0.86
1:A:129:VAL:HG12	1:A:145:LEU:HD22	1.58	0.86
1:B:1139:LYS:HD3	1:B:1145:LEU:HD12	1.58	0.85
1:A:195:MSE:HB2	1:A:198:GLN:HG3	1.57	0.84
1:A:113:MSE:HE1	1:A:157:PHE:CD2	2.21	0.75
1:A:130:GLU:O	1:A:132:LEU:N	2.20	0.74
1:B:1113:MSE:HE1	1:B:1157:PHE:HD2	1.51	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:LEU:HG	1:B:1119:GLN:HG3	1.71	0.72
1:B:1125:MSE:HE3	1:B:1152:VAL:HG21	1.69	0.72
1:A:117:LEU:HG	1:A:119:GLN:HG3	1.70	0.71
1:B:1208:ARG:HH21	1:B:1213:ASP:HA	1.54	0.71
1:A:208:ARG:HH21	1:A:213:ASP:HA	1.56	0.71
1:B:1111:LEU:HD11	1:B:1262:GLN:HE21	1.55	0.70
1:B:1113:MSE:HE1	1:B:1157:PHE:CD2	2.27	0.69
1:A:183:THR:HB	1:A:240:TYR:O	1.93	0.68
1:A:125:MSE:HE3	1:A:152:VAL:HG21	1.76	0.67
1:A:113:MSE:HE2	1:A:260:PHE:CE1	2.31	0.65
1:A:144:LYS:HD3	1:A:144:LYS:C	2.20	0.65
1:B:1144:LYS:C	1:B:1144:LYS:HD3	2.22	0.65
1:B:1125:MSE:HE3	1:B:1152:VAL:CG2	2.26	0.64
1:A:167:HIS:CE1	1:A:259:VAL:HG21	2.33	0.64
1:B:1239:MSE:HG2	1:B:1241:PHE:CZ	2.32	0.64
1:A:239:MSE:HG2	1:A:241:PHE:CZ	2.34	0.63
1:B:1141:ASP:O	1:B:1195:MSE:HE1	1.98	0.63
1:B:1183:THR:HB	1:B:1240:TYR:O	1.98	0.63
1:B:1139:LYS:HD3	1:B:1145:LEU:CD1	2.26	0.63
1:B:1196:THR:HG22	1:B:1196:THR:O	1.98	0.63
1:A:111:LEU:HD11	1:A:262:GLN:HE21	1.64	0.63
1:A:112:GLU:HG2	1:A:257:SER:HB2	1.81	0.62
1:B:1112:GLU:HG2	1:B:1257:SER:HB2	1.80	0.62
1:A:164:GLN:HB3	1:A:261:ASN:HB2	1.82	0.62
1:A:188:THR:HB	1:A:191:LEU:HG	1.82	0.62
1:B:1164:GLN:HB3	1:B:1261:ASN:HB2	1.81	0.60
1:B:1104:ASP:N	3:B:353:CAC:C1	2.66	0.59
1:A:239:MSE:HG2	1:A:241:PHE:CE1	2.40	0.56
1:A:127:LEU:O	1:A:130:GLU:HB2	2.06	0.56
1:B:1179:THR:HG23	1:B:1205:ILE:HG12	1.87	0.55
1:A:125:MSE:HE3	1:A:152:VAL:CG2	2.36	0.55
1:A:179:THR:HG23	1:A:205:ILE:HG12	1.89	0.55
1:A:167:HIS:NE2	1:A:259:VAL:HG21	2.23	0.54
1:A:155:LEU:HB3	1:A:239:MSE:HB3	1.88	0.54
1:B:1113:MSE:HE2	1:B:1260:PHE:CE1	2.42	0.54
1:A:157:PHE:CZ	1:A:239:MSE:HB2	2.42	0.53
1:B:1239:MSE:HG2	1:B:1241:PHE:CE1	2.42	0.53
1:A:139:LYS:HE3	1:A:141:ASP:O	2.08	0.53
1:A:130:GLU:O	1:A:131:SER:C	2.52	0.53
1:A:140:GLN:HB3	1:A:143:GLU:HB2	1.91	0.52
1:A:157:PHE:CE1	1:A:239:MSE:HB2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1131:SER:O	1:B:1135:ARG:HG2	2.09	0.52
1:A:186:ASN:HB3	1:B:1210:GLU:OE2	2.10	0.51
1:B:1155:LEU:HB3	1:B:1239:MSE:HB3	1.91	0.51
1:B:1118:ASP:OD1	1:B:1121:LEU:HB3	2.09	0.51
1:B:1195:MSE:C	1:B:1197:ARG:H	2.19	0.50
1:A:112:GLU:HG3	1:A:259:VAL:HG22	1.93	0.50
1:B:1129:VAL:HG12	1:B:1145:LEU:HD22	1.94	0.49
1:B:1157:PHE:CE1	1:B:1239:MSE:HB2	2.46	0.49
1:B:1208:ARG:NH2	1:B:1213:ASP:HA	2.24	0.49
1:A:118:ASP:OD1	1:A:121:LEU:HB3	2.13	0.49
1:B:1135:ARG:HB3	1:B:1137:GLU:OE2	2.13	0.48
1:B:1157:PHE:CZ	1:B:1239:MSE:HB2	2.48	0.48
1:A:208:ARG:NH2	1:A:213:ASP:HA	2.26	0.48
1:A:187:TRP:CD1	1:A:192:THR:HB	2.48	0.48
1:A:135:ARG:HB3	1:A:137:GLU:OE2	2.14	0.48
1:A:124:GLN:NE2	3:A:351:CAC:C2	2.77	0.48
1:B:1171:VAL:HA	1:B:1215:MSE:HE2	1.96	0.48
1:A:129:VAL:HG12	1:A:145:LEU:CD2	2.35	0.47
1:A:195:MSE:HB3	1:A:197:ARG:HG2	1.97	0.47
1:A:187:TRP:HD1	1:A:192:THR:HB	1.80	0.47
1:A:105:GLY:C	1:A:107:GLN:H	2.21	0.46
1:A:125:MSE:HE2	1:A:187:TRP:HH2	1.80	0.46
1:A:164:GLN:OE1	1:A:263:LEU:HD21	2.16	0.46
1:A:126:ARG:O	1:A:129:VAL:HG22	2.16	0.46
1:B:1112:GLU:HG3	1:B:1259:VAL:HG22	1.99	0.45
1:B:1164:GLN:OE1	1:B:1263:LEU:HD21	2.17	0.45
1:A:164:GLN:O	1:A:165:PHE:HB3	2.15	0.45
1:B:1105:GLY:C	1:B:1107:GLN:H	2.23	0.45
1:A:164:GLN:HB2	1:A:263:LEU:HD21	1.99	0.45
1:A:167:HIS:HD2	1:A:168:TRP:O	2.00	0.44
1:A:129:VAL:C	1:A:130:GLU:O	2.59	0.44
1:A:207:TRP:CZ3	1:A:217:TRP:HA	2.53	0.44
1:A:121:LEU:O	1:A:125:MSE:HG3	2.16	0.44
1:A:159:GLN:HE22	1:A:262:GLN:NE2	2.15	0.44
1:B:1183:THR:HG21	1:B:1187:TRP:HE3	1.83	0.44
1:A:183:THR:HG21	1:A:187:TRP:HE3	1.84	0.43
1:B:1188:THR:HG22	1:B:1190:ASP:OD2	2.19	0.43
1:A:201:ASP:HA	1:A:202:PRO:HA	1.72	0.43
1:A:165:PHE:CZ	1:A:226:GLY:HA3	2.54	0.43
1:A:159:GLN:O	1:A:163:LEU:HG	2.20	0.42
1:B:1139:LYS:O	1:B:1140:GLN:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1159:GLN:O	1:B:1163:LEU:HG	2.19	0.42
1:B:1201:ASP:HA	1:B:1202:PRO:HA	1.71	0.42
1:A:190:ASP:HB3	1:B:1177:LYS:HD3	2.02	0.42
1:B:1159:GLN:HE22	1:B:1262:GLN:NE2	2.18	0.42
1:B:1114:PRO:HA	1:B:1257:SER:HA	2.03	0.41
1:B:1210:GLU:O	1:B:1210:GLU:HG2	2.20	0.41
1:A:115:LEU:HD22	1:A:155:LEU:HB2	2.02	0.41
1:A:167:HIS:CE1	1:A:259:VAL:HG11	2.55	0.41
1:A:211:ASP:O	1:A:212:SER:HB2	2.20	0.40
1:A:159:GLN:O	1:A:160:GLN:C	2.63	0.40
1:A:167:HIS:CE1	1:A:259:VAL:CG2	3.04	0.40
1:B:1196:THR:O	1:B:1196:THR:CG2	2.68	0.40
1:A:184:SER:C	1:A:186:ASN:H	2.29	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	158/162 (98%)	135 (85%)	15 (10%)	8 (5%)	1	13
1	B	158/162 (98%)	135 (85%)	18 (11%)	5 (3%)	3	21
All	All	316/324 (98%)	270 (85%)	33 (10%)	13 (4%)	2	17

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	SER
1	A	210	GLU
1	A	212	SER
1	A	130	GLU
1	A	141	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	219	GLU
1	A	108	LYS
1	A	160	GLN
1	B	1108	LYS
1	B	1196	THR
1	B	1219	GLU
1	B	1160	GLN
1	B	1165	PHE

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	143/139 (103%)	131 (92%)	12 (8%)	10	38
1	B	143/139 (103%)	133 (93%)	10 (7%)	14	45
All	All	286/278 (103%)	264 (92%)	22 (8%)	12	41

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ASP
1	A	116	VAL
1	A	125	MSE
1	A	137	GLU
1	A	144	LYS
1	A	170	VAL
1	A	183	THR
1	A	192	THR
1	A	193	ASN
1	A	196	THR
1	A	213	ASP
1	A	239	MSE
1	B	1104	ASP
1	B	1116	VAL
1	B	1125	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1129	VAL
1	B	1137	GLU
1	B	1144	LYS
1	B	1170	VAL
1	B	1183	THR
1	B	1190	ASP
1	B	1239	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	164	GLN
1	A	186	ASN
1	A	262	GLN
1	B	1164	GLN
1	B	1186	ASN
1	B	1262	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 22 are monoatomic - leaving 4 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	CAC	A	352	2	2,4,4	3.15	2 (100%)	4,6,6	4.88	4 (100%)
3	CAC	A	354	2	2,4,4	4.06	2 (100%)	4,6,6	4.13	4 (100%)
3	CAC	A	351	2	2,4,4	3.52	2 (100%)	4,6,6	4.04	4 (100%)
3	CAC	B	353	2	2,4,4	3.09	2 (100%)	4,6,6	4.60	4 (100%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	354	CAC	AS-C1	4.73	2.01	1.90
3	A	351	CAC	AS-C1	4.26	2.00	1.90
3	A	352	CAC	AS-C1	3.53	1.98	1.90
3	B	353	CAC	AS-C1	3.50	1.98	1.90
3	A	354	CAC	AS-C2	3.27	1.98	1.90
3	A	352	CAC	AS-C2	2.72	1.96	1.90
3	B	353	CAC	AS-C2	2.61	1.96	1.90
3	A	351	CAC	AS-C2	2.56	1.96	1.90

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	352	CAC	O1-AS-C1	-8.49	100.94	111.50
3	B	353	CAC	O1-AS-C1	-7.79	101.81	111.50
3	A	354	CAC	O1-AS-C1	-6.61	103.28	111.50
3	A	351	CAC	O1-AS-C1	-6.38	103.57	111.50
3	A	352	CAC	O2-AS-C1	3.37	114.00	105.84
3	A	351	CAC	O2-AS-C1	3.29	113.81	105.84
3	B	353	CAC	O2-AS-C1	3.17	113.53	105.84
3	A	354	CAC	O2-AS-C2	2.97	113.02	105.84
3	A	354	CAC	O1-AS-C2	-2.95	107.83	111.50
3	A	351	CAC	O2-AS-C2	2.83	112.69	105.84
3	B	353	CAC	O1-AS-C2	-2.82	108.00	111.50
3	A	352	CAC	O1-AS-C2	-2.76	108.07	111.50
3	A	354	CAC	O2-AS-C1	2.67	112.30	105.84
3	A	351	CAC	O1-AS-C2	-2.42	108.48	111.50
3	B	353	CAC	O2-AS-C2	2.39	111.62	105.84
3	A	352	CAC	O2-AS-C2	2.01	110.71	105.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	CAC	1	0
3	B	353	CAC	1	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, 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	155/162 (95%)	1.16	25 (16%) 4 3	7, 26, 47, 65	0
1	B	155/162 (95%)	1.06	20 (12%) 7 6	7, 27, 49, 66	0
All	All	310/324 (95%)	1.11	45 (14%) 6 5	7, 26, 48, 66	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	GLN	4.4
1	A	104	ASP	4.2
1	B	1190	ASP	3.8
1	B	1127	LEU	3.5
1	A	174	LYS	3.5
1	A	173	ASP	3.2
1	A	137	GLU	3.0
1	A	213	ASP	3.0
1	A	138	LYS	3.0
1	B	1104	ASP	3.0
1	A	109	GLN	3.0
1	A	164	GLN	2.8
1	A	162	LYS	2.7
1	B	1147	ARG	2.6
1	B	1213	ASP	2.6
1	A	255	LYS	2.6
1	B	1256	ALA	2.6
1	B	1169	ASN	2.6
1	B	1174	LYS	2.6
1	A	211	ASP	2.6
1	A	226	GLY	2.6
1	A	263	LEU	2.5
1	A	159	GLN	2.5
1	B	1197	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	147	ARG	2.5
1	A	140	GLN	2.4
1	A	209	LYS	2.4
1	B	1160	GLN	2.4
1	B	1233	ALA	2.4
1	A	108	LYS	2.3
1	B	1158	ILE	2.3
1	A	134	GLN	2.3
1	B	1120	ASP	2.3
1	B	1189	PRO	2.2
1	A	193	ASN	2.2
1	B	1232	LEU	2.2
1	A	151	SER	2.2
1	A	145	LEU	2.2
1	B	1123	GLN	2.1
1	B	1237	LYS	2.1
1	A	233	ALA	2.1
1	B	1173	ASP	2.1
1	A	210	GLU	2.1
1	B	1137	GLU	2.1
1	B	1192	THR	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](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	307	1/1	0.58	0.20	92,92,92,92	0
2	ZN	B	320	1/1	0.62	0.22	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	313	1/1	0.69	0.20	104,104,104,104	0
2	ZN	A	316	1/1	0.72	0.16	88,88,88,88	0
2	ZN	A	321	1/1	0.73	0.14	61,61,61,61	0
2	ZN	B	308	1/1	0.76	0.08	73,73,73,73	0
2	ZN	A	317	1/1	0.77	0.10	61,61,61,61	0
2	ZN	B	312	1/1	0.78	0.13	62,62,62,62	0
2	ZN	A	302	1/1	0.79	0.24	69,69,69,69	0
2	ZN	A	319	1/1	0.82	0.07	30,30,30,30	0
2	ZN	A	301	1/1	0.82	0.10	41,41,41,41	0
2	ZN	B	309	1/1	0.89	0.07	57,57,57,57	0
2	ZN	B	322	1/1	0.93	0.06	47,47,47,47	0
2	ZN	A	311	1/1	0.94	0.16	78,78,78,78	0
2	ZN	A	318	1/1	0.94	0.06	47,47,47,47	0
2	ZN	A	303	1/1	0.94	0.07	49,49,49,49	0
2	ZN	A	315	1/1	0.94	0.06	45,45,45,45	0
2	ZN	A	304	1/1	0.94	0.08	45,45,45,45	0
2	ZN	B	306	1/1	0.95	0.09	33,33,33,33	0
2	ZN	A	314	1/1	0.95	0.05	34,34,34,34	0
2	ZN	B	310	1/1	0.95	0.05	25,25,25,25	0
3	CAC	A	354	5/5	0.95	0.11	32,34,50,51	0
2	ZN	A	305	1/1	0.97	0.04	30,30,30,30	0
3	CAC	A	352	5/5	0.98	0.09	33,41,46,47	0
3	CAC	A	351	5/5	0.98	0.09	13,23,25,33	0
3	CAC	B	353	5/5	0.98	0.06	2,11,22,33	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.