



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:01 PM UTC

PDB ID : 3UX7 / pdb_00003ux7
Title : Crystal structure of a dimeric myotoxic component of the Vipera ammodytes meridionalis venom reveals determinants of myotoxicity and membrane damaging activity
Authors : Georgieva, D.; Coronado, M.; Oberthuer, D.; Buck, F.; Duhalov, D.; Arni, R.K.; Genov, N.; Betzel, C.
Deposited on : 2011-12-04
Resolution : 2.97 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

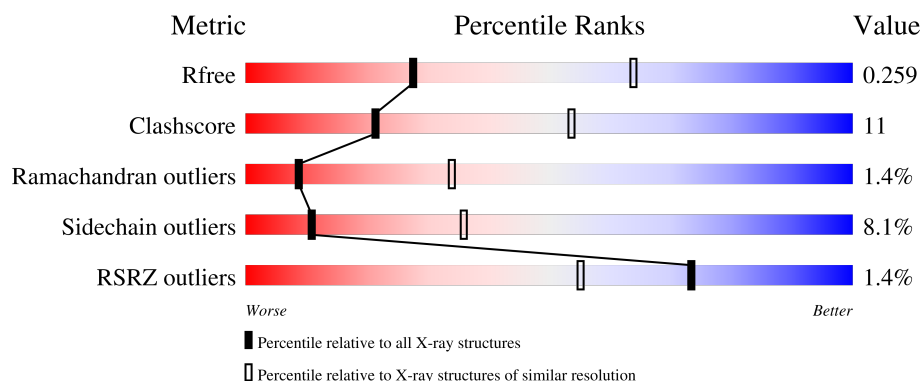
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	122	
1	B	122	
1	C	122	
1	D	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	122	
1	F	122	
1	G	122	
1	H	122	

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
2	SO4	F	125	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7657 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 Ammodytin L(1) isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			933	580	159	179	15			
1	B	122	Total	C	N	O	S	0	0	0
			932	580	159	178	15			
1	C	122	Total	C	N	O	S	3	0	0
			933	580	159	179	15			
1	D	122	Total	C	N	O	S	4	0	0
			933	580	159	179	15			
1	E	122	Total	C	N	O	S	5	0	0
			933	580	159	179	15			
1	F	122	Total	C	N	O	S	2	0	0
			933	580	159	179	15			
1	G	122	Total	C	N	O	S	12	1	0
			942	586	161	180	15			
1	H	122	Total	C	N	O	S	0	0	0
			933	580	159	179	15			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

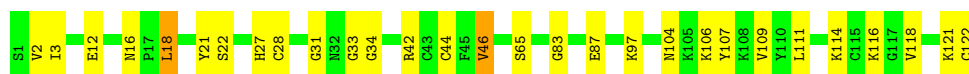
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	8	Total O 8 8	0	0
3	C	8	Total O 8 8	0	0
3	D	13	Total O 13 13	0	0
3	E	11	Total O 11 11	0	0
3	F	10	Total O 10 10	0	0
3	G	14	Total O 14 14	0	0
3	H	15	Total O 15 15	0	0

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.

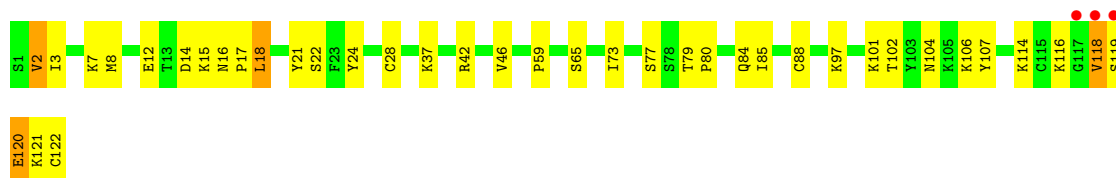
- Molecule 1: Ammodytin L(1) isoform

Chain A: 



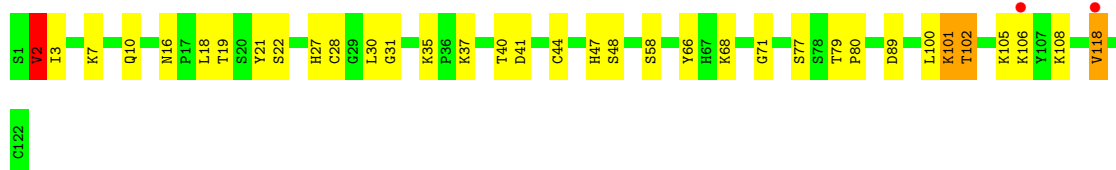
- Molecule 1: Ammodytin L(1) isoform

Chain B: 



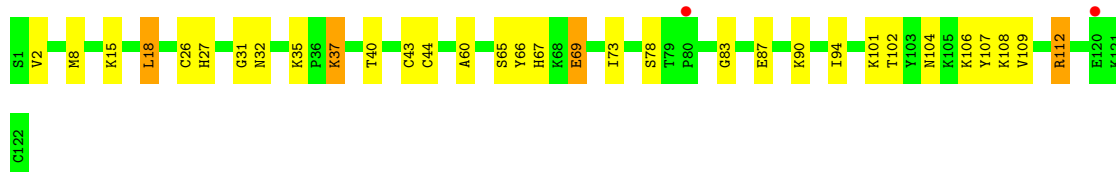
- Molecule 1: Ammodytin L(1) isoform

Chain C: 

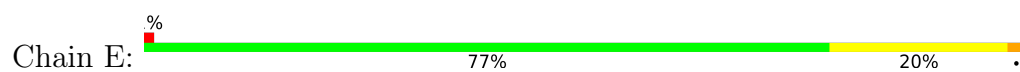


- Molecule 1: Ammodytin L(1) isoform

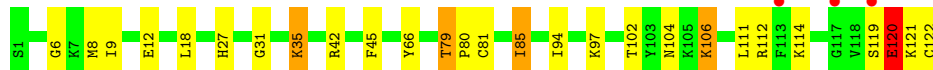
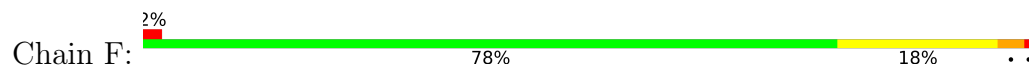
Chain D: 



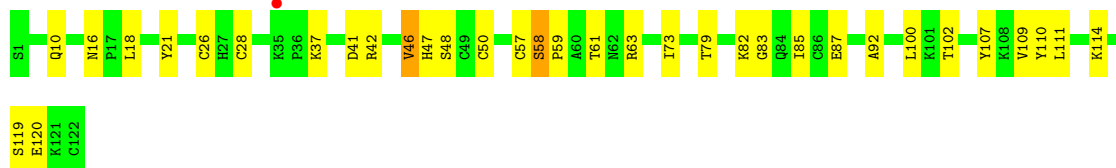
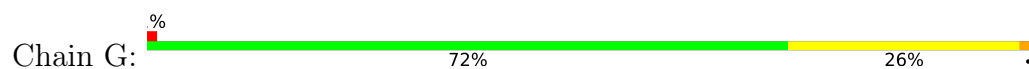
- Molecule 1: Ammodytin L(1) isoform



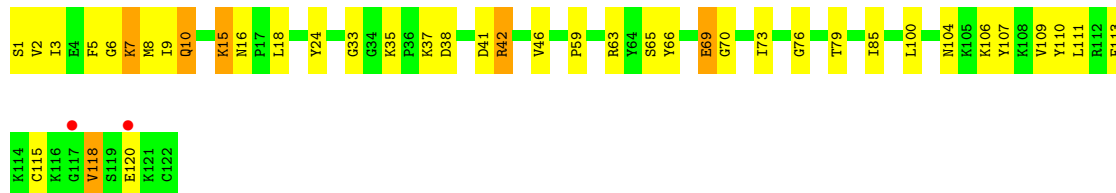
- Molecule 1: Ammodytin L(1) isoform



- Molecule 1: Ammodytin L(1) isoform



- Molecule 1: Ammodytin L(1) isoform



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.97 Å 47.67 Å 126.62 Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	40.00 – 2.97 40.00 – 2.97	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.00-2.97) 97.0 (40.00-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.95 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.261 0.226 , 0.259	Depositor DCC
R_{free} test set	971 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7657	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2936e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.49	0/952	0.95	2/1273 (0.2%)
1	B	0.54	0/951	0.96	2/1273 (0.2%)
1	C	0.53	0/952	1.02	7/1273 (0.5%)
1	D	0.49	0/952	0.91	0/1273
1	E	0.59	1/952 (0.1%)	0.92	1/1273 (0.1%)
1	F	0.55	0/952	0.94	3/1273 (0.2%)
1	G	0.52	0/961	0.91	2/1284 (0.2%)
1	H	0.51	0/952	0.98	5/1273 (0.4%)
All	All	0.53	1/7624 (0.0%)	0.95	22/10195 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	114	LYS	CA-CB	-6.73	1.43	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	114	LYS	N-CA-CB	7.94	121.52	110.56
1	C	79	THR	CA-C-N	7.75	129.52	119.84
1	C	79	THR	C-N-CA	7.75	129.52	119.84
1	F	120	GLU	CB-CG-CD	6.85	124.25	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	79	THR	CA-C-N	6.48	127.94	119.84
1	F	79	THR	C-N-CA	6.48	127.94	119.84
1	B	79	THR	CA-C-N	6.26	127.67	119.84
1	B	79	THR	C-N-CA	6.26	127.67	119.84
1	A	16	ASN	CA-C-N	6.12	125.84	119.05
1	A	16	ASN	C-N-CA	6.12	125.84	119.05
1	H	79	THR	CA-C-N	5.88	127.19	119.84
1	H	79	THR	C-N-CA	5.88	127.19	119.84
1	H	69	GLU	N-CA-C	5.64	116.65	107.23
1	C	101	LYS	N-CA-C	-5.53	102.83	110.35
1	H	16	ASN	CA-C-N	5.51	124.97	119.24
1	H	16	ASN	C-N-CA	5.51	124.97	119.24
1	C	58	SER	CA-C-N	5.28	125.60	119.47
1	C	58	SER	C-N-CA	5.28	125.60	119.47
1	G	16	ASN	CA-C-N	5.28	124.73	119.24
1	G	16	ASN	C-N-CA	5.28	124.73	119.24
1	C	35	LYS	CA-C-N	5.03	125.31	119.93
1	C	35	LYS	C-N-CA	5.03	125.31	119.93

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	120	GLU	Sidechain

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	933	0	895	14	0
1	B	932	0	895	34	0
1	C	933	0	895	28	0
1	D	933	0	895	24	0
1	E	933	0	895	15	0
1	F	933	0	895	18	0
1	G	942	0	907	16	0
1	H	933	0	895	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	0	0	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	1	0
2	F	15	0	0	2	0
2	G	15	0	0	0	0
2	H	10	0	0	0	0
3	A	11	0	0	0	0
3	B	8	0	0	1	0
3	C	8	0	0	3	0
3	D	13	0	0	0	0
3	E	11	0	0	0	0
3	F	10	0	0	0	0
3	G	14	0	0	1	0
3	H	15	0	0	0	0
All	All	7657	0	7172	160	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 11.

All (160) 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:35:LYS:HB3	1:F:35:LYS:HZ3	1.31	0.94
1:C:105:LYS:HE3	3:C:132:HOH:O	1.74	0.86
1:B:3:ILE:HG22	1:B:7:LYS:HE3	1.60	0.81
1:F:35:LYS:HB3	1:F:35:LYS:NZ	1.97	0.79
1:A:104:ASN:HB3	1:A:107:TYR:HD2	1.48	0.79
1:G:87:GLU:HG3	3:G:133:HOH:O	1.82	0.77
1:F:104:ASN:OD1	1:F:106:LYS:HG2	1.85	0.76
1:C:105:LYS:CE	3:C:132:HOH:O	2.32	0.76
1:D:37:LYS:HG3	1:D:107:TYR:CE1	2.22	0.74
1:D:37:LYS:CG	1:D:107:TYR:CE1	2.73	0.72
1:H:7:LYS:HD2	1:H:66:TYR:OH	1.90	0.71
1:C:16:ASN:HD21	1:C:18:LEU:HB2	1.55	0.71
1:B:14:ASP:HB3	1:D:67:HIS:CD2	2.26	0.70
1:E:104:ASN:HB3	1:E:107:TYR:HD2	1.57	0.70
1:F:35:LYS:NZ	1:F:35:LYS:CB	2.55	0.70
1:B:120:GLU:HG2	1:H:111:LEU:HG	1.75	0.68
1:H:42:ARG:HH21	1:H:42:ARG:HG2	1.57	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ASN:HB3	1:D:107:TYR:HD2	1.59	0.67
1:C:18:LEU:O	1:C:22:SER:HB3	1.96	0.65
1:B:3:ILE:O	1:B:7:LYS:HG3	1.97	0.64
1:B:14:ASP:HB3	1:D:67:HIS:HD2	1.62	0.64
1:D:83:GLY:O	1:D:87:GLU:HG2	1.99	0.63
1:C:105:LYS:HG3	1:C:108:LYS:HD2	1.82	0.61
1:A:83:GLY:O	1:A:87:GLU:HG3	2.01	0.61
1:C:102:THR:HG21	1:H:106:LYS:NZ	2.16	0.60
1:B:21:TYR:O	1:B:28:CYS:HB3	2.02	0.59
1:C:102:THR:O	1:C:102:THR:OG1	2.20	0.59
1:H:42:ARG:O	1:H:46:VAL:HG23	2.02	0.59
1:A:27:HIS:NE2	1:A:34:GLY:O	2.29	0.57
1:H:37:LYS:HD3	1:H:107:TYR:CE1	2.39	0.57
1:G:63:ARG:O	1:G:82:LYS:HE3	2.05	0.56
1:C:19:THR:HG22	1:G:46:VAL:HG21	1.86	0.56
1:D:37:LYS:HG3	1:D:107:TYR:HE1	1.69	0.56
1:E:1:SER:N	1:E:62:ASN:O	2.34	0.56
1:C:102:THR:CG2	1:H:106:LYS:HZ3	2.18	0.56
1:C:102:THR:CG2	1:H:106:LYS:NZ	2.68	0.56
1:A:104:ASN:HB3	1:A:107:TYR:CD2	2.35	0.56
1:C:118:VAL:HG11	1:F:97:LYS:HG2	1.87	0.56
1:E:104:ASN:HB3	1:E:107:TYR:CD2	2.40	0.56
1:B:104:ASN:OD1	1:B:106:LYS:HB3	2.06	0.56
1:B:84:GLN:NE2	3:B:129:HOH:O	2.38	0.55
1:D:37:LYS:HG2	1:D:107:TYR:CE1	2.41	0.55
1:A:27:HIS:O	1:A:44:CYS:HB3	2.07	0.55
1:F:121:LYS:O	1:F:122:CYS:HB3	2.07	0.55
1:A:104:ASN:OD1	1:A:106:LYS:HG2	2.07	0.54
1:B:59:PRO:HA	1:B:85:ILE:HD13	1.89	0.54
1:D:104:ASN:HD21	1:D:106:LYS:HE3	1.73	0.54
1:H:42:ARG:HH21	1:H:42:ARG:CG	2.19	0.54
1:A:3:ILE:HD12	1:E:80:PRO:HA	1.88	0.54
1:G:37:LYS:HD2	1:G:110:TYR:CZ	2.43	0.54
1:D:109:VAL:HG21	1:F:45:PHE:HE2	1.73	0.53
1:B:120:GLU:OE2	1:B:122:CYS:N	2.42	0.53
1:E:2:VAL:HG22	1:E:60:ALA:O	2.09	0.52
1:D:37:LYS:CG	1:D:107:TYR:HE1	2.21	0.52
1:F:31:GLY:HA2	1:F:112:ARG:HH11	1.75	0.52
1:E:42:ARG:O	1:E:46:VAL:HG12	2.08	0.52
1:G:47:HIS:HB2	1:G:92:ALA:HB2	1.92	0.52
1:G:111:LEU:HB2	1:G:114:LYS:HE3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:HD13	1:E:67:HIS:HB2	1.91	0.52
1:B:37:LYS:HE2	1:B:107:TYR:HE1	1.74	0.51
1:C:68:LYS:HE3	1:C:71:GLY:HA2	1.92	0.51
1:C:21:TYR:O	1:C:28:CYS:HB3	2.10	0.51
1:E:42:ARG:NH2	2:E:123:SO4:O4	2.43	0.51
1:C:47:HIS:HE1	1:C:89:ASP:OD2	1.94	0.50
1:D:2:VAL:HG13	1:D:60:ALA:HA	1.93	0.50
1:A:42:ARG:O	1:A:46:VAL:HG12	2.10	0.50
1:B:8:MET:SD	1:B:73:ILE:HD13	2.52	0.50
1:C:105:LYS:HE3	1:C:108:LYS:NZ	2.26	0.49
1:B:119:SER:HB3	1:B:120:GLU:HA	1.95	0.49
1:H:37:LYS:HD2	1:H:110:TYR:CZ	2.48	0.49
1:C:16:ASN:ND2	1:C:18:LEU:HB2	2.26	0.49
1:B:120:GLU:OE2	1:B:121:LYS:N	2.46	0.48
1:B:15:LYS:HE2	1:D:69:GLU:HG3	1.95	0.48
1:H:37:LYS:N	1:H:41:ASP:OD1	2.36	0.48
1:H:7:LYS:HE3	1:H:7:LYS:HB2	1.56	0.48
1:H:69:GLU:HA	1:H:70:GLY:HA2	1.54	0.48
1:F:27:HIS:HA	1:F:31:GLY:O	2.14	0.48
1:D:104:ASN:HB3	1:D:107:TYR:CD2	2.45	0.48
1:F:42:ARG:NH2	2:F:125:SO4:S	2.87	0.48
1:H:15:LYS:HD2	1:H:100:LEU:HD21	1.96	0.48
1:H:38:ASP:O	1:H:42:ARG:HB2	2.13	0.48
1:A:18:LEU:O	1:A:22:SER:HB2	2.14	0.47
1:H:1:SER:OG	1:H:63:ARG:HD3	2.14	0.47
1:F:35:LYS:HZ3	1:F:35:LYS:CB	2.11	0.47
1:D:104:ASN:HD22	1:D:107:TYR:HE2	1.62	0.47
1:H:6:GLY:O	1:H:10:GLN:HB2	2.15	0.47
1:B:42:ARG:NE	2:B:124:SO4:O1	2.47	0.47
1:B:104:ASN:HB3	1:B:107:TYR:HD2	1.80	0.47
1:B:121:LYS:O	1:B:122:CYS:HB2	2.14	0.47
1:E:7:LYS:HD2	1:E:66:TYR:OH	2.14	0.47
1:G:57:CYS:HB3	1:G:85:ILE:HD11	1.96	0.47
1:A:12:GLU:O	1:A:97:LYS:HD2	2.14	0.47
1:C:108:LYS:NZ	3:C:132:HOH:O	2.48	0.47
1:G:42:ARG:O	1:G:46:VAL:HG12	2.14	0.47
1:G:79:THR:O	1:G:83:GLY:N	2.46	0.47
1:A:111:LEU:O	1:A:114:LYS:HG3	2.15	0.46
1:A:121:LYS:H	1:A:121:LYS:HD2	1.80	0.46
1:E:59:PRO:HA	1:E:85:ILE:HD13	1.97	0.46
1:F:42:ARG:NH2	2:F:125:SO4:O2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLU:O	1:B:97:LYS:HD2	2.16	0.46
1:B:119:SER:CB	1:B:120:GLU:HA	2.46	0.46
1:B:24:TYR:O	1:B:28:CYS:HB2	2.16	0.45
1:H:104:ASN:HB3	1:H:107:TYR:CD2	2.52	0.45
1:D:31:GLY:CA	1:D:112:ARG:NH1	2.79	0.45
1:B:106:LYS:CG	1:B:106:LYS:O	2.63	0.45
1:D:40:THR:O	1:D:43:CYS:HB2	2.15	0.45
1:E:35:LYS:HA	1:E:36:PRO:HD3	1.83	0.45
1:C:27:HIS:HA	1:C:31:GLY:O	2.16	0.45
1:F:8:MET:HE2	1:F:66:TYR:CD2	2.52	0.45
1:E:16:ASN:HA	1:E:17:PRO:HD3	1.88	0.45
1:C:106:LYS:HG3	1:C:106:LYS:O	2.16	0.45
1:G:58:SER:N	1:G:59:PRO:HD3	2.32	0.45
1:G:21:TYR:O	1:G:28:CYS:HB3	2.16	0.45
1:B:106:LYS:NZ	1:G:102:THR:CG2	2.80	0.44
1:B:101:LYS:HG3	1:B:102:THR:HG23	2.00	0.44
1:H:5:PHE:CE1	1:H:9:ILE:HD11	2.52	0.44
1:B:16:ASN:HA	1:B:17:PRO:HD3	1.85	0.44
1:F:81:CYS:O	1:F:85:ILE:HG12	2.17	0.44
1:C:3:ILE:O	1:C:7:LYS:HG3	2.17	0.44
1:G:37:LYS:HD3	1:G:107:TYR:CE1	2.54	0.43
1:A:18:LEU:HG	1:E:50:CYS:SG	2.58	0.43
1:B:18:LEU:O	1:B:22:SER:HB2	2.18	0.43
1:D:27:HIS:O	1:D:44:CYS:HB3	2.19	0.43
1:E:27:HIS:NE2	1:E:34:GLY:O	2.33	0.43
1:B:106:LYS:O	1:B:106:LYS:HG3	2.19	0.43
1:C:105:LYS:HE3	1:C:108:LYS:HZ2	1.83	0.43
1:B:65:SER:H	1:B:77:SER:HG	1.65	0.43
1:F:111:LEU:O	1:F:114:LYS:HG2	2.18	0.43
1:C:2:VAL:HG23	1:C:3:ILE:HD12	2.01	0.42
1:C:41:ASP:O	1:C:44:CYS:HB2	2.20	0.42
1:D:8:MET:HE2	1:D:66:TYR:CD2	2.54	0.42
1:H:37:LYS:HD2	1:H:110:TYR:CE2	2.54	0.42
1:B:3:ILE:H	1:B:3:ILE:HD12	1.84	0.42
1:D:18:LEU:HD12	1:D:18:LEU:O	2.20	0.42
1:E:57:CYS:HB3	1:E:85:ILE:HD11	2.01	0.42
1:G:58:SER:HB3	1:G:61:THR:OG1	2.18	0.42
1:D:26:CYS:SG	1:D:37:LYS:HD3	2.59	0.42
1:C:7:LYS:HD2	1:C:66:TYR:OH	2.20	0.42
1:H:8:MET:SD	1:H:73:ILE:HD13	2.59	0.42
1:B:120:GLU:CD	1:B:122:CYS:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:THR:HG21	1:H:106:LYS:HZ3	1.83	0.41
1:H:65:SER:HB2	1:H:76:GLY:O	2.20	0.41
1:B:104:ASN:HB3	1:B:107:TYR:CD2	2.54	0.41
1:B:118:VAL:HG13	1:B:120:GLU:HB3	2.02	0.41
1:H:24:TYR:HA	1:H:107:TYR:O	2.19	0.41
1:H:3:ILE:HD12	1:H:3:ILE:HA	1.85	0.41
1:B:120:GLU:HB2	1:B:121:LYS:H	1.55	0.41
1:G:26:CYS:H	1:G:41:ASP:CG	2.29	0.41
1:H:59:PRO:HA	1:H:85:ILE:HD13	2.03	0.41
1:B:85:ILE:O	1:B:88:CYS:HB2	2.20	0.41
1:C:18:LEU:HD23	1:G:50:CYS:SG	2.61	0.41
1:C:101:LYS:O	1:C:102:THR:HG23	2.20	0.41
1:H:33:GLY:O	1:H:115:CYS:HB3	2.21	0.41
1:D:109:VAL:HG21	1:F:45:PHE:CE2	2.54	0.41
1:F:6:GLY:HA2	1:F:9:ILE:HD12	2.03	0.41
1:H:111:LEU:HD23	1:H:113:PHE:HE2	1.86	0.41
1:D:73:ILE:HB	1:D:90:LYS:HG3	2.03	0.40
1:D:101:LYS:HG3	1:D:102:THR:HG23	2.03	0.40
1:A:21:TYR:O	1:A:28:CYS:HB3	2.21	0.40
1:F:12:GLU:OE2	1:F:94:ILE:HD13	2.21	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	120/122 (98%)	112 (93%)	6 (5%)	2 (2%)	7	30
1	B	120/122 (98%)	107 (89%)	11 (9%)	2 (2%)	7	30
1	C	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	7	30
1	D	120/122 (98%)	112 (93%)	6 (5%)	2 (2%)	7	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	F	120/122 (98%)	110 (92%)	7 (6%)	3 (2%)	4	21
1	G	121/122 (99%)	111 (92%)	9 (7%)	1 (1%)	16	47
1	H	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	47
All	All	961/976 (98%)	884 (92%)	64 (7%)	13 (1%)	9	34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLY
1	C	2	VAL
1	F	119	SER
1	A	33	GLY
1	D	108	LYS
1	C	80	PRO
1	D	32	ASN
1	F	120	GLU
1	B	80	PRO
1	G	73	ILE
1	H	118	VAL
1	F	80	PRO
1	B	2	VAL

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	104/104 (100%)	96 (92%)	8 (8%)	12	38
1	B	104/104 (100%)	97 (93%)	7 (7%)	15	44
1	C	104/104 (100%)	95 (91%)	9 (9%)	9	33
1	D	104/104 (100%)	95 (91%)	9 (9%)	9	33
1	E	104/104 (100%)	96 (92%)	8 (8%)	12	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	104/104 (100%)	97 (93%)	7 (7%)	15	44
1	G	105/104 (101%)	96 (91%)	9 (9%)	10	34
1	H	104/104 (100%)	94 (90%)	10 (10%)	8	29
All	All	833/832 (100%)	766 (92%)	67 (8%)	11	36

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	18	LEU
1	A	46	VAL
1	A	65	SER
1	A	109	VAL
1	A	116	LYS
1	A	118	VAL
1	A	122	CYS
1	B	2	VAL
1	B	18	LEU
1	B	46	VAL
1	B	114	LYS
1	B	116	LYS
1	B	118	VAL
1	B	120	GLU
1	C	2	VAL
1	C	10	GLN
1	C	30	LEU
1	C	37	LYS
1	C	40	THR
1	C	48	SER
1	C	77	SER
1	C	102	THR
1	C	118	VAL
1	D	15	LYS
1	D	18	LEU
1	D	35	LYS
1	D	37	LYS
1	D	65	SER
1	D	69	GLU
1	D	78	SER
1	D	94	ILE
1	D	112	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	2	VAL
1	E	10	GLN
1	E	46	VAL
1	E	65	SER
1	E	102	THR
1	E	109	VAL
1	E	114	LYS
1	E	118	VAL
1	F	18	LEU
1	F	35	LYS
1	F	79	THR
1	F	85	ILE
1	F	102	THR
1	F	106	LYS
1	F	120	GLU
1	G	10	GLN
1	G	18	LEU
1	G	46	VAL
1	G	48	SER
1	G	58	SER
1	G	100	LEU
1	G	109	VAL
1	G	119	SER
1	G	120	GLU
1	H	2	VAL
1	H	7	LYS
1	H	10	GLN
1	H	15	LYS
1	H	18	LEU
1	H	35	LYS
1	H	42	ARG
1	H	109	VAL
1	H	118	VAL
1	H	120	GLU

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	67	HIS
1	A	99	ASN
1	B	84	GLN
1	C	10	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	47	HIS
1	D	67	HIS
1	D	99	ASN
1	D	104	ASN
1	F	16	ASN
1	G	84	GLN
1	G	99	ASN
1	H	47	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](#)

19 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	H	123	-	4,4,4	0.36	0	6,6,6	0.25	0
2	SO4	A	124	-	4,4,4	0.32	0	6,6,6	0.14	0
2	SO4	G	123	-	4,4,4	0.36	0	6,6,6	0.06	0
2	SO4	F	123	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	H	124	-	4,4,4	0.46	0	6,6,6	0.09	0
2	SO4	A	123	-	4,4,4	0.35	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	G	124	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	C	123	-	4,4,4	0.35	0	6,6,6	0.09	0
2	SO4	D	123	-	4,4,4	0.36	0	6,6,6	0.15	0
2	SO4	A	126	-	4,4,4	0.37	0	6,6,6	0.12	0
2	SO4	C	124	-	4,4,4	0.44	0	6,6,6	0.09	0
2	SO4	F	124	-	4,4,4	0.39	0	6,6,6	0.12	0
2	SO4	B	123	-	4,4,4	0.34	0	6,6,6	0.12	0
2	SO4	A	125	-	4,4,4	0.36	0	6,6,6	0.18	0
2	SO4	E	123	-	4,4,4	0.37	0	6,6,6	0.19	0
2	SO4	G	125	-	4,4,4	0.30	0	6,6,6	0.18	0
2	SO4	D	124	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	F	125	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	B	124	-	4,4,4	0.56	0	6,6,6	0.29	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	123	SO4	1	0
2	F	125	SO4	2	0
2	B	124	SO4	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	122/122 (100%)	0.07	0 100 100	14, 25, 53, 80	0
1	B	122/122 (100%)	0.23	3 (2%) 58 39	10, 25, 56, 69	0
1	C	122/122 (100%)	0.09	2 (1%) 70 51	14, 26, 42, 62	1 (0%)
1	D	122/122 (100%)	0.02	2 (1%) 70 51	10, 23, 43, 66	1 (0%)
1	E	122/122 (100%)	0.07	1 (0%) 82 67	12, 24, 55, 67	1 (0%)
1	F	122/122 (100%)	0.07	3 (2%) 58 39	13, 23, 62, 76	1 (0%)
1	G	122/122 (100%)	0.09	1 (0%) 82 67	14, 24, 51, 61	2 (1%)
1	H	122/122 (100%)	-0.02	2 (1%) 70 51	14, 21, 53, 77	0
All	All	976/976 (100%)	0.08	14 (1%) 73 55	10, 24, 55, 80	6 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	GLU	3.2
1	D	80	PRO	3.1
1	F	117	GLY	2.9
1	B	118	VAL	2.6
1	H	117	GLY	2.5
1	E	113	PHE	2.5
1	B	119	SER	2.3
1	C	106	LYS	2.3
1	F	113	PHE	2.2
1	C	118	VAL	2.2
1	G	35	LYS	2.1
1	F	119	SER	2.1
1	B	117	GLY	2.0
1	H	120	GLU	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](#)

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	SO4	F	123	5/5	0.43	0.19	124,124,126,126	0
2	SO4	H	124	5/5	0.68	0.16	82,82,84,86	0
2	SO4	C	124	5/5	0.75	0.13	76,76,76,77	0
2	SO4	B	123	5/5	0.78	0.24	93,95,96,98	0
2	SO4	C	123	5/5	0.83	0.21	86,86,89,90	0
2	SO4	B	124	5/5	0.84	0.15	74,76,79,80	0
2	SO4	A	126	5/5	0.85	0.12	75,78,79,80	0
2	SO4	H	123	5/5	0.87	0.19	43,45,52,53	0
2	SO4	F	124	5/5	0.87	0.15	65,65,66,68	0
2	SO4	G	125	5/5	0.88	0.23	55,55,57,61	0
2	SO4	D	123	5/5	0.89	0.16	54,59,62,62	0
2	SO4	A	125	5/5	0.90	0.15	42,48,49,49	0
2	SO4	G	123	5/5	0.91	0.13	67,67,68,69	0
2	SO4	G	124	5/5	0.92	0.13	49,50,52,55	0
2	SO4	A	123	5/5	0.92	0.08	79,79,81,84	0
2	SO4	E	123	5/5	0.93	0.07	53,54,55,57	0
2	SO4	F	125	5/5	0.94	0.09	59,59,59,59	0
2	SO4	A	124	5/5	0.94	0.19	65,66,66,67	0
2	SO4	D	124	5/5	0.96	0.06	56,59,60,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.