



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:15 AM UTC

PDB ID : 3CFI / pdb_00003cfi
Title : Nanobody-aided structure determination of the EPSI:EPSJ pseudopilin heterodimer from *Vibrio Vulnificus*
Authors : Lam, A.Y.; Pardon, E.; Korotkov, K.V.; Steyaert, J.; Hol, W.G.J.
Deposited on : 2008-03-03
Resolution : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

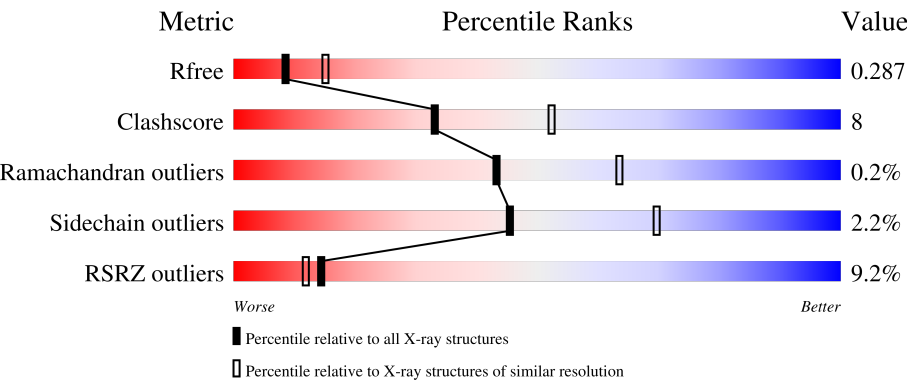
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	84	8% 64% 26% 10%
1	D	84	13% 63% 29% 5%
1	G	84	17% 67% 19% 12%
1	J	84	15% 79% 15%
2	B	164	7% 81% 16%

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Mol	Chain	Length	Quality of chain
2	E	164	5% 86% 10%
2	H	164	7% 82% 13%
2	K	164	4% 84% 9% 7%
3	C	116	8% 83% 16%
3	F	116	16% 78% 18%
3	I	116	7% 84% 16%
3	L	116	9% 84% 10% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11229 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 Type II secretory pathway, pseudopilin EpsI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	76	Total	C	N	O	S	0	0	0
			587	376	96	110	5			
1	D	80	Total	C	N	O	S	0	0	0
			611	392	99	115	5			
1	G	74	Total	C	N	O	S	0	0	0
			573	367	94	107	5			
1	J	81	Total	C	N	O	S	0	0	0
			624	400	102	117	5			

- Molecule 2 is a protein called Type II secretory pathway, PSEUDOPILIN EpsJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1322	836	236	247	3			
2	E	158	Total	C	N	O	S	0	0	0
			1306	823	235	245	3			
2	H	157	Total	C	N	O	S	0	0	0
			1303	826	233	241	3			
2	K	153	Total	C	N	O	S	0	0	0
			1270	807	225	235	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	86	ASN	SER	SEE REMARK 999	UNP Q7MPZ0
H	167	THR	ALA	SEE REMARK 999	UNP Q7MPZ0
E	86	ASN	SER	SEE REMARK 999	UNP Q7MPZ0
E	167	THR	ALA	SEE REMARK 999	UNP Q7MPZ0
K	86	ASN	SER	SEE REMARK 999	UNP Q7MPZ0
K	167	THR	ALA	SEE REMARK 999	UNP Q7MPZ0
B	86	ASN	SER	SEE REMARK 999	UNP Q7MPZ0
B	167	THR	ALA	SEE REMARK 999	UNP Q7MPZ0

- Molecule 3 is a protein called Nanobody NBPSIJ_11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	115	Total	C	N	O	S	0	0	0
			879	550	158	167	4			
3	F	114	Total	C	N	O	S	0	0	0
			872	547	157	164	4			
3	I	116	Total	C	N	O	S	0	0	0
			888	555	160	169	4			
3	L	109	Total	C	N	O	S	0	0	0
			835	523	151	157	4			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		
4	K	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	16	Total	O	0	0
			16	16		
5	C	17	Total	O	0	0
			17	17		
5	D	5	Total	O	0	0
			5	5		
5	E	19	Total	O	0	0
			19	19		
5	F	7	Total	O	0	0
			7	7		
5	G	9	Total	O	0	0
			9	9		
5	H	21	Total	O	0	0
			21	21		
5	I	14	Total	O	0	0
			14	14		

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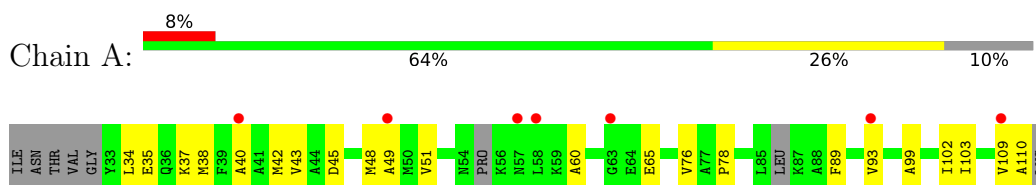
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	7	Total 7	O 7	0	0
5	K	22	Total 22	O 22	0	0
5	L	7	Total 7	O 7	0	0

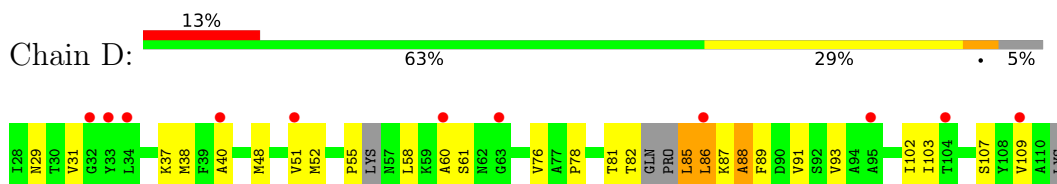
3 Residue-property plots [i](#)

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.

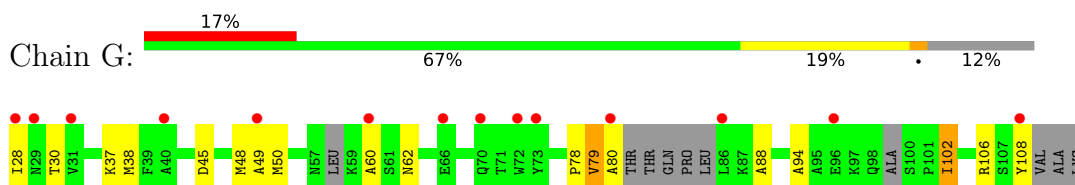
- Molecule 1: Type II secretory pathway, pseudopilin EpsI



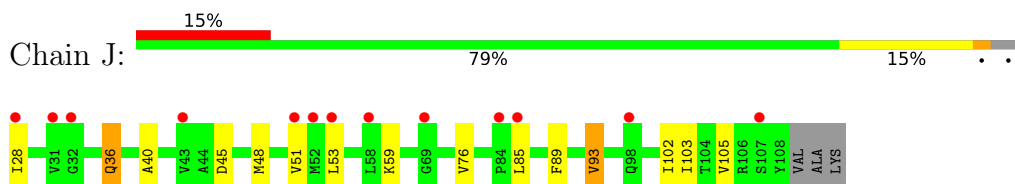
- Molecule 1: Type II secretory pathway, pseudopilin EpsI



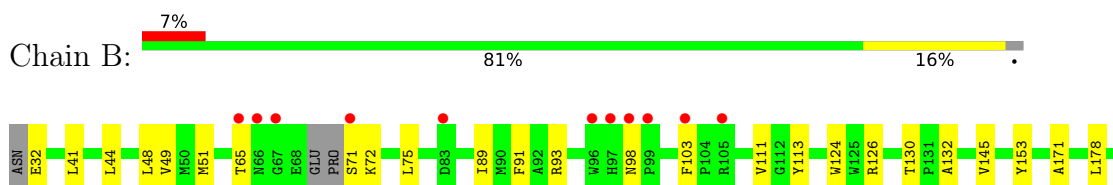
- Molecule 1: Type II secretory pathway, pseudopilin EpsI



- Molecule 1: Type II secretory pathway, pseudopilin EpsI

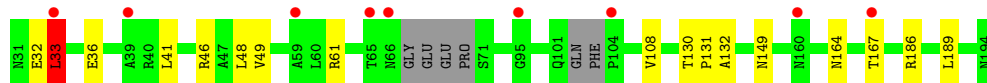
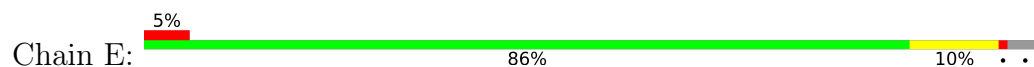


- Molecule 2: Type II secretory pathway, PSEUDOPILIN EpsJ

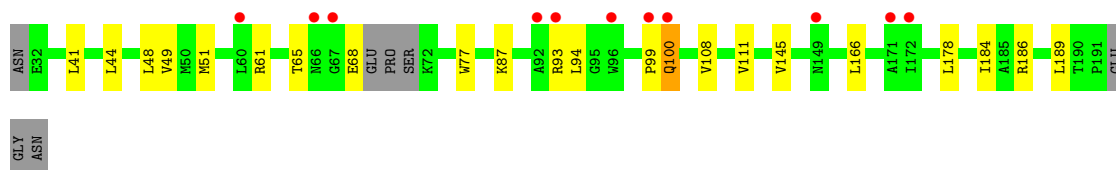
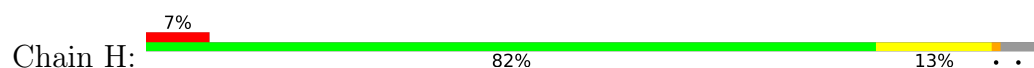




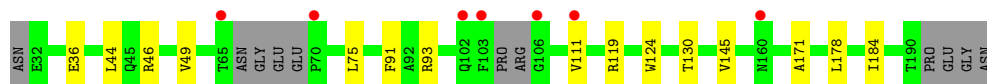
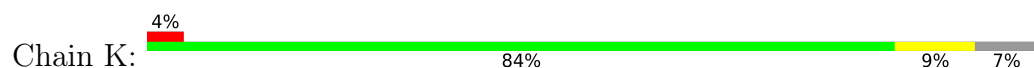
- Molecule 2: Type II secretory pathway, PSEUDOPILIN EpsJ



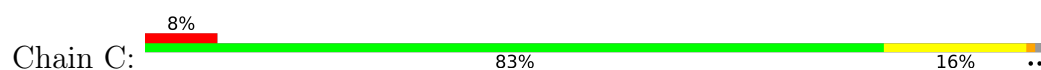
- Molecule 2: Type II secretory pathway, PSEUDOPILIN EpsJ



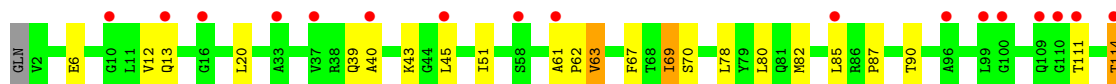
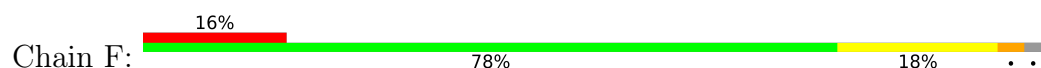
- Molecule 2: Type II secretory pathway, PSEUDOPILIN EpsJ



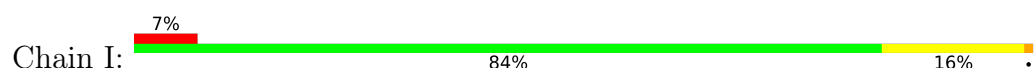
- Molecule 3: Nanobody NBEPSIJ_11

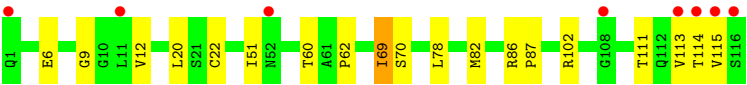


- Molecule 3: Nanobody NBEPSIJ_11

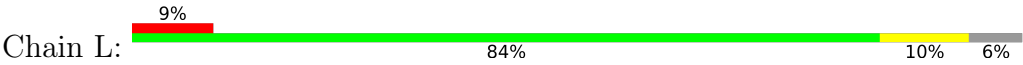


- Molecule 3: Nanobody NBEPSIJ_11





● Molecule 3: Nanobody NBEPSIJ_11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.72Å 67.24Å 128.25Å 96.54° 91.62° 90.20°	Depositor
Resolution (Å)	19.97 – 2.58 19.97 – 2.58	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.97-2.58) 95.9 (19.97-2.58)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.279 0.235 , 0.287	Depositor DCC
R_{free} test set	2645 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11229	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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

5.1 Standard geometry

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

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	0.43	0/596	0.65	0/805
1	D	0.45	0/620	0.68	0/840
1	G	0.46	0/581	0.66	0/782
1	J	0.51	1/636 (0.2%)	0.69	0/864
2	B	0.44	0/1351	0.60	0/1829
2	E	0.43	0/1333	0.63	0/1802
2	H	0.44	0/1332	0.59	0/1804
2	K	0.41	0/1297	0.62	0/1754
3	C	0.44	0/899	0.62	0/1215
3	F	0.44	0/892	0.62	0/1207
3	I	0.44	0/908	0.63	0/1227
3	L	0.43	0/854	0.65	0/1151
All	All	0.44	1/11299 (0.0%)	0.63	0/15280

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
2	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	36	GLN	CD-OE1	5.08	1.33	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	33	LEU	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	587	0	589	19	0
1	D	611	0	615	24	0
1	G	573	0	572	19	0
1	J	624	0	631	12	0
2	B	1322	0	1298	23	0
2	E	1306	0	1284	12	0
2	H	1303	0	1284	25	0
2	K	1270	0	1254	12	0
3	C	879	0	847	13	0
3	F	872	0	842	15	0
3	I	888	0	858	16	0
3	L	835	0	800	8	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
5	A	11	0	0	1	0
5	B	16	0	0	1	0
5	C	17	0	0	1	0
5	D	5	0	0	0	0
5	E	19	0	0	0	0
5	F	7	0	0	0	0
5	G	9	0	0	1	0
5	H	21	0	0	0	0
5	I	14	0	0	1	0
5	J	7	0	0	0	0
5	K	22	0	0	2	0
5	L	7	0	0	0	0
All	All	11229	0	10874	171	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 8.

All (171) 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)
2:B:49:VAL:HG21	2:K:49:VAL:HG21	1.49	0.94
1:G:49:ALA:HB1	2:H:189:LEU:HD11	1.55	0.89
3:F:63:VAL:HG13	3:F:67:PHE:HB2	1.57	0.85
2:E:49:VAL:HG11	2:H:49:VAL:HG21	1.58	0.84
2:H:48:LEU:HD23	2:H:51:MET:HE2	1.62	0.81
3:F:85:LEU:HD23	3:F:115:VAL:HG11	1.64	0.80
2:E:164:ASN:OD1	2:E:167:THR:HG22	1.82	0.79
3:C:82:MET:HE2	3:C:85:LEU:HD21	1.64	0.79
1:A:93:VAL:HG22	1:A:103:ILE:HG22	1.65	0.77
3:F:69:ILE:HD11	3:F:78:LEU:HD11	1.68	0.74
3:C:45:LEU:HD23	3:C:104:TRP:CZ2	2.23	0.73
1:A:93:VAL:HG22	1:A:103:ILE:CG2	2.17	0.73
3:I:22:CYS:SG	5:I:125:HOH:O	2.48	0.70
1:A:40:ALA:HB2	1:A:102:ILE:HD11	1.73	0.69
3:I:69:ILE:HD13	3:I:70:SER:N	2.08	0.68
3:F:51:ILE:HB	3:F:69:ILE:HD12	1.74	0.68
1:J:45:ASP:HA	1:J:48:MET:HE3	1.75	0.68
1:D:93:VAL:HG22	1:D:103:ILE:HG22	1.76	0.67
2:B:48:LEU:HD23	2:B:51:MET:CE	2.23	0.67
3:I:60:THR:HG23	3:I:102:ARG:HH12	1.57	0.67
2:K:145:VAL:HG22	2:K:178:LEU:HD22	1.75	0.67
1:G:49:ALA:HB1	2:H:189:LEU:CD1	2.23	0.67
1:G:38:MET:CE	2:H:41:LEU:HD22	2.25	0.67
1:D:40:ALA:HB2	1:D:102:ILE:HD11	1.77	0.66
2:E:46:ARG:HG2	2:H:49:VAL:HG12	1.78	0.66
1:J:51:VAL:HG21	1:J:89:PHE:CE1	2.30	0.65
3:I:20:LEU:HG	3:I:82:MET:HE2	1.79	0.64
3:C:39:GLN:HB2	3:C:45:LEU:HD12	1.80	0.63
2:K:130:THR:HG22	5:K:205:HOH:O	2.00	0.62
3:F:69:ILE:HD13	3:F:70:SER:N	2.15	0.60
1:D:51:VAL:HG21	1:D:89:PHE:CE1	2.37	0.60
2:H:93:ARG:HD2	2:H:111:VAL:HG11	1.84	0.60
1:D:93:VAL:HG22	1:D:103:ILE:CG2	2.32	0.60
3:L:67:PHE:CE1	3:L:82:MET:HE3	2.37	0.60
1:D:51:VAL:HG11	1:D:76:VAL:HG21	1.85	0.59
2:B:49:VAL:HG12	2:K:46:ARG:HG2	1.85	0.59
3:F:6:GLU:HB2	3:F:111:THR:HG23	1.85	0.59
2:B:145:VAL:HG22	2:B:178:LEU:HD22	1.84	0.59
3:F:87:PRO:HA	3:F:115:VAL:HG23	1.85	0.58
3:C:82:MET:HE2	3:C:85:LEU:CD2	2.33	0.58
3:F:20:LEU:HD12	3:F:80:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:ILE:HD12	1:G:28:ILE:N	2.20	0.57
2:E:130:THR:HG22	2:E:132:ALA:H	1.70	0.57
1:G:38:MET:HE1	2:H:41:LEU:HD22	1.85	0.57
2:B:111:VAL:HG12	2:B:124:TRP:HD1	1.69	0.56
2:B:75:LEU:HD23	2:B:91:PHE:HB3	1.86	0.56
3:I:9:GLY:HA2	3:I:113:VAL:HG22	1.86	0.56
1:A:93:VAL:CG2	1:A:103:ILE:HG22	2.35	0.55
1:J:53:LEU:HD21	2:K:171:ALA:HB2	1.89	0.55
3:F:61:ALA:HB3	3:F:62:PRO:HD3	1.88	0.55
1:D:87:LYS:O	1:D:88:ALA:HB2	2.07	0.55
3:I:69:ILE:HD11	3:I:78:LEU:HD11	1.88	0.55
1:G:38:MET:HE2	2:H:41:LEU:HD22	1.89	0.54
2:H:48:LEU:HD23	2:H:51:MET:CE	2.35	0.54
2:B:93:ARG:HD3	2:B:111:VAL:HG11	1.88	0.54
1:D:55:PRO:HB3	1:D:109:VAL:HG21	1.89	0.54
3:I:87:PRO:HA	3:I:115:VAL:HG13	1.88	0.54
1:A:45:ASP:HA	1:A:48:MET:HE3	1.89	0.54
2:H:48:LEU:HD22	2:H:186:ARG:HD2	1.88	0.54
1:A:51:VAL:HG11	1:A:89:PHE:CE1	2.42	0.53
1:G:45:ASP:HA	1:G:48:MET:HE3	1.89	0.53
3:L:67:PHE:CZ	3:L:82:MET:HE3	2.43	0.53
3:I:6:GLU:HB2	3:I:111:THR:HG23	1.89	0.53
1:A:37:LYS:HZ3	1:J:105:VAL:HG11	1.74	0.53
1:G:38:MET:CE	2:H:44:LEU:HD23	2.38	0.53
2:K:93:ARG:HD2	2:K:111:VAL:HG11	1.90	0.53
3:L:61:ALA:HB3	3:L:62:PRO:HD3	1.90	0.53
1:D:93:VAL:CG2	1:D:103:ILE:HG22	2.38	0.53
2:E:48:LEU:HD22	2:E:186:ARG:CD	2.39	0.53
3:I:51:ILE:HB	3:I:69:ILE:HD12	1.90	0.53
1:A:38:MET:HE1	2:B:44:LEU:HD23	1.91	0.52
2:E:48:LEU:HD22	2:E:186:ARG:HD2	1.92	0.52
1:J:28:ILE:HG23	1:J:28:ILE:O	2.09	0.52
1:A:38:MET:CE	2:B:44:LEU:HD23	2.40	0.52
1:D:38:MET:CE	2:E:41:LEU:HD22	2.39	0.52
1:D:81:THR:HG23	1:D:82:THR:H	1.75	0.52
2:B:145:VAL:HG22	2:B:178:LEU:CD2	2.40	0.51
1:G:88:ALA:HB2	1:G:108:TYR:CD1	2.45	0.51
3:C:87:PRO:HA	3:C:115:VAL:HG13	1.93	0.51
3:I:60:THR:HG23	3:I:102:ARG:NH1	2.26	0.51
1:G:49:ALA:CB	2:H:189:LEU:HD11	2.35	0.50
1:A:43:VAL:HG13	1:A:65:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:130:THR:HG23	2:E:131:PRO:HD2	1.93	0.50
1:D:61:SER:OG	1:D:76:VAL:HG12	2.11	0.50
2:H:99:PRO:O	2:H:100:GLN:HB2	2.12	0.50
2:B:111:VAL:HG12	2:B:124:TRP:CD1	2.47	0.50
1:D:109:VAL:HG22	1:D:109:VAL:O	2.11	0.50
3:L:51:ILE:HG21	3:L:78:LEU:HD11	1.93	0.50
1:G:30:THR:HG22	5:G:119:HOH:O	2.12	0.50
1:G:60:ALA:HB2	1:G:78:PRO:HD2	1.94	0.50
3:C:60:THR:HG22	3:C:62:PRO:HD2	1.95	0.49
2:B:65:THR:O	2:B:65:THR:HG23	2.12	0.49
2:E:61:ARG:HD2	2:E:108:VAL:HG11	1.95	0.49
3:L:6:GLU:HB2	3:L:111:THR:HG23	1.95	0.49
2:K:119:ARG:CZ	5:K:215:HOH:O	2.60	0.48
3:F:85:LEU:HD23	3:F:115:VAL:CG1	2.40	0.48
1:A:42:MET:HE1	2:B:184:ILE:CG2	2.43	0.48
3:I:60:THR:HG22	3:I:62:PRO:CD	2.44	0.48
2:H:145:VAL:HG22	2:H:178:LEU:HD22	1.96	0.48
2:B:130:THR:HG22	2:B:132:ALA:H	1.78	0.48
2:H:48:LEU:HD22	2:H:186:ARG:CD	2.44	0.48
1:A:35:GLU:HG2	2:B:41:LEU:HD11	1.95	0.47
1:J:93:VAL:HG22	1:J:103:ILE:HG22	1.96	0.47
3:L:60:THR:HG22	3:L:102:ARG:NH1	2.30	0.47
1:D:55:PRO:CB	1:D:109:VAL:HG21	2.46	0.46
2:K:111:VAL:HG12	2:K:124:TRP:HD1	1.81	0.46
1:D:29:ASN:HB2	1:D:31:VAL:HG12	1.98	0.46
2:B:124:TRP:CZ3	2:B:126:ARG:HG2	2.51	0.46
3:I:86:ARG:O	3:I:115:VAL:HG11	2.16	0.46
1:A:38:MET:CE	2:B:41:LEU:HD22	2.46	0.46
1:D:38:MET:HE1	2:E:41:LEU:HD22	1.98	0.46
1:A:40:ALA:HB1	1:A:93:VAL:CG2	2.45	0.46
1:D:52:MET:HB2	2:E:189:LEU:HD11	1.98	0.45
1:G:79:VAL:HG13	1:G:80:ALA:H	1.82	0.45
2:K:93:ARG:CD	2:K:111:VAL:HG11	2.47	0.45
2:H:99:PRO:O	2:H:100:GLN:CB	2.64	0.45
1:D:48:MET:HE1	1:G:37:LYS:HD3	1.99	0.45
3:C:68:THR:HG23	5:C:127:HOH:O	2.16	0.44
1:G:79:VAL:HG21	1:G:106:ARG:CZ	2.46	0.44
1:D:48:MET:HE3	1:D:107:SER:HB2	1.99	0.44
3:F:39:GLN:HG3	3:F:45:LEU:HD22	1.99	0.44
1:D:37:LYS:HE2	1:G:48:MET:HE1	1.99	0.44
1:J:51:VAL:HG11	1:J:76:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:20:LEU:HG	3:F:82:MET:HE2	2.00	0.44
1:A:49:ALA:HB1	2:B:189:LEU:CD1	2.47	0.44
3:C:90:THR:HG23	3:C:114:THR:HA	2.00	0.44
1:J:40:ALA:HB1	1:J:93:VAL:CG2	2.48	0.44
1:D:85:LEU:O	1:D:86:LEU:CB	2.66	0.44
2:B:98:ASN:HB2	5:B:200:HOH:O	2.18	0.43
1:D:58:LEU:HD21	1:D:89:PHE:HB3	1.98	0.43
1:G:94:ALA:HA	1:G:102:ILE:HD13	1.98	0.43
3:I:12:VAL:O	3:I:115:VAL:HG23	2.19	0.43
1:J:36:GLN:HG2	1:J:102:ILE:HD13	1.98	0.43
2:E:32:GLU:C	2:E:33:LEU:HD13	2.43	0.43
1:D:81:THR:HG23	1:D:82:THR:N	2.33	0.43
1:G:38:MET:HE1	2:H:44:LEU:HD23	2.00	0.43
1:D:60:ALA:HB2	1:D:78:PRO:HD2	2.01	0.42
3:I:60:THR:HG22	3:I:62:PRO:HD2	2.01	0.42
1:A:99:ALA:HB1	5:A:115:HOH:O	2.19	0.42
3:F:40:ALA:HB3	3:F:43:LYS:CE	2.49	0.42
3:C:45:LEU:HD23	3:C:104:TRP:CE2	2.55	0.42
1:A:35:GLU:CG	2:B:41:LEU:HD11	2.50	0.42
2:H:94:LEU:HD12	2:H:108:VAL:HG22	2.00	0.42
3:C:20:LEU:HD21	3:C:113:VAL:HG21	2.01	0.42
3:C:61:ALA:HB3	3:C:62:PRO:HD3	2.02	0.42
1:J:51:VAL:HG21	1:J:89:PHE:CZ	2.54	0.42
3:C:36:TRP:CG	3:C:80:LEU:HD22	2.55	0.41
2:K:44:LEU:HD21	2:K:184:ILE:CD1	2.50	0.41
2:H:65:THR:HG23	2:H:65:THR:O	2.20	0.41
1:D:48:MET:HG3	1:D:91:VAL:HG21	2.03	0.41
1:J:85:LEU:HD23	1:J:85:LEU:O	2.20	0.41
2:K:75:LEU:HD23	2:K:91:PHE:HB3	2.03	0.41
2:K:111:VAL:HG12	2:K:124:TRP:CD1	2.56	0.41
2:B:153:TYR:HB3	2:B:171:ALA:HB3	2.01	0.41
3:F:12:VAL:HG23	3:F:115:VAL:HG12	2.02	0.41
2:H:61:ARG:HD3	2:H:108:VAL:HG11	2.03	0.41
3:F:90:THR:HG23	3:F:114:THR:HA	2.03	0.41
2:H:77:TRP:CH2	2:H:87:LYS:HB3	2.55	0.41
1:A:60:ALA:HB2	1:A:78:PRO:HD2	2.03	0.41
2:H:48:LEU:HA	2:H:51:MET:HE2	2.03	0.41
3:L:6:GLU:OE1	3:L:6:GLU:N	2.54	0.41
1:G:38:MET:HE3	2:H:44:LEU:HD23	2.02	0.40
2:H:166:LEU:HD12	2:H:166:LEU:N	2.36	0.40
3:I:82:MET:HE1	3:I:113:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:LEU:HD22	3:C:22:CYS:SG	2.61	0.40
3:I:60:THR:HG22	3:I:62:PRO:HD3	2.03	0.40
3:L:47:TRP:O	3:L:60:THR:HG21	2.22	0.40
1:A:109:VAL:HG22	1:A:110:ALA:H	1.85	0.40
2:B:71:SER:OG	2:B:72:LYS:N	2.54	0.40
2:B:89:ILE:HG22	2:B:113:TYR:HB2	2.04	0.40
1:J:36:GLN:CG	1:J:102:ILE:HD13	2.51	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	70/84 (83%)	68 (97%)	2 (3%)	0	100	100
1	D	74/84 (88%)	69 (93%)	3 (4%)	2 (3%)	4	6
1	G	66/84 (79%)	61 (92%)	5 (8%)	0	100	100
1	J	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
2	B	156/164 (95%)	150 (96%)	6 (4%)	0	100	100
2	E	152/164 (93%)	148 (97%)	4 (3%)	0	100	100
2	H	153/164 (93%)	147 (96%)	5 (3%)	1 (1%)	18	36
2	K	147/164 (90%)	145 (99%)	2 (1%)	0	100	100
3	C	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
3	F	112/116 (97%)	108 (96%)	4 (4%)	0	100	100
3	I	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
3	L	105/116 (90%)	100 (95%)	5 (5%)	0	100	100
All	All	1341/1456 (92%)	1291 (96%)	47 (4%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	86	LEU
1	D	88	ALA
2	H	100	GLN

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	61/68 (90%)	59 (97%)	2 (3%)	33	59
1	D	64/68 (94%)	63 (98%)	1 (2%)	55	77
1	G	60/68 (88%)	56 (93%)	4 (7%)	15	31
1	J	66/68 (97%)	64 (97%)	2 (3%)	36	62
2	B	141/145 (97%)	139 (99%)	2 (1%)	59	79
2	E	140/145 (97%)	137 (98%)	3 (2%)	47	71
2	H	139/145 (96%)	137 (99%)	2 (1%)	59	79
2	K	136/145 (94%)	135 (99%)	1 (1%)	76	88
3	C	90/91 (99%)	89 (99%)	1 (1%)	65	83
3	F	89/91 (98%)	85 (96%)	4 (4%)	24	47
3	I	91/91 (100%)	89 (98%)	2 (2%)	45	70
3	L	84/91 (92%)	83 (99%)	1 (1%)	63	82
All	All	1161/1216 (96%)	1136 (98%)	25 (2%)	45	70

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	76	VAL
2	B	32	GLU
2	B	103	PHE
3	C	45	LEU
1	D	85	LEU
2	E	33	LEU
2	E	36	GLU

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Mol	Chain	Res	Type
2	E	149	ASN
3	F	13	GLN
3	F	63	VAL
3	F	69	ILE
3	F	114	THR
1	G	50	MET
1	G	62	ASN
1	G	79	VAL
1	G	102	ILE
2	H	68	GLU
2	H	184	ILE
3	I	69	ILE
3	I	114	THR
1	J	59	LYS
1	J	93	VAL
2	K	36	GLU
3	L	113	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	97	HIS
3	C	81	GLN
3	C	83	ASN
1	D	57	ASN
1	D	62	ASN
2	E	35	GLN
2	E	101	GLN
3	F	52	ASN
2	H	101	GLN
3	I	5	GLN
3	I	76	ASN
3	I	81	GLN
3	I	83	ASN
2	K	102	GLN

5.3.3 RNA ⓘ

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	76/84 (90%)	1.15	7 (9%) 14 12	62, 65, 73, 88	0
1	D	80/84 (95%)	1.19	11 (13%) 6 5	63, 65, 72, 74	0
1	G	74/84 (88%)	1.29	14 (18%) 3 2	61, 65, 75, 79	0
1	J	81/84 (96%)	1.08	13 (16%) 5 4	62, 65, 74, 79	0
2	B	160/164 (97%)	0.91	11 (6%) 23 19	62, 65, 75, 83	0
2	E	158/164 (96%)	0.69	9 (5%) 29 25	60, 65, 72, 84	0
2	H	157/164 (95%)	0.83	11 (7%) 22 19	36, 65, 74, 80	1 (0%)
2	K	153/164 (93%)	0.75	7 (4%) 37 33	61, 65, 69, 92	0
3	C	115/116 (99%)	0.93	9 (7%) 19 16	61, 65, 70, 85	0
3	F	114/116 (98%)	1.34	18 (15%) 5 4	6, 65, 71, 79	1 (0%)
3	I	116/116 (100%)	0.86	8 (6%) 23 19	58, 65, 73, 81	1 (0%)
3	L	109/116 (93%)	0.98	10 (9%) 14 12	62, 65, 71, 75	0
All	All	1393/1456 (95%)	0.96	128 (9%) 14 12	6, 65, 73, 92	3 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	16	GLY	15.7
2	H	149	ASN	5.7
1	G	80	ALA	4.3
1	J	32	GLY	4.0
1	D	32	GLY	4.0
1	G	108	TYR	4.0
3	I	115	VAL	3.8
3	L	85	LEU	3.7
3	C	116	SER	3.6
1	J	84	PRO	3.6
3	F	114	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	57	ASN	3.5
1	J	85	LEU	3.5
1	D	34	LEU	3.5
2	B	103	PHE	3.5
3	L	11	LEU	3.4
3	F	111	THR	3.3
1	D	95	ALA	3.3
1	A	63	GLY	3.3
1	D	63	GLY	3.2
3	L	110	GLY	3.2
2	K	65	THR	3.1
3	F	96	ALA	3.0
3	L	113	VAL	3.0
3	F	110	GLY	3.0
2	B	99	PRO	3.0
2	E	66	ASN	3.0
2	E	160	ASN	3.0
3	F	10	GLY	3.0
2	B	66	ASN	3.0
2	B	67	GLY	3.0
3	F	85	LEU	2.9
3	I	113	VAL	2.9
2	H	67	GLY	2.9
1	G	28	ILE	2.9
2	H	99	PRO	2.9
1	J	31	VAL	2.8
2	E	104	PRO	2.8
1	G	40	ALA	2.8
3	L	40	ALA	2.8
1	A	49	ALA	2.7
2	H	172	ILE	2.7
1	G	72	TRP	2.7
1	G	49	ALA	2.7
3	L	111	THR	2.7
1	J	28	ILE	2.7
3	C	17	SER	2.7
3	F	115	VAL	2.7
2	H	66	ASN	2.7
3	F	33	ALA	2.7
3	F	40	ALA	2.7
3	I	114	THR	2.7
1	G	29	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	60	ALA	2.6
3	C	112	GLN	2.6
2	K	106	GLY	2.6
3	I	1	GLN	2.6
1	G	96	GLU	2.5
1	A	40	ALA	2.5
1	A	58	LEU	2.5
3	F	37	VAL	2.5
3	L	33	ALA	2.5
3	F	109	GLN	2.5
2	E	65	THR	2.5
1	J	58	LEU	2.4
2	B	96	TRP	2.4
1	D	104	THR	2.4
1	J	69	GLY	2.4
1	G	86	LEU	2.4
2	K	102	GLN	2.4
2	K	103	PHE	2.4
3	F	58	SER	2.4
3	C	110	GLY	2.4
3	F	45	LEU	2.4
3	F	99	LEU	2.4
2	K	160	ASN	2.4
3	F	61	ALA	2.4
3	L	87	PRO	2.4
1	J	107	SER	2.4
2	B	71	SER	2.4
3	I	108	GLY	2.4
1	J	51	VAL	2.4
1	D	60	ALA	2.3
1	D	86	LEU	2.3
2	E	167	THR	2.3
1	J	98	GLN	2.3
1	D	109	VAL	2.3
1	J	43	VAL	2.3
3	L	96	ALA	2.2
3	C	108	GLY	2.2
2	B	98	ASN	2.2
3	C	91	ALA	2.2
1	G	70	GLN	2.2
2	E	59	ALA	2.2
1	J	52	MET	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	13	GLN	2.2
2	B	65	THR	2.2
2	H	60	LEU	2.2
1	G	31	VAL	2.1
2	E	95	GLY	2.1
3	I	11	LEU	2.1
2	B	105	ARG	2.1
2	H	100	GLN	2.1
2	E	39	ALA	2.1
1	J	53	LEU	2.1
3	I	116	SER	2.1
1	D	51	VAL	2.1
3	L	100	GLY	2.1
1	G	73	TYR	2.1
2	B	83	ASP	2.1
2	B	97	HIS	2.1
2	K	111	VAL	2.1
3	C	113	VAL	2.1
2	H	171	ALA	2.1
1	G	66	GLU	2.1
1	D	40	ALA	2.0
2	H	93	ARG	2.0
2	E	33	LEU	2.0
2	H	96	TRP	2.0
3	F	100	GLY	2.0
1	D	33	TYR	2.0
2	K	70	PRO	2.0
1	A	93	VAL	2.0
1	A	109	VAL	2.0
2	H	92	ALA	2.0
3	I	52	ASN	2.0
3	C	60	THR	2.0
3	C	41	PRO	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(Å ²)	Q<0.9
4	CL	E	1	1/1	0.96	0.07	43,43,43,43	0
4	CL	H	1	1/1	0.96	0.09	48,48,48,48	0
4	CL	K	1	1/1	0.96	0.08	45,45,45,45	0
4	CL	B	1	1/1	0.98	0.06	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.