



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 08:55 PM EDT

PDB ID : 2X7A  
Title : Structural basis of HIV-1 tethering to membranes by the Bst2-tetherin ectodomain  
Authors : Natrajan, G.; McCarthy, A.A.; Weissenhorn, W.  
Deposited on : 2010-02-25  
Resolution : 2.77 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

<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>.

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

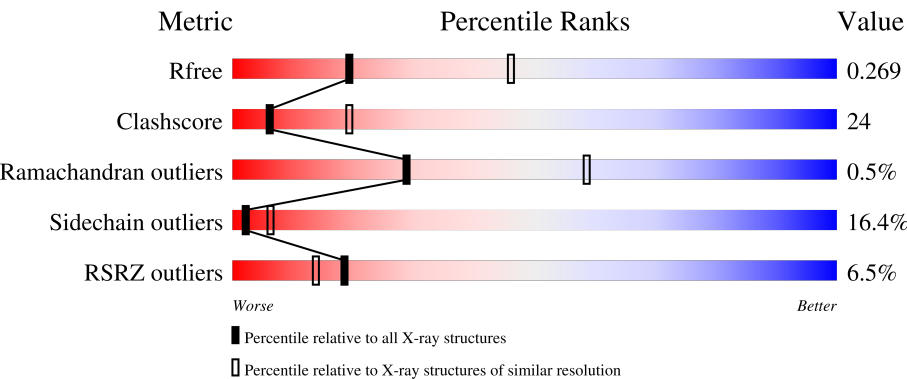
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

# 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 2.77 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))
$R_{free}$	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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  $\geq 3$ , 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	61	
1	B	61	
1	C	61	
1	D	61	
1	E	61	

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Mol	Chain	Length	Quality of chain
1	F	61	
1	G	61	
1	H	61	
1	I	61	
1	J	61	
1	K	61	

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	CL	F	1149	-	-	-	X
3	CL	H	1145	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4673 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 BONE MARROW STROMAL ANTIGEN 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	59	Total	C	N	O	S	Se	0	0	0
			446	270	80	93	1	2			
1	B	59	Total	C	N	O	S	Se	0	0	0
			450	271	83	93	1	2			
1	C	48	Total	C	N	O	S	Se	0	0	0
			363	219	64	77	1	2			
1	D	56	Total	C	N	O	S	Se	0	0	0
			410	248	73	86	1	2			
1	E	59	Total	C	N	O	S	Se	0	0	0
			452	273	83	93	1	2			
1	F	59	Total	C	N	O	S	Se	0	0	0
			452	273	83	93	1	2			
1	G	54	Total	C	N	O	S	Se	0	0	0
			412	248	76	85	1	2			
1	H	54	Total	C	N	O	S	Se	0	0	0
			409	246	74	86	1	2			
1	I	59	Total	C	N	O	S	Se	0	0	0
			458	276	86	93	1	2			
1	J	59	Total	C	N	O	S	Se	0	0	0
			458	276	86	93	1	2			
1	K	39	Total	C	N	O	S	Se	0	0	0
			282	171	48	60	1	2			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

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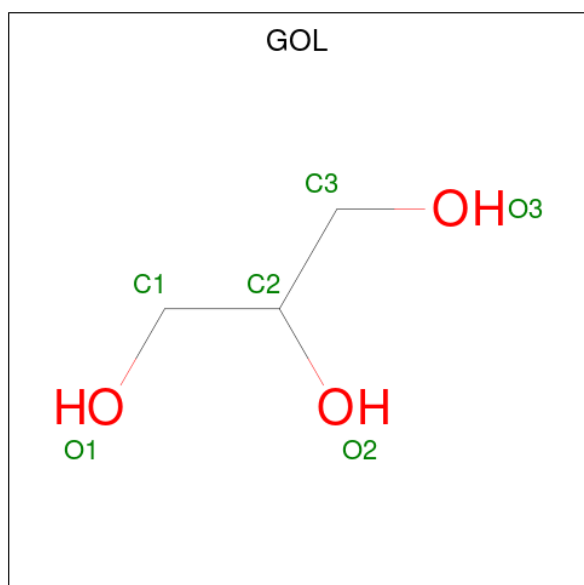
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Na	0	0
			1	1		
2	H	1	Total	Na	0	0
			1	1		
2	I	1	Total	Na	0	0
			1	1		
2	J	1	Total	Na	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	G	2	Total	Cl	0	0
			2	2		
3	H	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

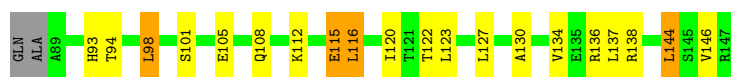
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		
6	B	8	Total	O	0	0
			8	8		
6	C	2	Total	O	0	0
			2	2		
6	D	7	Total	O	0	0
			7	7		
6	E	5	Total	O	0	0
			5	5		
6	F	8	Total	O	0	0
			8	8		
6	G	9	Total	O	0	0
			9	9		
6	H	5	Total	O	0	0
			5	5		
6	I	6	Total	O	0	0
			6	6		
6	J	4	Total	O	0	0
			4	4		
6	K	3	Total	O	0	0
			3	3		

### 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.

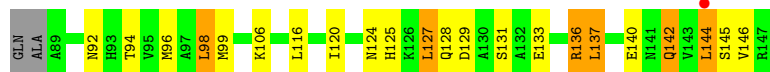
#### • Molecule 1: BONE MARROW STROMAL ANTIGEN 2

Chain A: 



#### • Molecule 1: BONE MARROW STROMAL ANTIGEN 2

Chain B: 



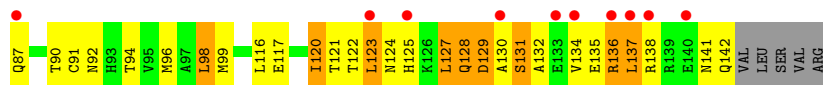
#### • Molecule 1: BONE MARROW STROMAL ANTIGEN 2

Chain C: 



#### • Molecule 1: BONE MARROW STROMAL ANTIGEN 2

Chain D: 



#### • Molecule 1: BONE MARROW STROMAL ANTIGEN 2

Chain E: 



#### • Molecule 1: BONE MARROW STROMAL ANTIGEN 2



- Molecule 1: BONE MARROW STROMAL ANTIGEN 2



- Molecule 1: BONE MARROW STROMAL ANTIGEN 2



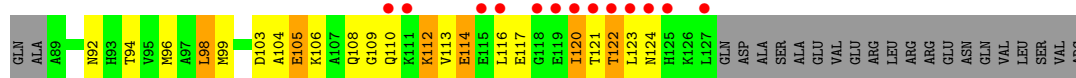
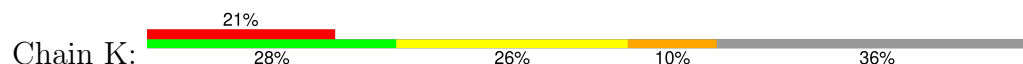
- Molecule 1: BONE MARROW STROMAL ANTIGEN 2



- Molecule 1: BONE MARROW STROMAL ANTIGEN 2



- Molecule 1: BONE MARROW STROMAL ANTIGEN 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.89Å 85.93Å 123.31Å 90.00° 126.94° 90.00°	Depositor
Resolution (Å)	44.88 – 2.77 44.88 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.88-2.77) 94.4 (44.88-2.65)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.236 , 0.273 0.231 , 0.269	Depositor DCC
$R_{free}$ test set	1968 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.8	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 69.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% 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, 0.333 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, NA, GOL, MG

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	0.46	0/445	0.57	0/595
1	B	0.47	0/448	0.61	0/596
1	C	0.50	0/362	0.62	0/482
1	D	0.44	0/409	0.59	0/547
1	E	0.64	1/451 (0.2%)	0.69	0/602
1	F	0.51	0/451	0.64	0/602
1	G	0.53	0/410	0.66	0/544
1	H	0.56	0/407	0.60	0/541
1	I	0.54	0/457	0.63	0/609
1	J	0.50	0/455	0.64	0/603
1	K	0.47	0/280	0.58	0/373
All	All	0.52	1/4575 (0.0%)	0.62	0/6094

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	GLU	CD-OE2	7.51	1.33	1.25

There are no bond angle outliers.

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	446	0	440	23	0
1	B	450	0	443	25	0
1	C	363	0	358	42	0
1	D	410	0	392	55	0
1	E	452	0	454	22	0
1	F	452	0	451	28	0
1	G	412	0	407	26	0
1	H	409	0	397	30	1
1	I	458	0	462	20	0
1	J	458	0	460	23	1
1	K	282	0	273	16	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	1	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
4	G	6	0	8	0	0
5	I	1	0	0	0	0
6	A	3	0	0	1	0
6	B	8	0	0	0	0
6	C	2	0	0	1	0
6	D	7	0	0	3	0
6	E	5	0	0	0	0
6	F	8	0	0	1	0
6	G	9	0	0	0	0
6	H	5	0	0	0	0
6	I	6	0	0	3	0
6	J	4	0	0	0	0
6	K	3	0	0	0	0
All	All	4673	0	4545	224	1

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 24.

All (224) 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:H:136:ARG:HG3	1:H:136:ARG:HH11	1.17	1.04
1:C:127:LEU:HD21	1:D:127:LEU:HB2	1.39	1.04
1:C:134:VAL:HG22	1:D:134:VAL:HG11	1.36	1.03
1:J:144:LEU:C	1:J:145:SER:N	2.15	0.99
1:F:99:MSE:HE2	1:H:94:THR:HG21	1.48	0.96
1:C:123:LEU:HD23	1:D:123:LEU:HD11	1.50	0.94
1:C:90:THR:HG22	1:E:103:ASP:OD1	1.70	0.92
1:D:125:HIS:O	1:D:129:ASP:HB3	1.67	0.92
1:C:94:THR:HG21	1:E:99:MSE:HE2	1.51	0.91
1:C:94:THR:HG21	1:E:99:MSE:CE	2.03	0.88
1:J:146:VAL:C	1:J:147:ARG:N	2.30	0.84
1:C:99:MSE:HE2	1:J:90:THR:HG22	1.57	0.83
1:G:136:ARG:HH11	1:G:136:ARG:HG2	1.41	0.82
1:C:95:VAL:O	1:C:99:MSE:HG3	1.80	0.82
1:F:99:MSE:CE	1:H:94:THR:HG21	2.09	0.81
1:G:136:ARG:HH11	1:G:136:ARG:CG	1.93	0.81
1:C:99:MSE:HE1	1:J:94:THR:HB	1.62	0.80
1:D:92:ASN:HB3	1:E:96:MSE:HE2	1.64	0.79
1:D:99:MSE:HE2	1:F:94:THR:CB	2.13	0.79
1:D:99:MSE:CE	1:F:94:THR:HG21	2.14	0.77
1:D:99:MSE:HG2	1:F:90:THR:HG22	1.66	0.77
1:A:94:THR:OG1	1:H:99:MSE:HE2	1.85	0.76
1:E:94:THR:HG21	1:G:99:MSE:CE	2.16	0.76
1:H:136:ARG:HG3	1:H:136:ARG:NH1	1.97	0.76
1:K:109:GLY:O	1:K:113:VAL:HG23	1.87	0.74
1:H:138:ARG:HG2	1:H:139:ARG:N	2.03	0.74
1:C:90:THR:CG2	1:E:103:ASP:OD1	2.35	0.74
1:D:99:MSE:HE2	1:F:94:THR:OG1	1.88	0.74
1:D:127:LEU:O	1:D:131:SER:HB3	1.87	0.74
1:E:94:THR:HG21	1:G:99:MSE:HE1	1.70	0.72
1:A:144:LEU:HD22	1:B:144:LEU:HB3	1.73	0.71
1:G:95:VAL:HG13	1:G:99:MSE:HE3	1.70	0.71
1:B:99:MSE:CE	1:G:94:THR:HG21	2.21	0.71
1:D:94:THR:HG21	1:I:99:MSE:CE	2.21	0.70
1:H:136:ARG:HH11	1:H:136:ARG:CG	1.99	0.70
1:C:99:MSE:HE1	1:J:94:THR:CB	2.22	0.70
1:B:92:ASN:O	1:B:96:MSE:HG2	1.91	0.70
1:K:105:GLU:HG3	1:K:105:GLU:O	1.92	0.68
1:C:109:GLY:HA2	1:C:112:LYS:HE2	1.76	0.68
1:E:140:GLU:HG2	1:F:141:ASN:ND2	2.08	0.68
1:C:128:GLN:HA	1:C:128:GLN:NE2	2.08	0.68
1:A:144:LEU:CD2	1:B:144:LEU:HB3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LEU:HD12	1:D:124:ASN:N	2.09	0.67
1:I:112:LYS:O	1:I:116:LEU:HD22	1.94	0.67
1:K:117:GLU:O	1:K:121:THR:HG23	1.95	0.66
1:H:136:ARG:HD2	1:H:136:ARG:C	2.16	0.66
1:C:108:GLN:HE21	1:C:112:LYS:HZ2	1.42	0.65
1:D:123:LEU:HD12	1:D:123:LEU:C	2.16	0.65
1:D:117:GLU:C	6:D:2007:HOH:O	2.34	0.64
1:D:128:GLN:O	1:D:132:ALA:HB3	1.96	0.64
1:D:136:ARG:HA	1:D:136:ARG:CZ	2.26	0.64
1:I:134:VAL:HG23	1:J:134:VAL:HG23	1.78	0.64
1:J:96:MSE:HE3	1:K:92:ASN:OD1	1.98	0.64
1:G:136:ARG:HG2	1:G:136:ARG:NH1	2.07	0.63
1:B:142:GLN:O	1:B:145:SER:HB3	1.99	0.62
1:C:94:THR:CG2	1:E:99:MSE:HE2	2.27	0.61
1:J:146:VAL:O	1:J:147:ARG:HA	2.01	0.60
1:D:136:ARG:HA	1:D:136:ARG:NH1	2.16	0.60
1:I:94:THR:HG21	6:I:2003:HOH:O	2.02	0.60
1:C:123:LEU:CD2	1:D:123:LEU:HD11	2.30	0.59
1:D:120:ILE:HG22	1:D:121:THR:N	2.18	0.59
1:I:116:LEU:HD22	1:I:116:LEU:H	1.67	0.59
1:A:105:GLU:CG	1:B:106:LYS:HE2	2.33	0.59
1:A:94:THR:HG21	1:H:99:MSE:CE	2.33	0.58
1:C:125:HIS:HB2	6:C:2002:HOH:O	2.01	0.58
1:D:120:ILE:N	6:D:2007:HOH:O	2.36	0.58
1:C:116:LEU:O	1:C:120:ILE:HG12	2.04	0.58
1:F:92:ASN:ND2	1:G:96:MSE:HE3	2.18	0.58
1:H:110:GLN:HA	1:H:110:GLN:NE2	2.17	0.58
1:H:136:ARG:HE	1:H:137:LEU:HD23	1.68	0.58
1:B:99:MSE:HE2	1:G:94:THR:OG1	2.04	0.58
1:F:142:GLN:NE2	1:F:142:GLN:HA	2.19	0.58
1:J:124:ASN:O	1:J:128:GLN:HG3	2.04	0.58
1:G:134:VAL:HG23	1:H:134:VAL:HG23	1.85	0.57
1:D:130:ALA:O	1:D:134:VAL:N	2.33	0.57
1:K:112:LYS:O	1:K:116:LEU:HG	2.05	0.57
1:B:142:GLN:HA	1:B:142:GLN:OE1	2.04	0.56
1:H:136:ARG:HD3	1:H:140:GLU:OE2	2.04	0.56
1:E:102:LEU:HD13	1:F:102:LEU:HD13	1.86	0.56
1:D:94:THR:CB	1:I:99:MSE:HE2	2.35	0.56
1:E:94:THR:HG21	1:G:99:MSE:HE2	1.87	0.56
1:H:136:ARG:HE	1:H:137:LEU:CD2	2.18	0.56
1:C:94:THR:HG21	1:E:99:MSE:HE1	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:94:THR:HG22	1:I:98:LEU:HD22	1.87	0.56
1:D:127:LEU:HD23	1:D:128:GLN:N	2.21	0.56
1:H:127:LEU:O	1:H:131:SER:HB2	2.05	0.55
1:A:120:ILE:HG13	1:B:120:ILE:HD11	1.87	0.55
1:A:94:THR:HG21	1:H:99:MSE:HE1	1.89	0.55
1:F:94:THR:HG22	1:F:98:LEU:HD22	1.89	0.55
1:D:121:THR:N	6:D:2007:HOH:O	2.39	0.54
1:C:127:LEU:HD21	1:D:127:LEU:CB	2.23	0.54
1:D:99:MSE:HE1	1:F:94:THR:HG21	1.88	0.54
1:C:123:LEU:HB3	1:D:123:LEU:HD13	1.90	0.54
1:E:110:GLN:HA	1:E:110:GLN:NE2	2.23	0.54
1:A:127:LEU:HA	1:B:127:LEU:HD23	1.90	0.54
1:B:99:MSE:HE2	1:G:94:THR:HG21	1.90	0.54
1:C:123:LEU:HB3	1:D:123:LEU:CD1	2.38	0.54
1:D:94:THR:HG21	1:I:99:MSE:HE2	1.89	0.54
1:B:133:GLU:O	1:B:137:LEU:HB2	2.07	0.54
1:A:94:THR:HG22	1:A:98:LEU:HD22	1.89	0.54
1:H:136:ARG:NH1	1:H:136:ARG:CG	2.64	0.53
1:F:94:THR:HG22	1:F:98:LEU:CD2	2.38	0.53
1:G:108:GLN:HG3	1:G:109:GLY:N	2.24	0.53
1:I:145:SER:O	1:I:146:VAL:HG22	2.09	0.53
1:F:96:MSE:HE3	1:G:92:ASN:ND2	2.24	0.53
1:I:116:LEU:H	1:I:116:LEU:CD2	2.21	0.53
1:F:99:MSE:HE2	1:H:94:THR:CG2	2.30	0.53
1:A:93:HIS:HB3	6:A:2001:HOH:O	2.07	0.52
1:F:89:ALA:N	6:F:2001:HOH:O	2.41	0.52
1:B:94:THR:HG22	1:B:98:LEU:HD22	1.92	0.52
1:C:111:LYS:CG	1:C:112:LYS:N	2.74	0.51
1:G:132:ALA:O	1:G:135:GLU:HG2	2.11	0.51
1:G:134:VAL:HG12	1:G:135:GLU:N	2.25	0.51
6:I:2003:HOH:O	1:J:95:VAL:HG11	2.10	0.51
1:D:99:MSE:CE	1:F:94:THR:CB	2.87	0.51
1:K:121:THR:C	1:K:123:LEU:H	2.14	0.51
1:C:108:GLN:HE21	1:C:112:LYS:NZ	2.07	0.50
1:C:116:LEU:HD12	1:D:116:LEU:HB2	1.92	0.50
1:D:91:CYS:HB2	6:I:2005:HOH:O	2.11	0.50
1:I:136:ARG:HA	1:I:139:ARG:HG2	1.93	0.50
1:A:94:THR:CB	1:H:99:MSE:CE	2.89	0.50
1:D:99:MSE:CE	1:F:94:THR:CG2	2.87	0.50
1:J:114:GLU:HA	1:J:117:GLU:CG	2.42	0.50
1:A:94:THR:CB	1:H:99:MSE:HE2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:MSE:HE2	1:G:94:THR:CB	2.42	0.50
1:B:99:MSE:HE1	1:G:94:THR:HG21	1.92	0.50
1:D:137:LEU:HD23	1:D:138:ARG:N	2.26	0.50
1:D:94:THR:OG1	1:I:99:MSE:HE2	2.12	0.49
1:D:94:THR:HG22	1:D:98:LEU:CD2	2.42	0.49
1:J:114:GLU:HA	1:J:117:GLU:HG2	1.94	0.49
1:C:102:LEU:HG	1:C:106:LYS:HE3	1.95	0.49
1:D:96:MSE:SE	1:E:96:MSE:HE3	2.63	0.49
1:D:137:LEU:HD23	1:D:137:LEU:C	2.34	0.49
1:C:127:LEU:N	1:C:127:LEU:HD23	2.27	0.48
1:D:87:GLN:O	1:D:87:GLN:HG3	2.12	0.48
1:C:99:MSE:CE	1:J:91:CYS:HA	2.44	0.48
1:K:103:ASP:O	1:K:106:LYS:HB2	2.14	0.48
1:F:99:MSE:HG2	1:H:90:THR:HG22	1.96	0.47
1:B:116:LEU:O	1:B:120:ILE:HG12	2.14	0.47
1:G:102:LEU:HD13	1:H:102:LEU:HA	1.96	0.47
1:H:135:GLU:O	1:H:138:ARG:HG2	2.14	0.47
1:H:125:HIS:O	1:H:128:GLN:HG2	2.14	0.47
1:J:111:LYS:O	1:J:115:GLU:HB3	2.15	0.47
1:D:123:LEU:O	1:D:127:LEU:N	2.43	0.47
1:F:102:LEU:HD12	1:F:102:LEU:O	2.15	0.47
1:G:95:VAL:CG1	1:G:99:MSE:HE3	2.42	0.47
1:A:105:GLU:HG3	1:B:106:LYS:HE2	1.95	0.46
1:B:96:MSE:HA	1:B:96:MSE:HE2	1.96	0.46
1:D:131:SER:O	1:D:135:GLU:CB	2.63	0.46
1:K:112:LYS:HD3	1:K:113:VAL:CG2	2.46	0.46
1:F:89:ALA:HB2	3:F:1149:CL:CL	2.53	0.46
1:I:142:GLN:O	1:I:145:SER:HB2	2.15	0.46
1:C:129:ASP:OD2	1:C:130:ALA:N	2.49	0.46
1:G:127:LEU:HD13	1:H:127:LEU:HA	1.97	0.46
1:H:122:THR:HG22	1:H:126:LYS:HE3	1.98	0.45
1:K:120:ILE:O	1:K:123:LEU:HG	2.15	0.45
1:C:113:VAL:HG12	1:C:114:GLU:N	2.30	0.45
1:H:137:LEU:O	1:H:138:ARG:C	2.55	0.45
1:D:99:MSE:HE2	1:F:94:THR:HB	1.97	0.45
1:K:104:ALA:C	1:K:106:LYS:N	2.70	0.45
1:I:146:VAL:HG23	1:I:146:VAL:O	2.17	0.44
1:K:110:GLN:O	1:K:114:GLU:HB2	2.17	0.44
1:E:137:LEU:HB3	1:F:137:LEU:HD13	2.00	0.44
1:A:123:LEU:HD21	1:B:124:ASN:OD1	2.17	0.44
1:A:136:ARG:HG3	1:A:137:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLN:NE2	1:C:112:LYS:NZ	2.65	0.44
1:D:90:THR:HG22	1:I:99:MSE:HG2	2.00	0.44
1:E:137:LEU:HB3	1:F:137:LEU:HB3	1.98	0.44
1:D:120:ILE:O	1:D:123:LEU:N	2.50	0.44
1:B:125:HIS:CE1	1:B:129:ASP:OD2	2.71	0.44
1:D:129:ASP:OD2	1:D:129:ASP:C	2.55	0.44
1:C:99:MSE:CE	1:J:94:THR:OG1	2.66	0.43
1:E:130:ALA:O	1:E:134:VAL:HG23	2.18	0.43
1:C:90:THR:HG21	1:E:102:LEU:HB3	2.00	0.43
1:D:131:SER:O	1:D:135:GLU:HB3	2.18	0.43
1:I:139:ARG:O	1:I:143:VAL:HG13	2.18	0.43
1:J:146:VAL:C	1:J:147:ARG:CA	2.86	0.43
1:C:99:MSE:CE	1:J:94:THR:CB	2.95	0.43
1:C:123:LEU:HB2	1:D:123:LEU:HD21	2.01	0.43
1:D:94:THR:CG2	1:I:99:MSE:HE2	2.48	0.43
1:C:134:VAL:HG22	1:D:134:VAL:CG1	2.26	0.43
1:C:120:ILE:CD1	1:D:120:ILE:HG13	2.48	0.43
1:J:144:LEU:C	1:J:145:SER:CA	2.86	0.43
1:D:141:ASN:O	1:D:142:GLN:C	2.57	0.43
1:A:130:ALA:O	1:A:134:VAL:HG23	2.18	0.42
1:D:123:LEU:C	1:D:123:LEU:CD1	2.87	0.42
1:I:116:LEU:CD2	1:I:116:LEU:N	2.82	0.42
1:J:106:LYS:HE3	1:J:106:LYS:HB2	1.84	0.42
1:C:111:LYS:HG3	1:C:112:LYS:N	2.33	0.42
1:F:99:MSE:HA	1:H:90:THR:HG21	2.01	0.42
1:J:123:LEU:HD12	1:J:123:LEU:HA	1.81	0.42
1:C:120:ILE:O	1:C:124:ASN:HB2	2.20	0.42
1:A:136:ARG:HG3	1:A:137:LEU:H	1.85	0.42
1:A:146:VAL:HG23	1:A:146:VAL:O	2.20	0.42
1:I:144:LEU:HB3	1:J:144:LEU:HB3	2.01	0.42
1:A:116:LEU:HA	1:A:116:LEU:HD12	1.77	0.42
1:H:135:GLU:OE2	1:H:138:ARG:NH1	2.48	0.41
1:A:115:GLU:HG2	1:A:116:LEU:HD13	2.02	0.41
1:D:125:HIS:O	1:D:129:ASP:CB	2.55	0.41
1:E:88:ALA:HA	1:G:103:ASP:OD2	2.20	0.41
1:E:140:GLU:HG2	1:F:141:ASN:HD21	1.82	0.41
1:G:136:ARG:NH1	1:G:137:LEU:HD23	2.35	0.41
1:B:99:MSE:HE2	1:G:94:THR:CG2	2.50	0.41
1:F:95:VAL:CG1	1:F:99:MSE:HE3	2.50	0.41
1:K:96:MSE:HA	1:K:99:MSE:HE2	2.02	0.41
1:G:95:VAL:HG23	1:H:95:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ASP:OD2	1:C:129:ASP:C	2.59	0.41
1:K:104:ALA:O	1:K:106:LYS:N	2.53	0.41
1:B:136:ARG:O	1:B:137:LEU:C	2.59	0.41
1:C:123:LEU:O	1:C:126:LYS:HB2	2.21	0.41
1:I:137:LEU:HB3	1:J:137:LEU:HB3	2.02	0.41
1:K:94:THR:HG22	1:K:98:LEU:HD22	2.03	0.41
1:A:138:ARG:NH2	1:B:133:GLU:OE1	2.53	0.41
1:F:127:LEU:HA	1:F:127:LEU:HD12	1.78	0.40
1:G:116:LEU:HD12	1:G:116:LEU:HA	1.84	0.40
1:J:147:ARG:HH11	1:J:147:ARG:HB2	1.85	0.40
1:K:122:THR:C	1:K:124:ASN:H	2.24	0.40
1:A:144:LEU:HD23	1:B:144:LEU:HB3	2.00	0.40
1:C:115:GLU:O	1:C:116:LEU:C	2.58	0.40
1:E:116:LEU:HD12	1:E:116:LEU:HA	1.76	0.40
1:A:105:GLU:CD	1:B:106:LYS:HE2	2.42	0.40
1:D:96:MSE:SE	1:E:96:MSE:CE	3.20	0.40
1:D:129:ASP:O	1:D:131:SER:N	2.53	0.40
1:K:121:THR:C	1:K:123:LEU:N	2.74	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:GLU:OE1	1:J:147:ARG:NH1[4_657]	2.07	0.13

## 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	57/61 (93%)	55 (96%)	2 (4%)	0	100	100
1	B	55/61 (90%)	51 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	46/61 (75%)	43 (94%)	3 (6%)	0	100	100
1	D	54/61 (88%)	49 (91%)	4 (7%)	1 (2%)	8	23
1	E	57/61 (93%)	57 (100%)	0	0	100	100
1	F	57/61 (93%)	57 (100%)	0	0	100	100
1	G	50/61 (82%)	49 (98%)	1 (2%)	0	100	100
1	H	50/61 (82%)	47 (94%)	3 (6%)	0	100	100
1	I	57/61 (93%)	56 (98%)	0	1 (2%)	8	25
1	J	54/61 (88%)	52 (96%)	2 (4%)	0	100	100
1	K	37/61 (61%)	33 (89%)	3 (8%)	1 (3%)	5	15
All	All	574/671 (86%)	549 (96%)	22 (4%)	3 (0%)	29	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	120	ILE
1	K	122	THR
1	I	146	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	48/49 (98%)	40 (83%)	8 (17%)	2	6
1	B	48/49 (98%)	38 (79%)	10 (21%)	1	3
1	C	39/49 (80%)	34 (87%)	5 (13%)	4	12
1	D	41/49 (84%)	32 (78%)	9 (22%)	1	2
1	E	49/49 (100%)	38 (78%)	11 (22%)	1	2
1	F	49/49 (100%)	43 (88%)	6 (12%)	5	13
1	G	43/49 (88%)	38 (88%)	5 (12%)	5	15
1	H	43/49 (88%)	36 (84%)	7 (16%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	50/49 (102%)	44 (88%)	6 (12%)	5	14
1	J	50/49 (102%)	43 (86%)	7 (14%)	3	9
1	K	29/49 (59%)	23 (79%)	6 (21%)	1	3
All	All	489/539 (91%)	409 (84%)	80 (16%)	2	6

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LEU
1	A	101	SER
1	A	108	GLN
1	A	112	LYS
1	A	115	GLU
1	A	116	LEU
1	A	122	THR
1	A	144	LEU
1	B	98	LEU
1	B	127	LEU
1	B	128	GLN
1	B	131	SER
1	B	136	ARG
1	B	137	LEU
1	B	140	GLU
1	B	142	GLN
1	B	144	LEU
1	B	146	VAL
1	C	90	THR
1	C	110	GLN
1	C	113	VAL
1	C	116	LEU
1	C	123	LEU
1	D	98	LEU
1	D	122	THR
1	D	123	LEU
1	D	127	LEU
1	D	128	GLN
1	D	129	ASP
1	D	131	SER
1	D	136	ARG
1	D	137	LEU
1	E	98	LEU

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Mol	Chain	Res	Type
1	E	101	SER
1	E	112	LYS
1	E	116	LEU
1	E	121	THR
1	E	126	LYS
1	E	127	LEU
1	E	128	GLN
1	E	137	LEU
1	E	142	GLN
1	E	144	LEU
1	F	98	LEU
1	F	102	LEU
1	F	116	LEU
1	F	123	LEU
1	F	135	GLU
1	F	143	VAL
1	G	108	GLN
1	G	116	LEU
1	G	123	LEU
1	G	131	SER
1	G	136	ARG
1	H	101	SER
1	H	108	GLN
1	H	111	LYS
1	H	116	LEU
1	H	131	SER
1	H	136	ARG
1	H	141	ASN
1	I	98	LEU
1	I	108	GLN
1	I	116	LEU
1	I	123	LEU
1	I	124	ASN
1	I	137	LEU
1	J	98	LEU
1	J	108	GLN
1	J	115	GLU
1	J	123	LEU
1	J	136	ARG
1	J	137	LEU
1	J	147	ARG
1	K	98	LEU

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Mol	Chain	Res	Type
1	K	105	GLU
1	K	108	GLN
1	K	112	LYS
1	K	114	GLU
1	K	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	HIS
1	C	108	GLN
1	C	128	GLN
1	D	92	ASN
1	F	142	GLN
1	H	110	GLN
1	H	141	ASN
1	I	124	ASN
1	J	92	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 15 are monoatomic - leaving 1 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	$\# Z  > 2$
4	GOL	G	1142	-	5,5,5	0.35	0	5,5,5	0.64	0

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
4	GOL	G	1142	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1142	GOL	O1-C1-C2-C3
4	G	1142	GOL	O1-C1-C2-O2

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	J	2
1	H	1
1	G	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	138:ARG	C	139:ARG	N	2.85
1	G	138:ARG	C	139:ARG	N	2.82
1	B	142:GLN	C	143:VAL	N	2.78
1	J	146:VAL	C	147:ARG	N	2.30
1	J	144:LEU	C	145:SER	N	2.15

## 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	57/61 (93%)	0.19	0 100 100	33, 92, 134, 139	0
1	B	57/61 (93%)	0.36	1 (1%) 68 65	33, 86, 141, 177	0
1	C	46/61 (75%)	0.77	5 (10%) 5 4	37, 106, 204, 263	0
1	D	54/61 (88%)	0.88	10 (18%) 1 1	39, 105, 250, 260	0
1	E	57/61 (93%)	0.55	2 (3%) 44 38	35, 63, 100, 136	0
1	F	57/61 (93%)	0.49	1 (1%) 68 65	33, 64, 131, 191	0
1	G	52/61 (85%)	0.51	2 (3%) 40 35	29, 63, 156, 227	0
1	H	52/61 (85%)	0.66	3 (5%) 23 18	36, 77, 158, 196	0
1	I	57/61 (93%)	0.25	0 100 100	35, 74, 131, 149	0
1	J	57/61 (93%)	0.27	1 (1%) 68 65	36, 82, 113, 146	0
1	K	37/61 (60%)	2.06	13 (35%) 0 0	41, 141, 257, 285	0
All	All	583/671 (86%)	0.58	38 (6%) 18 14	29, 78, 187, 285	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	123	LEU	9.6
1	C	134	VAL	7.6
1	K	122	THR	6.0
1	K	121	THR	5.7
1	K	119	GLU	5.4
1	K	125	HIS	5.0
1	D	133	GLU	4.6
1	K	124	ASN	4.0
1	D	125	HIS	3.8
1	K	120	ILE	3.7
1	G	88	ALA	3.6
1	C	112	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	110	GLN	3.2
1	C	127	LEU	3.2
1	D	140	GLU	3.1
1	H	123	LEU	3.0
1	D	130	ALA	3.0
1	G	139	ARG	3.0
1	E	146	VAL	3.0
1	K	111	LYS	2.9
1	K	115	GLU	2.7
1	K	116	LEU	2.7
1	C	135	GLU	2.6
1	D	136	ARG	2.6
1	D	137	LEU	2.5
1	B	144	LEU	2.4
1	D	134	VAL	2.4
1	D	138	ARG	2.4
1	F	146	VAL	2.4
1	K	127	LEU	2.4
1	J	146	VAL	2.4
1	D	123	LEU	2.3
1	C	128	GLN	2.3
1	H	141	ASN	2.2
1	E	98	LEU	2.2
1	K	118	GLY	2.1
1	D	87	GLN	2.0
1	H	134	VAL	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 monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	F	1149	1/1	0.09	0.45	162,162,162,162	0
3	CL	H	1145	1/1	0.55	0.49	97,97,97,97	0
4	GOL	G	1142	6/6	0.60	0.26	107,107,107,107	0
2	NA	H	1144	1/1	0.66	0.30	83,83,83,83	0
3	CL	B	1149	1/1	0.77	0.20	115,115,115,115	0
2	NA	J	1148	1/1	0.81	0.24	86,86,86,86	0
2	NA	F	1148	1/1	0.82	0.31	86,86,86,86	0
3	CL	E	1147	1/1	0.86	0.14	106,106,106,106	0
3	CL	G	1144	1/1	0.88	0.38	93,93,93,93	0
2	NA	B	1148	1/1	0.89	0.20	98,98,98,98	0
2	NA	I	1149	1/1	0.90	0.37	93,93,93,93	0
3	CL	J	1149	1/1	0.92	0.28	98,98,98,98	0
2	NA	D	1143	1/1	0.94	0.34	107,107,107,107	0
2	NA	G	1145	1/1	0.95	0.32	81,81,81,81	0
3	CL	G	1143	1/1	0.95	0.25	95,95,95,95	0
5	MG	I	1148	1/1	0.96	0.18	65,65,65,65	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.