



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 02:16 am BST

PDB ID : 2X2C / pdb\_00002x2c  
Title : acetyl-CypA:cyclosporine complex  
Authors : Lammers, M.; Neumann, H.; Chin, J.W.; James, L.C.  
Deposited on : 2010-01-12  
Resolution : 2.41 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>.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

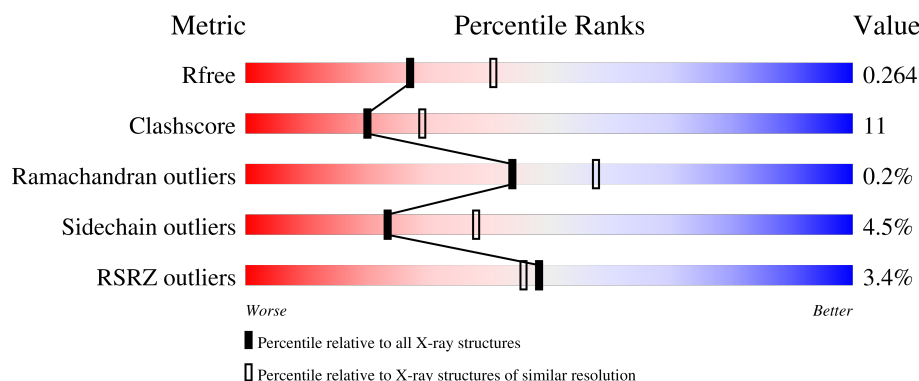
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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))
$R_{free}$	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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	B	11	<div> <div>18%</div> <div>45%</div> <div>36%</div> </div>
1	F	11	<div> <div>18%</div> <div>55%</div> <div>18%</div> <div>9%</div> </div>
1	L	11	<div> <div>64%</div> <div>36%</div> </div>
1	P	11	<div> <div>9%</div> <div>55%</div> <div>36%</div> </div>
1	R	11	<div> <div>27%</div> <div>27%</div> <div>45%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	K	165	
2	M	165	
2	O	165	
2	Q	165	
2	S	165	

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
1	SAR	L	7	-	-	X	-
1	MLE	L	8	-	-	X	-
2	ALY	K	125	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7267 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 CYCLOSPORIN A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	B	11	Total	C	N	O	0	0	0
			85	62	11	12			
1	F	11	Total	C	N	O	0	0	0
			85	62	11	12			
1	L	11	Total	C	N	O	0	0	0
			85	62	11	12			
1	P	11	Total	C	N	O	0	0	0
			85	62	11	12			
1	R	11	Total	C	N	O	0	0	0
			85	62	11	12			

- Molecule 2 is a protein called PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	165	Total	C	N	O	S	0	0	0
			1269	804	218	238	9			
2	M	165	Total	C	N	O	S	0	0	0
			1269	804	218	238	9			
2	O	165	Total	C	N	O	S	0	0	0
			1269	804	218	238	9			
2	Q	165	Total	C	N	O	S	0	0	0
			1269	804	218	238	9			
2	S	165	Total	C	N	O	S	0	0	0
			1269	804	218	238	9			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	O	0	0
			3	3		
3	F	3	Total	O	0	0
			3	3		

*Continued on next page...*

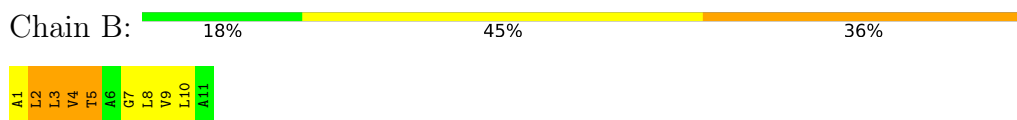
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	51	Total 51	O 51	0	0
3	L	9	Total 9	O 9	0	0
3	M	174	Total 174	O 174	0	0
3	O	85	Total 85	O 85	0	0
3	P	3	Total 3	O 3	0	0
3	Q	83	Total 83	O 83	0	0
3	R	1	Total 1	O 1	0	0
3	S	85	Total 85	O 85	0	0

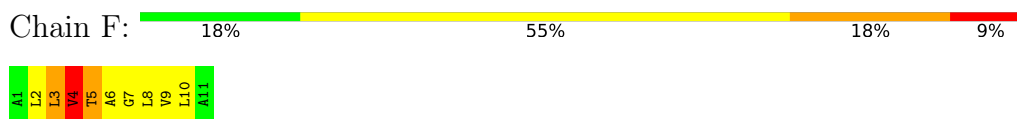
### 3 Residue-property plots [i](#)

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: CYCLOSPORIN A



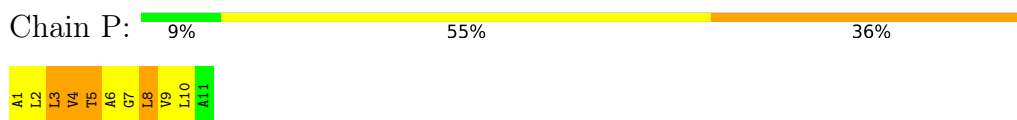
- Molecule 1: CYCLOSPORIN A



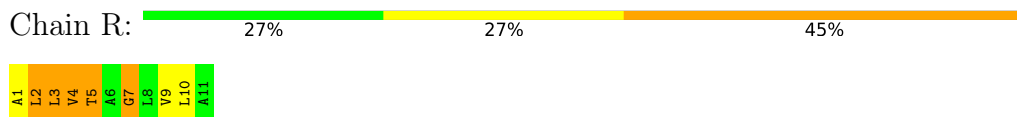
- Molecule 1: CYCLOSPORIN A



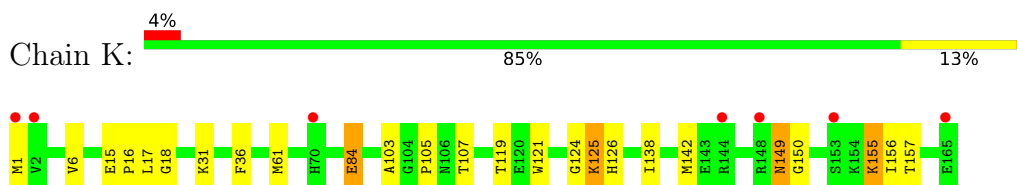
- Molecule 1: CYCLOSPORIN A



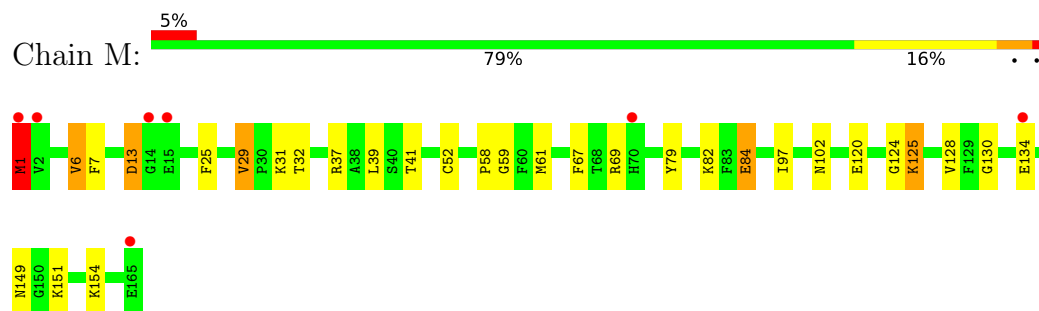
- Molecule 1: CYCLOSPORIN A



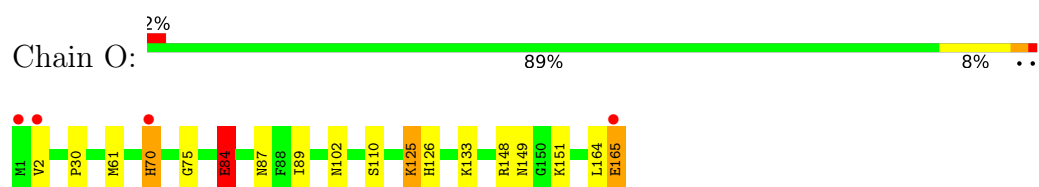
- Molecule 2: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A



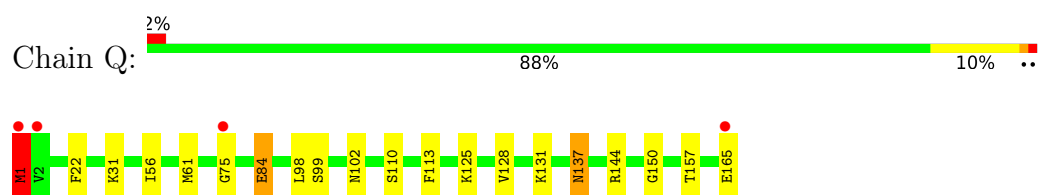
- Molecule 2: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A



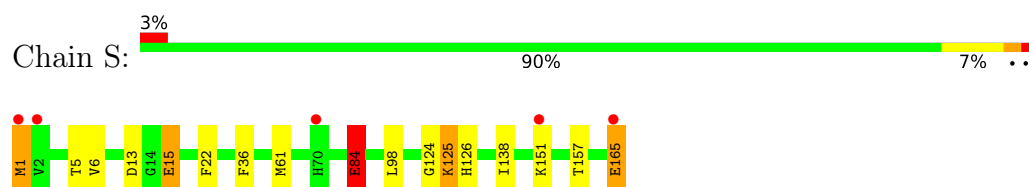
- Molecule 2: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A



- Molecule 2: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A



- Molecule 2: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.43Å 107.43Å 428.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.27 – 2.41 61.27 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.4 (61.27-2.41) 99.4 (61.27-2.41)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.206 , 0.264 0.211 , 0.264	Depositor DCC
$R_{free}$ test set	2921 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 34.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7267	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: MVA, MLE, SAR, ALY, BMT, ABA, DAL

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	B	0.95	0/10	1.25	0/11
1	F	1.35	0/10	1.23	0/11
1	L	1.27	0/10	0.69	0/11
1	P	1.20	0/10	0.80	0/11
1	R	1.69	0/10	1.10	0/11
2	K	0.91	1/1284 (0.1%)	0.82	0/1719
2	M	0.85	2/1284 (0.2%)	0.81	1/1719 (0.1%)
2	O	1.04	2/1284 (0.2%)	0.82	0/1719
2	Q	1.06	4/1284 (0.3%)	0.89	1/1719 (0.1%)
2	S	1.06	3/1284 (0.2%)	0.82	0/1719
All	All	0.99	12/6470 (0.2%)	0.84	2/8650 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
2	M	0	3
2	S	0	1
All	All	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	84	GLU	CG-CD	7.01	1.62	1.51
2	S	15	GLU	CG-CD	7.00	1.62	1.51
2	Q	84	GLU	CG-CD	6.96	1.62	1.51
2	K	84	GLU	CG-CD	6.68	1.61	1.51
2	O	84	GLU	CD-OE1	6.50	1.32	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	128	VAL	CB-CG2	6.12	1.65	1.52
2	M	134	GLU	CG-CD	6.11	1.61	1.51
2	M	84	GLU	CB-CG	5.53	1.62	1.52
2	O	84	GLU	CG-CD	5.34	1.59	1.51
2	S	165	GLU	CG-CD	5.19	1.59	1.51
2	Q	137	ASN	CG-OD1	5.06	1.35	1.24
2	Q	1	MET	CB-CG	5.01	1.67	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	144	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	M	37	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	4	MVA	Mainchain
2	M	1	MET	Peptide
2	M	124	GLY	Mainchain
2	M	125	ALY	Mainchain
2	S	124	GLY	Mainchain

## 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	B	85	0	109	7	0
1	F	85	0	109	6	0
1	L	85	0	109	26	1
1	P	85	0	110	12	0
1	R	85	0	109	6	0
2	K	1269	0	1238	27	0
2	M	1269	0	1238	24	0
2	O	1269	0	1236	20	0
2	Q	1269	0	1238	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	1269	0	1238	11	1
3	B	3	0	0	4	1
3	F	3	0	0	0	0
3	K	51	0	0	0	0
3	L	9	0	0	17	0
3	M	174	0	0	24	2
3	O	85	0	0	9	0
3	P	3	0	0	0	0
3	Q	83	0	0	2	0
3	R	1	0	0	0	0
3	S	85	0	0	3	0
All	All	7267	0	6734	146	3

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 (146) 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:L:9:VAL:O	3:L:2007:HOH:O	1.52	1.28
2:K:124:GLY:C	2:K:125:ALY:N	1.89	1.26
1:L:1:DAL:HB2	3:M:2073:HOH:O	1.25	1.25
1:L:7:SAR:HN3	3:L:2005:HOH:O	1.42	1.17
2:O:70:HIS:HB2	3:O:2033:HOH:O	1.48	1.11
1:L:7:SAR:CN	3:L:2005:HOH:O	1.98	1.09
2:K:124:GLY:C	2:K:125:ALY:H2	1.48	1.07
1:L:8:MLE:HB3	3:L:2006:HOH:O	1.56	1.04
2:O:30:PRO:HB3	3:O:2012:HOH:O	1.59	1.00
1:L:11:ALA:O	3:L:2009:HOH:O	1.84	0.95
2:M:120:GLU:OE1	3:M:2121:HOH:O	1.84	0.92
3:B:2002:HOH:O	1:L:8:MLE:CN	2.18	0.91
3:B:2002:HOH:O	1:L:8:MLE:HN2	1.70	0.89
2:K:103:ALA:HB2	3:L:2003:HOH:O	1.76	0.86
2:M:144:ARG:NH2	3:M:2157:HOH:O	2.13	0.80
1:L:4:MVA:C	1:L:5:BMT:CA	2.59	0.80
2:K:125:ALY:HH32	3:M:2086:HOH:O	1.81	0.79
1:P:4:MVA:C	1:P:5:BMT:CN	2.63	0.76
1:B:8:MLE:HN1	3:B:2002:HOH:O	1.85	0.75
2:M:120:GLU:OE2	3:M:2123:HOH:O	2.04	0.75
1:P:4:MVA:C	1:P:5:BMT:CA	2.64	0.74
2:M:29:VAL:HG11	3:M:2141:HOH:O	1.87	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:102:ASN:OD1	3:M:2101:HOH:O	2.06	0.73
2:M:31:LYS:NZ	2:M:84:GLU:OE2	2.20	0.73
2:K:125:ALY:O	2:K:126:HIS:N	2.21	0.73
1:L:4:MVA:C	1:L:5:BMT:CN	2.68	0.72
1:L:8:MLE:HD22	1:L:10:MLE:HD11	1.72	0.72
2:Q:31:LYS:NZ	2:Q:84:GLU:OE2	2.16	0.72
2:M:1:MET:SD	3:M:2026:HOH:O	2.48	0.70
2:K:125:ALY:C	2:K:126:HIS:CA	2.70	0.69
2:S:125:ALY:C	2:S:126:HIS:CA	2.68	0.69
2:Q:84:GLU:OE2	3:Q:2042:HOH:O	2.10	0.69
2:M:102:ASN:HB2	3:M:2105:HOH:O	1.92	0.68
2:M:120:GLU:CD	3:M:2121:HOH:O	2.27	0.67
1:L:8:MLE:HD13	3:L:2007:HOH:O	1.94	0.67
1:F:8:MLE:HD22	1:F:10:MLE:HD11	1.77	0.67
1:L:7:SAR:CA	3:L:2005:HOH:O	2.42	0.66
2:O:30:PRO:CB	3:O:2012:HOH:O	2.27	0.66
1:L:11:ALA:C	3:L:2009:HOH:O	2.28	0.65
1:L:7:SAR:C	3:L:2005:HOH:O	2.44	0.65
2:S:84:GLU:H	2:S:84:GLU:CD	2.01	0.64
2:Q:131:LYS:HE2	3:Q:2070:HOH:O	1.96	0.64
2:M:41:THR:HG22	3:M:2169:HOH:O	1.97	0.63
2:K:84:GLU:H	2:K:84:GLU:CD	2.02	0.63
1:P:8:MLE:HD22	1:P:10:MLE:HD11	1.81	0.62
2:M:59:GLY:HA2	3:M:2155:HOH:O	1.99	0.61
2:M:52:CYS:SG	3:M:2039:HOH:O	2.46	0.61
1:L:8:MLE:HN2	3:L:2006:HOH:O	2.02	0.59
2:M:79:TYR:OH	3:M:2073:HOH:O	2.16	0.59
2:S:6:VAL:HG21	2:S:36:PHE:HE2	1.67	0.58
1:L:8:MLE:CB	3:L:2006:HOH:O	2.30	0.58
2:K:17:LEU:CD2	2:K:138:ILE:HG23	2.35	0.56
3:M:2123:HOH:O	2:O:89:ILE:HG12	2.06	0.56
2:K:149:ASN:C	2:K:149:ASN:HD22	2.10	0.55
1:L:9:VAL:N	3:L:2007:HOH:O	2.40	0.54
2:S:125:ALY:HH32	3:S:2074:HOH:O	2.07	0.54
2:O:164:LEU:O	2:O:165:GLU:HB3	2.07	0.54
2:Q:75:GLY:HA3	2:Q:110:SER:OG	2.07	0.54
2:K:17:LEU:HD23	2:K:138:ILE:HG23	1.89	0.54
3:O:2061:HOH:O	2:Q:1:MET:HE3	2.09	0.53
2:O:125:ALY:C	2:O:126:HIS:CA	2.78	0.53
2:K:103:ALA:CB	3:L:2003:HOH:O	2.43	0.53
2:K:125:ALY:CH3	3:M:2086:HOH:O	2.46	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:32:THR:O	3:M:2029:HOH:O	2.18	0.52
1:B:8:MLE:HD22	1:B:10:MLE:HD11	1.92	0.52
2:M:69:ARG:CZ	3:M:2062:HOH:O	2.58	0.51
2:M:148:ARG:HB2	3:M:2160:HOH:O	2.10	0.51
2:K:156:ILE:HD13	2:K:156:ILE:N	2.24	0.51
2:S:125:ALY:N	2:S:126:HIS:N	2.58	0.51
2:S:22:PHE:CD1	2:S:98:LEU:HD22	2.47	0.50
2:S:1:MET:HB3	3:S:2001:HOH:O	2.11	0.50
2:O:133:LYS:NZ	3:O:2071:HOH:O	2.44	0.50
2:S:138:ILE:HG22	2:S:138:ILE:O	2.12	0.50
1:F:3:MLE:O	1:F:3:MLE:HN3	2.12	0.49
2:K:6:VAL:HG21	2:K:36:PHE:HE2	1.77	0.49
2:K:31:LYS:NZ	2:K:84:GLU:OE2	2.41	0.49
2:O:125:ALY:HE3	3:O:2068:HOH:O	2.13	0.48
1:L:9:VAL:C	3:L:2007:HOH:O	2.26	0.48
3:M:2123:HOH:O	2:O:89:ILE:CG1	2.61	0.48
2:Q:84:GLU:H	2:Q:84:GLU:CD	2.16	0.48
2:O:84:GLU:H	2:O:84:GLU:CD	2.18	0.47
2:K:103:ALA:HB1	1:L:5:BMT:HH3	1.97	0.47
1:L:5:BMT:HH1	3:L:2006:HOH:O	2.14	0.47
1:L:6:ABA:HA	1:L:7:SAR:HN1	1.67	0.47
2:O:75:GLY:HA3	2:O:110:SER:OG	2.14	0.47
1:P:4:MVA:HA	1:P:5:BMT:HN1	1.96	0.47
2:K:17:LEU:HD23	2:K:138:ILE:CG2	2.45	0.46
1:B:8:MLE:CN	3:B:2002:HOH:O	2.53	0.46
1:F:9:VAL:HA	1:F:10:MLE:HN1	1.78	0.46
2:M:32:THR:HG22	3:M:2029:HOH:O	2.16	0.46
2:K:105:PRO:O	2:K:107:THR:HG23	2.16	0.46
3:M:2123:HOH:O	2:O:89:ILE:CG2	2.63	0.46
1:P:9:VAL:HA	1:P:10:MLE:HN1	1.74	0.46
1:R:9:VAL:HA	1:R:10:MLE:HN1	1.73	0.46
1:R:1:DAL:HA	1:R:2:MLE:HN1	1.73	0.46
2:S:5:THR:HA	2:S:22:PHE:O	2.16	0.45
2:Q:22:PHE:CD1	2:Q:98:LEU:HD22	2.51	0.45
2:M:25:PHE:CD2	2:M:130:GLY:HA2	2.51	0.45
1:L:9:VAL:HA	1:L:10:MLE:HN1	1.65	0.45
2:O:149:ASN:OD1	2:O:149:ASN:C	2.55	0.44
2:O:102:ASN:O	1:P:5:BMT:HA	2.18	0.44
1:L:1:DAL:C	1:L:3:MLE:HN1	2.48	0.44
1:R:3:MLE:HB2	1:R:4:MVA:HN1	1.99	0.44
2:O:87:ASN:ND2	2:O:89:ILE:HD12	2.32	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:70:HIS:CG	3:O:2033:HOH:O	2.70	0.44
1:P:4:MVA:CA	1:P:5:BMT:HN1	2.46	0.44
2:S:6:VAL:HG21	2:S:36:PHE:CE2	2.50	0.43
2:K:125:ALY:N	2:K:126:HIS:N	2.66	0.43
1:P:1:DAL:HA	1:P:2:MLE:HN1	1.78	0.43
3:M:2123:HOH:O	2:O:89:ILE:HG21	2.19	0.43
1:B:4:MVA:HA	1:B:5:BMT:HN1	1.88	0.43
1:L:6:ABA:C	3:L:2003:HOH:O	2.67	0.43
1:P:2:MLE:HA	1:P:3:MLE:HN1	1.88	0.43
2:M:39:LEU:HD22	2:M:67:PHE:CE2	2.53	0.43
1:F:8:MLE:HD12	1:F:8:MLE:HA	1.87	0.42
2:S:125:ALY:CH3	3:S:2074:HOH:O	2.66	0.42
1:P:6:ABA:HA	1:P:7:SAR:HN1	1.61	0.42
2:M:13:ASP:OD2	2:M:154:LYS:HD2	2.19	0.42
1:P:10:MLE:O	1:P:10:MLE:HN3	2.20	0.42
2:K:15:GLU:O	2:K:16:PRO:C	2.56	0.42
2:M:97:ILE:HG23	2:M:128:VAL:HG13	2.02	0.42
3:M:2123:HOH:O	2:O:89:ILE:HD13	2.20	0.42
2:K:119:THR:HA	2:K:121:TRP:CZ3	2.55	0.42
2:Q:99:SER:HB3	2:Q:113:PHE:CZ	2.55	0.42
2:K:149:ASN:HD22	2:K:150:GLY:N	2.17	0.41
2:K:155:LYS:C	2:K:156:ILE:HD13	2.40	0.41
2:Q:102:ASN:O	1:R:5:BMT:HA	2.20	0.41
2:O:125:ALY:CE	3:O:2068:HOH:O	2.68	0.41
1:R:5:BMT:O	1:R:7:SAR:HN1	2.20	0.41
1:B:9:VAL:HA	1:B:10:MLE:HN1	1.73	0.41
1:R:3:MLE:HB2	1:R:4:MVA:CN	2.49	0.41
2:M:58:PRO:HA	2:M:143:GLU:OE1	2.21	0.41
1:B:1:DAL:HA	1:B:2:MLE:HN1	1.79	0.41
2:K:18:GLY:HA3	2:K:138:ILE:HD12	2.03	0.41
2:K:138:ILE:O	2:K:142:MET:HG3	2.21	0.41
1:L:1:DAL:HA	1:L:2:MLE:HN1	1.83	0.41
2:O:70:HIS:CD2	3:O:2033:HOH:O	2.74	0.41
2:K:15:GLU:HA	2:K:16:PRO:HD2	1.94	0.41
2:M:149:ASN:OD1	2:M:149:ASN:C	2.58	0.41
1:B:1:DAL:C	1:B:3:MLE:HN1	2.51	0.41
2:Q:56:ILE:O	2:Q:150:GLY:HA2	2.20	0.41
1:F:4:MVA:HA	1:F:5:BMT:HN1	1.85	0.40
1:F:6:ABA:HA	1:F:7:SAR:HN1	1.79	0.40
2:K:125:ALY:O	2:K:126:HIS:CA	2.68	0.40
2:M:6:VAL:HG23	2:M:7:PHE:N	2.36	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1:DAL:C	1:P:3:MLE:HN1	2.51	0.40

All (3) 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:L:5:BMT:CH	3:M:2103:HOH:O[10_554]	1.94	0.26
3:B:2003:HOH:O	3:M:2054:HOH:O[10_554]	2.11	0.09
2:S:15:GLU:OE2	2:S:15:GLU:OE2[10_664]	2.11	0.09

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	B	1/11 (9%)	1 (100%)	0	0	100	100
1	F	1/11 (9%)	1 (100%)	0	0	100	100
1	L	1/11 (9%)	1 (100%)	0	0	100	100
1	P	1/11 (9%)	1 (100%)	0	0	100	100
1	R	1/11 (9%)	1 (100%)	0	0	100	100
2	K	162/165 (98%)	156 (96%)	6 (4%)	0	100	100
2	M	162/165 (98%)	152 (94%)	9 (6%)	1 (1%)	22	31
2	O	162/165 (98%)	156 (96%)	6 (4%)	0	100	100
2	Q	162/165 (98%)	156 (96%)	6 (4%)	0	100	100
2	S	162/165 (98%)	152 (94%)	9 (6%)	1 (1%)	22	31
All	All	815/880 (93%)	777 (95%)	36 (4%)	2 (0%)	44	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	13	ASP
2	S	13	ASP

### 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	B	1/1 (100%)	1 (100%)	0	100	100
1	F	1/1 (100%)	1 (100%)	0	100	100
1	L	1/1 (100%)	1 (100%)	0	100	100
1	P	1/1 (100%)	1 (100%)	0	100	100
1	R	1/1 (100%)	1 (100%)	0	100	100
2	K	132/132 (100%)	127 (96%)	5 (4%)	28	45
2	M	132/132 (100%)	125 (95%)	7 (5%)	19	31
2	O	132/132 (100%)	125 (95%)	7 (5%)	19	31
2	Q	132/132 (100%)	127 (96%)	5 (4%)	28	45
2	S	132/132 (100%)	126 (96%)	6 (4%)	23	38
All	All	665/665 (100%)	635 (96%)	30 (4%)	23	38

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	1	MET
2	K	61	MET
2	K	149	ASN
2	K	155	LYS
2	K	157	THR
2	M	1	MET
2	M	6	VAL
2	M	29	VAL
2	M	61	MET
2	M	82	LYS
2	M	148	ARG
2	M	151	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	O	2	VAL
2	O	61	MET
2	O	70	HIS
2	O	84	GLU
2	O	148	ARG
2	O	151	LYS
2	O	165	GLU
2	Q	1	MET
2	Q	61	MET
2	Q	137	ASN
2	Q	157	THR
2	Q	165	GLU
2	S	1	MET
2	S	61	MET
2	S	84	GLU
2	S	151	LYS
2	S	157	THR
2	S	165	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	149	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

50 non-standard protein/DNA/RNA residues 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
1	SAR	F	7	1	4,4,5	0.59	0	1,3,5	1.79	0
1	ABA	L	6	1	4,5,6	0.66	0	1,5,7	0.53	0
1	MLE	B	3	1	7,8,9	0.73	0	6,9,11	1.21	1 (16%)
1	ABA	P	6	1	4,5,6	0.82	0	1,5,7	0.75	0
2	ALY	Q	125	2	10,11,12	2.06	3 (30%)	7,12,14	1.04	1 (14%)
1	SAR	P	7	1	4,4,5	0.77	0	1,3,5	1.66	0
1	MLE	F	2	1	7,8,9	0.80	0	6,9,11	1.30	1 (16%)
1	BMT	R	5	1	11,12,13	1.38	2 (18%)	12,14,16	1.21	1 (8%)
1	ABA	R	6	1	4,5,6	1.20	0	1,5,7	0.09	0
1	MLE	F	3	1	7,8,9	0.53	0	6,9,11	1.27	1 (16%)
1	SAR	B	7	1	4,4,5	0.54	0	1,3,5	2.36	1 (100%)
1	MLE	L	2	1	7,8,9	0.60	0	6,9,11	1.30	1 (16%)
1	MLE	B	2	1	7,8,9	0.54	0	6,9,11	1.10	1 (16%)
1	MLE	L	8	1	7,8,9	0.89	0	6,9,11	1.31	1 (16%)
2	ALY	K	125	2	10,11,12	1.05	1 (10%)	7,12,14	0.98	0
1	MVA	L	4	1	6,7,8	0.80	0	7,8,10	1.02	0
1	SAR	L	7	1	4,4,5	0.90	0	1,3,5	1.99	0
1	MVA	B	4	1	6,7,8	1.21	1 (16%)	7,8,10	2.82	3 (42%)
1	ABA	F	6	1	4,5,6	0.86	0	1,5,7	0.46	0
1	MVA	R	4	1	6,7,8	0.74	0	7,8,10	1.65	2 (28%)
1	MLE	B	10	1	7,8,9	0.60	0	6,9,11	0.99	0
1	MLE	P	3	1	7,8,9	0.64	0	6,9,11	1.25	1 (16%)
2	ALY	O	125	2	10,11,12	1.21	1 (10%)	7,12,14	0.67	0
1	MVA	F	4	1	6,7,8	1.15	1 (16%)	7,8,10	2.29	1 (14%)
1	MLE	R	10	1	7,8,9	0.42	0	6,9,11	0.73	0
1	MLE	R	3	1	7,8,9	0.56	0	6,9,11	1.20	1 (16%)
1	MLE	B	8	1	7,8,9	1.05	0	6,9,11	1.13	0
1	BMT	F	5	1	11,12,13	1.26	1 (9%)	12,14,16	1.26	1 (8%)
1	BMT	L	5	1	11,12,13	1.24	2 (18%)	12,14,16	1.78	3 (25%)
1	MLE	F	10	1	7,8,9	0.67	0	6,9,11	0.49	0
1	MLE	F	8	1	7,8,9	0.58	0	6,9,11	1.01	0
1	MLE	R	8	1	7,8,9	0.54	0	6,9,11	1.40	0
1	ABA	B	6	1	4,5,6	0.87	0	1,5,7	0.18	0
1	MLE	L	10	1	7,8,9	0.76	0	6,9,11	1.14	0
1	MLE	P	8	1	7,8,9	0.52	0	6,9,11	1.37	1 (16%)
1	BMT	P	5	1	11,12,13	0.88	1 (9%)	12,14,16	1.20	0
2	ALY	M	125	2	10,11,12	1.51	1 (10%)	7,12,14	0.66	0
2	ALY	S	125	2	10,11,12	1.51	2 (20%)	7,12,14	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	BMT	B	5	1	11,12,13	1.26	2 (18%)	12,14,16	1.75	3 (25%)
1	MLE	P	2	1	7,8,9	0.55	0	6,9,11	1.11	0
1	MVA	P	4	1	6,7,8	0.69	0	7,8,10	2.12	3 (42%)
1	SAR	R	7	1	4,4,5	0.66	0	1,3,5	2.13	1 (100%)
1	MLE	L	3	1	7,8,9	0.47	0	6,9,11	1.18	1 (16%)
1	MLE	P	10	1	7,8,9	0.40	0	6,9,11	0.87	0
1	MLE	R	2	1	7,8,9	0.91	0	6,9,11	1.22	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SAR	F	7	1	-	1/1/2/3	-
1	ABA	L	6	1	-	0/3/4/6	-
1	MLE	B	3	1	-	0/5/8/10	-
1	ABA	P	6	1	-	2/3/4/6	-
2	ALY	Q	125	2	-	3/9/10/12	-
1	SAR	P	7	1	-	1/1/2/3	-
1	MLE	F	2	1	-	0/5/8/10	-
1	BMT	R	5	1	-	1/13/16/18	-
1	ABA	R	6	1	-	0/3/4/6	-
1	MLE	F	3	1	-	0/5/8/10	-
1	SAR	B	7	1	-	1/1/2/3	-
1	MLE	L	2	1	-	0/5/8/10	-
1	MLE	B	2	1	-	0/5/8/10	-
1	MLE	L	8	1	-	4/5/8/10	-
2	ALY	K	125	2	-	2/9/10/12	-
1	MVA	L	4	1	-	1/6/8/10	-
1	SAR	L	7	1	-	1/1/2/3	-
1	MVA	B	4	1	-	1/6/8/10	-
1	ABA	F	6	1	-	0/3/4/6	-
1	MVA	R	4	1	-	3/6/8/10	-
1	MLE	B	10	1	-	0/5/8/10	-
1	MLE	P	3	1	-	0/5/8/10	-
2	ALY	O	125	2	-	2/9/10/12	-
1	MVA	F	4	1	-	1/6/8/10	-
1	MLE	R	10	1	-	0/5/8/10	-
1	MLE	R	3	1	-	0/5/8/10	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLE	B	8	1	-	5/5/8/10	-
1	BMT	F	5	1	-	1/13/16/18	-
1	BMT	L	5	1	-	1/13/16/18	-
1	MLE	F	10	1	-	0/5/8/10	-
1	MLE	F	8	1	-	5/5/8/10	-
1	MLE	R	8	1	-	5/5/8/10	-
1	ABA	B	6	1	-	0/3/4/6	-
1	MLE	L	10	1	-	0/5/8/10	-
1	MLE	P	8	1	-	5/5/8/10	-
1	BMT	P	5	1	-	1/13/16/18	-
2	ALY	M	125	2	-	1/9/10/12	-
2	ALY	S	125	2	-	3/9/10/12	-
1	BMT	B	5	1	-	2/13/16/18	-
1	MLE	P	2	1	-	0/5/8/10	-
1	MVA	P	4	1	-	2/6/8/10	-
1	SAR	R	7	1	-	1/1/2/3	-
1	MLE	L	3	1	-	0/5/8/10	-
1	MLE	P	10	1	-	0/5/8/10	-
1	MLE	R	2	1	-	0/5/8/10	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	125	ALY	CB-CA	3.99	1.58	1.53
2	Q	125	ALY	CH3-CH	3.60	1.58	1.50
2	M	125	ALY	CH3-CH	3.59	1.58	1.50
2	S	125	ALY	CH3-CH	3.48	1.57	1.50
2	O	125	ALY	CH3-CH	2.98	1.56	1.50
2	K	125	ALY	CH3-CH	2.55	1.55	1.50
1	B	4	MVA	CB-CA	-2.55	1.49	1.54
1	F	4	MVA	CB-CA	-2.50	1.49	1.54
1	B	5	BMT	CE-CZ	2.37	1.47	1.29
1	L	5	BMT	CA-N	-2.34	1.43	1.47
1	R	5	BMT	CE-CZ	2.33	1.47	1.29
1	L	5	BMT	CE-CZ	2.30	1.46	1.29
1	F	5	BMT	CE-CZ	2.28	1.46	1.29
2	S	125	ALY	CB-CA	2.27	1.56	1.53
1	P	5	BMT	CE-CZ	2.16	1.45	1.29
1	B	5	BMT	OG1-CB	-2.12	1.38	1.43
1	R	5	BMT	OG1-CB	-2.09	1.38	1.43
2	Q	125	ALY	CE-NZ	2.05	1.50	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	MVA	CB-CA-C	-6.25	105.20	113.04
1	F	4	MVA	CB-CA-C	-5.53	106.10	113.04
1	P	4	MVA	CB-CA-C	-3.92	108.13	113.04
1	L	5	BMT	CB-CA-N	-3.86	103.75	111.41
1	B	5	BMT	CG2-CD2-CE	3.64	119.58	113.98
1	P	4	MVA	CG2-CB-CA	-3.12	106.43	111.21
1	B	5	BMT	CB-CA-N	-2.97	105.52	111.41
1	R	4	MVA	CB-CA-N	2.90	114.95	111.17
1	B	4	MVA	CG2-CB-CA	-2.81	106.90	111.21
1	L	5	BMT	CD1-CG2-CD2	-2.64	106.11	110.54
1	P	8	MLE	CG-CB-CA	2.58	121.78	115.34
1	L	8	MLE	CG-CB-CA	2.51	121.59	115.34
1	L	3	MLE	O-C-CA	-2.49	118.24	124.78
1	R	2	MLE	O-C-CA	-2.43	118.40	124.78
1	B	5	BMT	CD2-CG2-CB	2.41	115.09	110.39
1	R	5	BMT	O-C-CA	-2.40	118.14	124.83
1	B	7	SAR	O-C-CA	-2.36	118.59	125.42
1	B	3	MLE	O-C-CA	-2.36	118.61	124.78
1	F	5	BMT	OG1-CB-CA	-2.34	104.35	109.32
1	R	3	MLE	O-C-CA	-2.28	118.81	124.78
1	P	4	MVA	CB-CA-N	2.22	114.06	111.17
1	F	3	MLE	O-C-CA	-2.22	118.97	124.78
1	R	4	MVA	CG2-CB-CA	-2.16	107.90	111.21
1	B	2	MLE	O-C-CA	-2.15	119.13	124.78
1	B	4	MVA	CB-CA-N	2.15	113.97	111.17
1	R	7	SAR	O-C-CA	-2.13	119.25	125.42
1	P	3	MLE	O-C-CA	-2.10	119.27	124.78
1	L	2	MLE	O-C-CA	-2.04	119.44	124.78
2	Q	125	ALY	OH-CH-CH3	-2.03	118.29	122.06
1	L	5	BMT	CD1-CG2-CB	2.01	115.26	111.54
1	F	2	MLE	CD1-CG-CB	2.01	118.49	111.11

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	8	MLE	C-CA-CB-CG
1	B	8	MLE	O-C-CA-CB
1	F	8	MLE	C-CA-CB-CG
1	F	8	MLE	O-C-CA-CB
1	L	7	SAR	C-CA-N-CN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	L	8	MLE	C-CA-CB-CG
1	L	8	MLE	O-C-CA-CB
1	P	6	ABA	O-C-CA-CB
1	P	8	MLE	C-CA-CB-CG
1	P	8	MLE	O-C-CA-CB
2	Q	125	ALY	O-C-CA-CB
1	R	4	MVA	CB-CA-N-CN
1	R	4	MVA	N-CA-CB-CG1
1	R	8	MLE	C-CA-CB-CG
1	R	8	MLE	O-C-CA-CB
1	L	8	MLE	N-CA-CB-CG
1	B	8	MLE	N-CA-CB-CG
1	P	8	MLE	N-CA-CB-CG
2	Q	125	ALY	CG-CD-CE-NZ
2	S	125	ALY	CG-CD-CE-NZ
2	K	125	ALY	CG-CD-CE-NZ
1	R	8	MLE	N-CA-CB-CG
1	F	8	MLE	CA-CB-CG-CD1
2	S	125	ALY	CA-CB-CG-CD
1	P	8	MLE	CA-CB-CG-CD1
1	F	8	MLE	CA-CB-CG-CD2
1	B	8	MLE	CA-CB-CG-CD1
1	F	8	MLE	N-CA-CB-CG
1	R	8	MLE	CA-CB-CG-CD1
2	K	125	ALY	CA-CB-CG-CD
1	L	8	MLE	CA-CB-CG-CD1
2	Q	125	ALY	CA-CB-CG-CD
2	O	125	ALY	CE-CD-CG-CB
2	O	125	ALY	CG-CD-CE-NZ
1	B	5	BMT	CB-CA-N-CN
1	F	5	BMT	CB-CA-N-CN
1	L	5	BMT	CB-CA-N-CN
1	P	5	BMT	CB-CA-N-CN
1	R	5	BMT	CB-CA-N-CN
1	B	4	MVA	CB-CA-N-CN
1	F	4	MVA	CB-CA-N-CN
1	L	4	MVA	CB-CA-N-CN
1	P	4	MVA	CB-CA-N-CN
1	P	8	MLE	CA-CB-CG-CD2
2	M	125	ALY	CE-CD-CG-CB
1	B	5	BMT	OG1-CB-CG2-CD1
2	S	125	ALY	C-CA-CB-CG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	P	6	ABA	N-CA-CB-CG
1	R	8	MLE	CA-CB-CG-CD2
1	B	8	MLE	CA-CB-CG-CD2
1	B	7	SAR	C-CA-N-CN
1	F	7	SAR	C-CA-N-CN
1	P	7	SAR	C-CA-N-CN
1	R	7	SAR	C-CA-N-CN
1	P	4	MVA	N-CA-CB-CG1
1	R	4	MVA	N-CA-CB-CG2

There are no ring outliers.

38 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	7	SAR	1	0
1	L	6	ABA	2	0
1	B	3	MLE	1	0
1	P	6	ABA	1	0
1	P	7	SAR	1	0
1	R	5	BMT	2	0
1	F	3	MLE	1	0
1	L	2	MLE	1	0
1	B	2	MLE	1	0
1	L	8	MLE	7	0
2	K	125	ALY	8	0
1	L	4	MVA	2	0
1	L	7	SAR	5	0
1	B	4	MVA	1	0
1	F	6	ABA	1	0
1	R	4	MVA	2	0
1	B	10	MLE	2	0
1	P	3	MLE	2	0
2	O	125	ALY	3	0
1	F	4	MVA	1	0
1	R	10	MLE	1	0
1	R	3	MLE	2	0
1	B	8	MLE	3	0
1	F	5	BMT	1	0
1	L	5	BMT	4	1
1	F	10	MLE	2	0
1	F	8	MLE	2	0
1	L	10	MLE	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	8	MLE	1	0
1	P	5	BMT	5	0
2	S	125	ALY	4	0
1	B	5	BMT	1	0
1	P	2	MLE	2	0
1	P	4	MVA	4	0
1	R	7	SAR	1	0
1	L	3	MLE	1	0
1	P	10	MLE	3	0
1	R	2	MLE	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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
2	K	2
2	S	2
2	O	1
1	L	1
1	B	1
1	P	1
1	F	1
1	R	1
2	M	1

All chain breaks are listed below:



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	124:GLY	C	125:ALY	N	1.89
1	K	125:ALY	C	126:HIS	N	1.75
1	O	125:ALY	C	126:HIS	N	1.71
1	L	4:MVA	C	5:BMT	N	1.70
1	B	4:MVA	C	5:BMT	N	1.67
1	P	4:MVA	C	5:BMT	N	1.67
1	S	125:ALY	C	126:HIS	N	1.67
1	S	124:GLY	C	125:ALY	N	1.65
1	F	4:MVA	C	5:BMT	N	1.64
1	R	4:MVA	C	5:BMT	N	1.62
1	M	124:GLY	C	125:ALY	N	1.60

## 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	B	2/11 (18%)	-0.01	0 100 100	32, 32, 32, 37	0
1	F	2/11 (18%)	-0.09	0 100 100	29, 29, 29, 33	0
1	L	2/11 (18%)	0.25	0 100 100	35, 35, 35, 38	0
1	P	2/11 (18%)	-0.54	0 100 100	23, 23, 23, 30	0
1	R	2/11 (18%)	-0.76	0 100 100	20, 20, 20, 27	0
2	K	164/165 (99%)	0.32	7 (4%) 40 38	28, 39, 55, 73	0
2	M	164/165 (99%)	0.41	8 (4%) 36 33	28, 43, 58, 71	0
2	O	164/165 (99%)	-0.45	4 (2%) 59 57	20, 27, 37, 63	0
2	Q	164/165 (99%)	-0.58	4 (2%) 59 57	15, 23, 36, 56	0
2	S	164/165 (99%)	-0.24	5 (3%) 52 50	19, 30, 44, 61	0
All	All	830/880 (94%)	-0.11	28 (3%) 48 46	15, 32, 54, 73	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	1	MET	9.1
2	Q	1	MET	7.5
2	S	1	MET	6.9
2	M	1	MET	6.8
2	M	2	VAL	5.3
2	O	165	GLU	5.1
2	O	1	MET	5.0
2	Q	165	GLU	4.5
2	K	2	VAL	4.5
2	S	2	VAL	4.3
2	S	165	GLU	4.2
2	K	165	GLU	4.0
2	Q	2	VAL	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	M	70	HIS	3.2
2	M	134	GLU	3.1
2	K	70	HIS	2.9
2	O	2	VAL	2.9
2	M	148	ARG	2.6
2	K	144	ARG	2.6
2	S	70	HIS	2.5
2	K	148	ARG	2.5
2	M	15	GLU	2.5
2	K	153	SER	2.4
2	M	14	GLY	2.4
2	M	165	GLU	2.3
2	S	151	LYS	2.3
2	O	70	HIS	2.1
2	Q	75	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
2	ALY	M	125	12/13	0.83	0.20	38,45,64,64	0
2	ALY	O	125	12/13	0.86	0.20	32,41,68,70	0
2	ALY	K	125	12/13	0.87	0.19	40,48,77,78	0
2	ALY	Q	125	12/13	0.88	0.19	26,37,66,67	0
2	ALY	S	125	12/13	0.88	0.19	27,38,66,66	0
1	DAL	L	1	5/6	0.91	0.10	35,36,37,37	0
1	MLE	L	10	9/10	0.92	0.12	35,36,40,40	0
1	MVA	B	4	8/9	0.92	0.10	23,25,26,27	0
1	DAL	B	1	5/6	0.92	0.10	33,33,33,35	0
1	MLE	L	8	9/10	0.92	0.13	33,33,34,38	0
1	BMT	L	5	13/14	0.93	0.10	21,26,28,28	0
1	MLE	B	10	9/10	0.93	0.10	33,35,36,37	0
1	MLE	L	2	9/10	0.93	0.10	27,32,33,33	0
1	MLE	B	8	9/10	0.94	0.10	29,32,33,34	0
1	SAR	B	7	5/6	0.94	0.09	30,30,32,34	0
1	MLE	L	3	9/10	0.94	0.09	25,29,29,30	0
1	MLE	F	2	9/10	0.94	0.09	24,25,28,28	0
1	MVA	F	4	8/9	0.94	0.09	17,20,21,22	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLE	F	10	9/10	0.94	0.09	28,31,32,32	0
1	ABA	L	6	6/7	0.95	0.09	26,28,29,29	0
1	BMT	P	5	13/14	0.95	0.07	12,17,19,19	0
1	SAR	L	7	5/6	0.95	0.09	30,30,32,32	0
1	SAR	F	7	5/6	0.95	0.08	22,23,25,27	0
1	ABA	B	6	6/7	0.95	0.09	24,28,28,28	0
1	DAL	F	1	5/6	0.95	0.09	29,29,30,31	0
1	MLE	B	3	9/10	0.95	0.08	24,26,27,29	0
1	DAL	P	1	5/6	0.95	0.08	25,25,26,27	0
1	SAR	R	7	5/6	0.96	0.06	17,18,20,21	0
1	MLE	R	8	9/10	0.96	0.08	18,21,26,32	0
1	MLE	R	10	9/10	0.96	0.08	22,24,25,26	0
1	BMT	B	5	13/14	0.96	0.08	22,25,29,29	0
1	MLE	B	2	9/10	0.96	0.08	21,27,31,31	0
1	MLE	P	10	9/10	0.96	0.07	25,28,31,32	0
1	MVA	L	4	8/9	0.96	0.08	25,26,27,28	0
1	MLE	R	2	9/10	0.96	0.06	14,18,19,20	0
1	DAL	R	1	5/6	0.96	0.07	22,23,24,25	0
1	BMT	R	5	13/14	0.97	0.06	10,15,18,18	0
1	MLE	P	2	9/10	0.97	0.07	16,19,22,22	0
1	BMT	F	5	13/14	0.97	0.07	20,21,23,25	0
1	ABA	P	6	6/7	0.97	0.06	18,19,19,20	0
1	SAR	P	7	5/6	0.97	0.07	20,20,21,21	0
1	ABA	F	6	6/7	0.97	0.07	20,20,22,22	0
1	MLE	F	3	9/10	0.97	0.06	20,23,24,24	0
1	MLE	F	8	9/10	0.97	0.07	23,26,27,30	0
1	MLE	R	3	9/10	0.97	0.06	14,17,21,21	0
1	MVA	R	4	8/9	0.97	0.06	14,15,16,17	0
1	MLE	P	3	9/10	0.98	0.06	17,17,20,21	0
1	MLE	P	8	9/10	0.98	0.06	21,22,24,25	0
1	ABA	R	6	6/7	0.98	0.05	14,15,16,16	0
1	MVA	P	4	8/9	0.98	0.05	10,13,15,16	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.