



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:43 PM BST

PDB ID : 4NZB
Title : NS9283 bound to Ls-AChBP
Authors : Olsen, J.A.; Kastrup, J.S.; Gajhede, M.
Deposited on : 2013-12-11
Resolution : 2.68 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

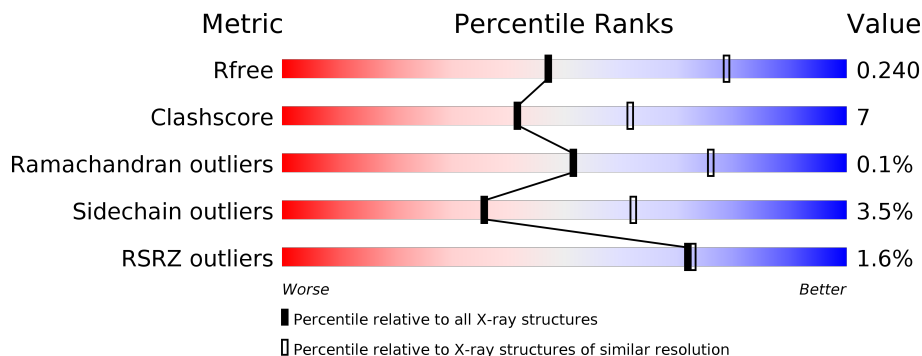
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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.







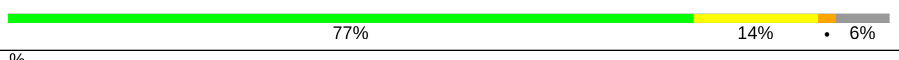
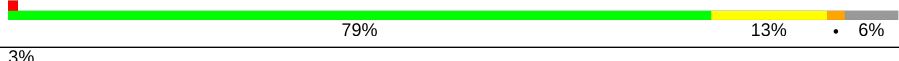

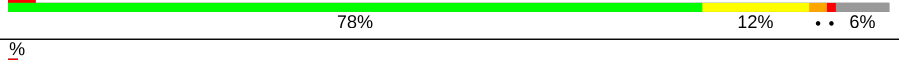

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 on 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	210	 77% 15% • 6%
1	B	210	 2% 77% 14% • 6%
1	C	210	 % 77% 14% •• 6%
1	D	210	 80% 11% • 6%
1	E	210	 2% 76% 14% •• 6%
1	F	210	 2% 77% 15% •• 5%

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Mol	Chain	Length	Quality of chain	
1	G	210		%
1	H	210		%
1	I	210		2%
1	J	210		%
1	K	210		%
1	L	210		%
1	M	210		3%
1	N	210		3%
1	O	210		%

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
4	SO4	F	302	-	-	-	X

2 Entry composition [i](#)

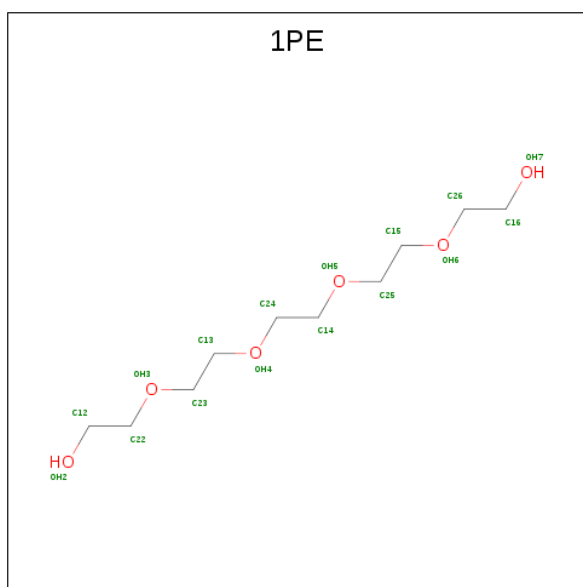
There are 9 unique types of molecules in this entry. The entry contains 24523 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	198	Total 1591	C 1002	N 272	O 312	S 5	0	1	0
1	D	197	Total 1578	C 991	N 271	O 311	S 5	0	0	0
1	E	198	Total 1586	C 997	N 272	O 312	S 5	0	0	0
1	A	198	Total 1586	C 997	N 272	O 312	S 5	0	0	0
1	B	198	Total 1586	C 997	N 272	O 312	S 5	0	0	0
1	C	198	Total 1586	C 997	N 272	O 312	S 5	0	0	0
1	F	200	Total 1607	C 1010	N 274	O 318	S 5	0	1	0
1	H	198	Total 1586	C 997	N 272	O 312	S 5	0	0	0
1	I	195	Total 1568	C 988	N 269	O 308	S 3	0	0	0
1	J	198	Total 1586	C 997	N 272	O 312	S 5	0	0	0
1	K	197	Total 1571	C 989	N 268	O 309	S 5	0	0	0
1	L	198	Total 1591	C 1000	N 272	O 314	S 5	0	1	0
1	M	194	Total 1566	C 988	N 268	O 307	S 3	0	1	0
1	N	198	Total 1586	C 997	N 272	O 312	S 5	0	0	0
1	O	198	Total 1586	C 997	N 272	O 312	S 5	0	0	0

- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



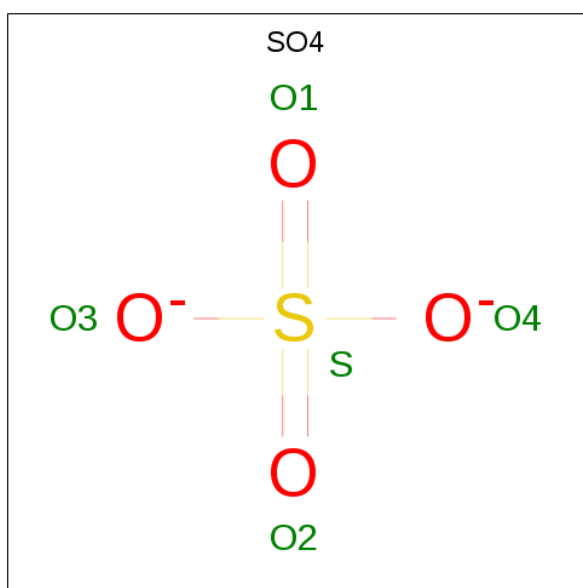
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			16	10	6		
2	D	1	Total	C	O	0	0
			16	10	6		
2	E	1	Total	C	O	0	0
			16	10	6		
2	A	1	Total	C	O	0	0
			16	10	6		
2	B	1	Total	C	O	0	0
			16	10	6		
2	C	1	Total	C	O	0	0
			16	10	6		
2	H	1	Total	C	O	0	0
			16	10	6		
2	I	1	Total	C	O	0	0
			16	10	6		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	G	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



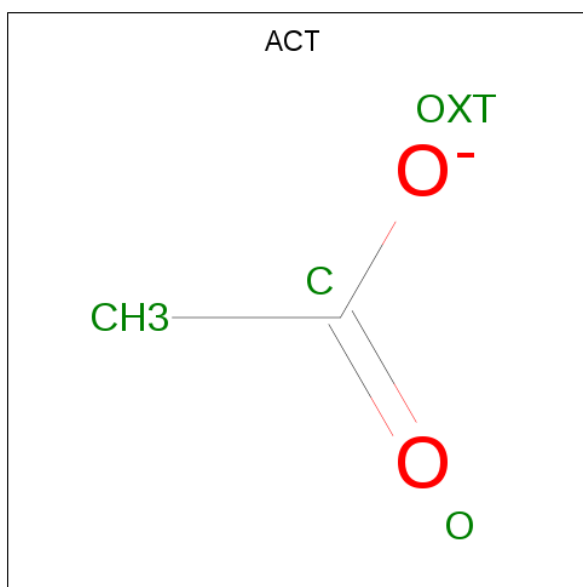
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	G	1	5	4	1	0	0
4	G	1	5	4	1	0	0

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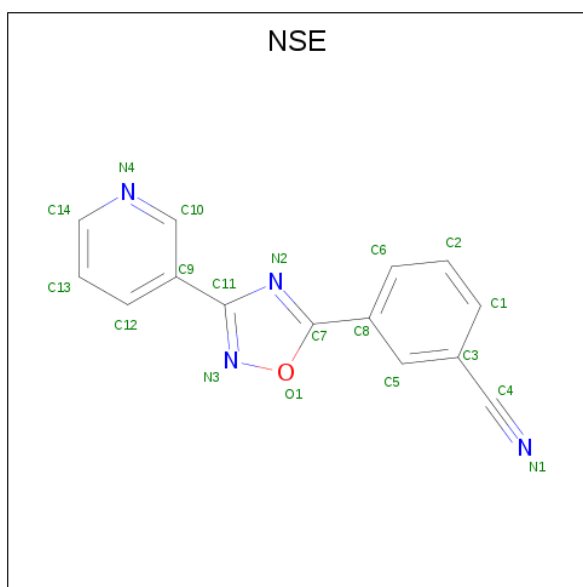
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	I	1	Total 5	O 4	S 1	0	0
4	J	1	Total 5	O 4	S 1	0	0
4	M	1	Total 5	O 4	S 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0

- Molecule 6 is 3-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]benzotrile (three-letter code: NSE) (formula: C₁₄H₈N₄O).

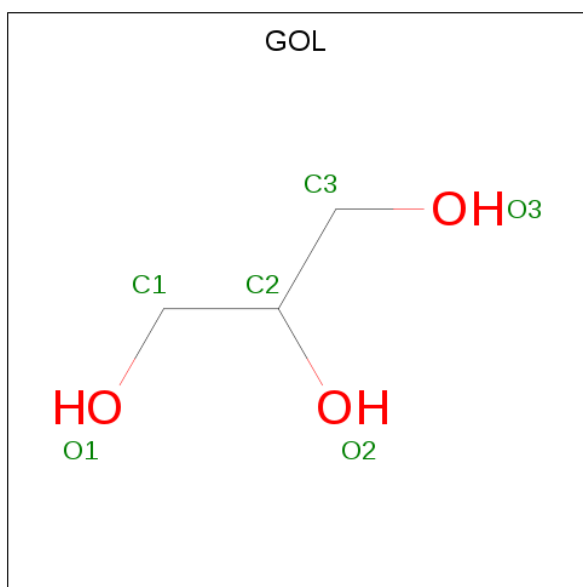


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	E	1	19	14	4	1	0	0
6	A	1	19	14	4	1	0	0
6	B	1	19	14	4	1	0	0
6	I	1	19	14	4	1	0	0
6	K	1	19	14	4	1	0	0
6	M	1	19	14	4	1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	A	1	1	1	0	0
7	L	1	1	1	0	0
7	K	1	1	1	0	0
7	N	1	1	1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	28	Total	O	0	0
			28	28		
9	D	27	Total	O	0	0
			27	27		
9	E	23	Total	O	0	0
			23	23		
9	A	28	Total	O	0	0
			28	28		
9	B	19	Total	O	0	0
			19	19		
9	C	22	Total	O	0	0
			22	22		
9	F	31	Total	O	0	0
			31	31		
9	H	26	Total	O	0	0
			26	26		
9	I	21	Total	O	0	0
			21	21		
9	J	21	Total	O	0	0
			21	21		
9	K	26	Total	O	0	0
			26	26		

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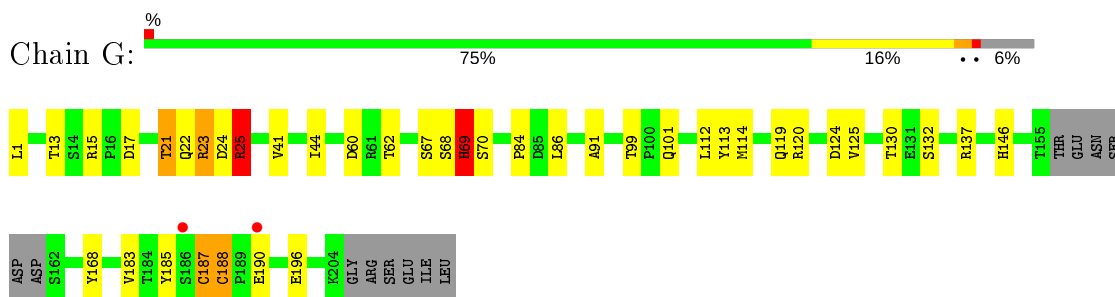
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	24	Total 24	O 24	0	0
9	M	21	Total 21	O 21	0	0
9	N	5	Total 5	O 5	0	0
9	O	13	Total 13	O 13	0	0

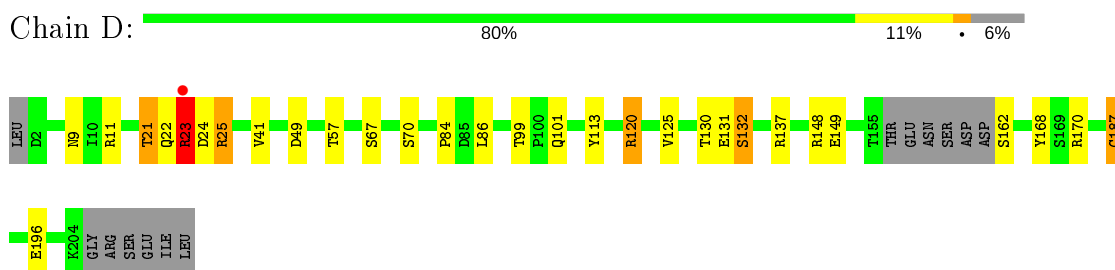
3 Residue-property plots [i](#)

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.

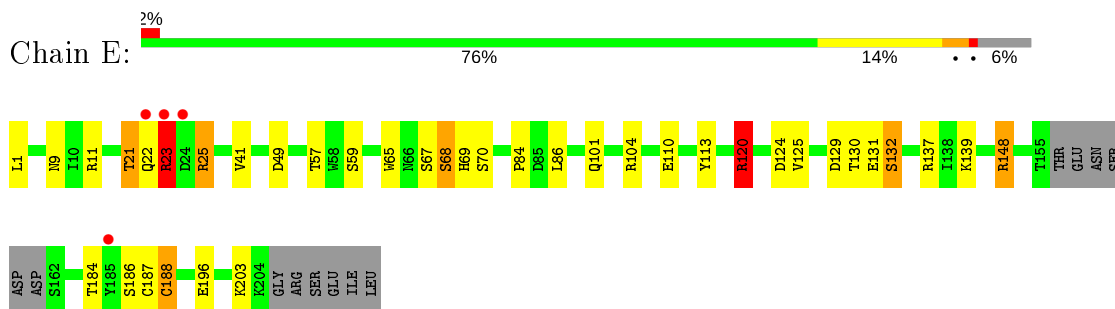
- Molecule 1: Acetylcholine-binding protein



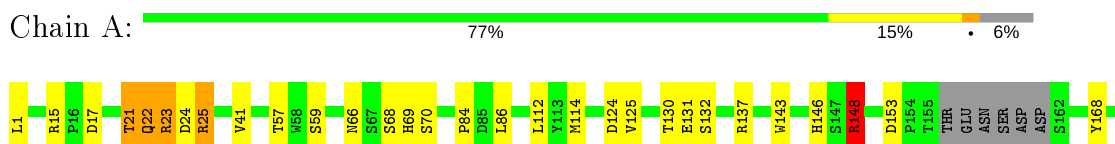
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein

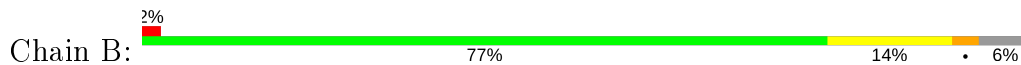


- Molecule 1: Acetylcholine-binding protein

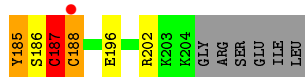
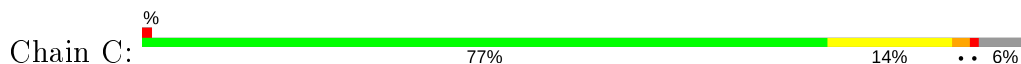




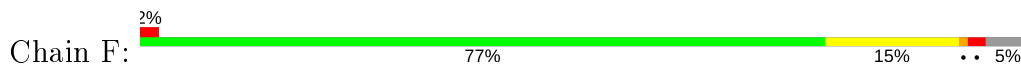
• Molecule 1: Acetylcholine-binding protein



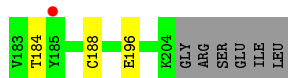
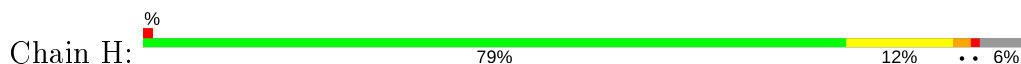
• Molecule 1: Acetylcholine-binding protein



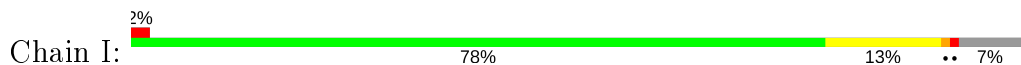
• Molecule 1: Acetylcholine-binding protein

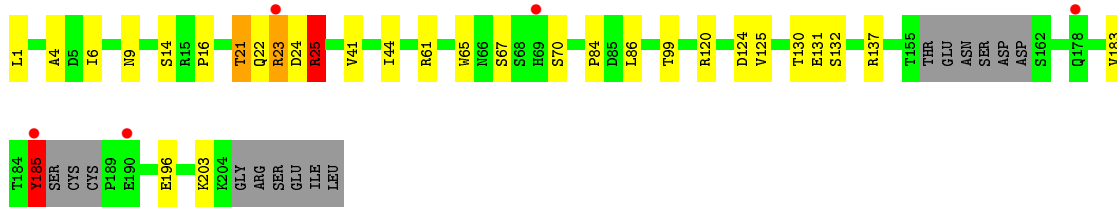


• Molecule 1: Acetylcholine-binding protein

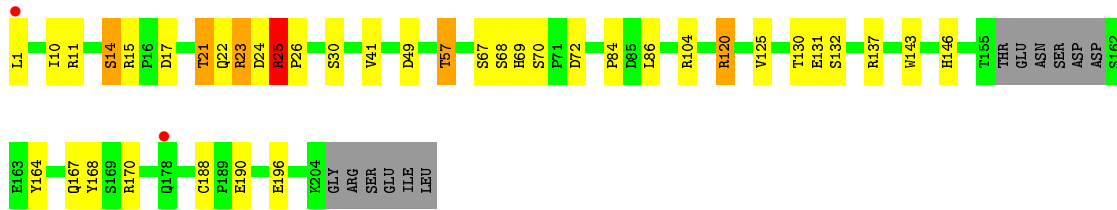
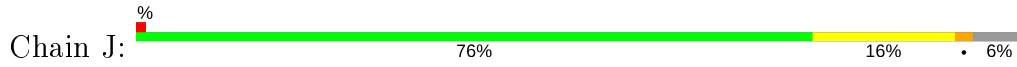


• Molecule 1: Acetylcholine-binding protein

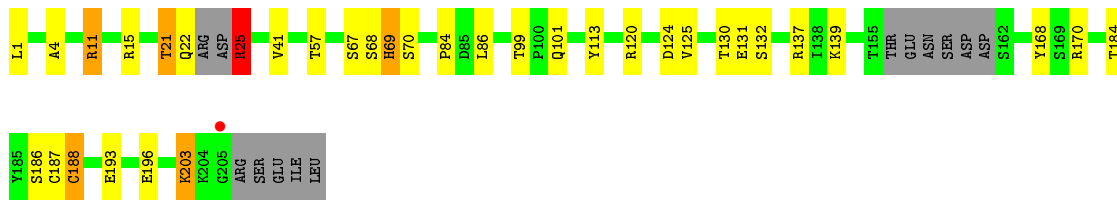
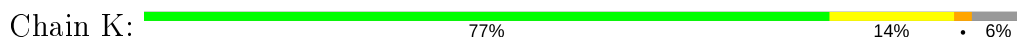




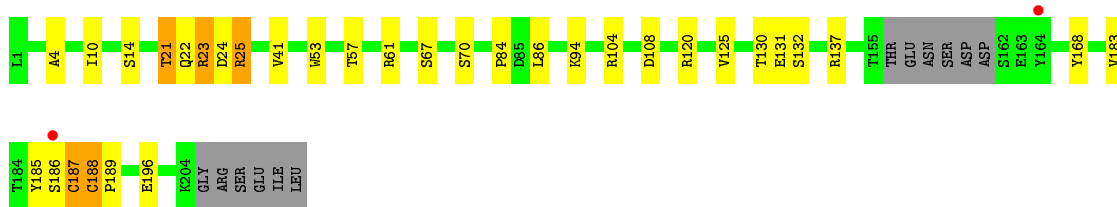
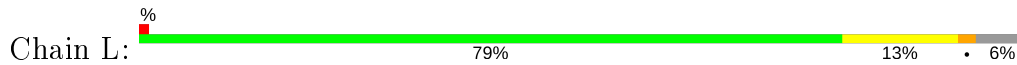
• Molecule 1: Acetylcholine-binding protein



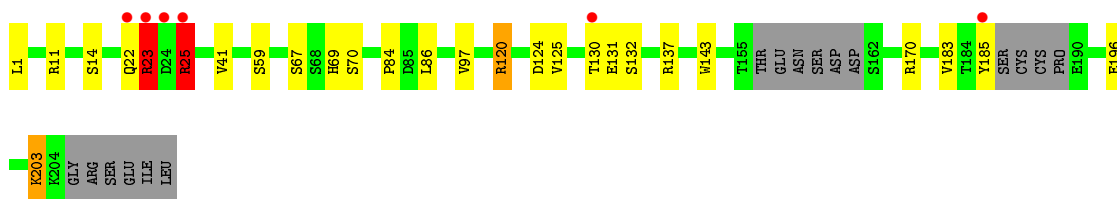
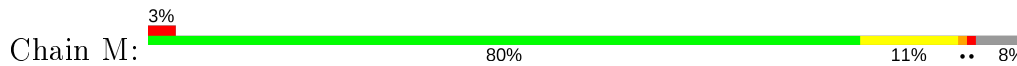
• Molecule 1: Acetylcholine-binding protein



• Molecule 1: Acetylcholine-binding protein

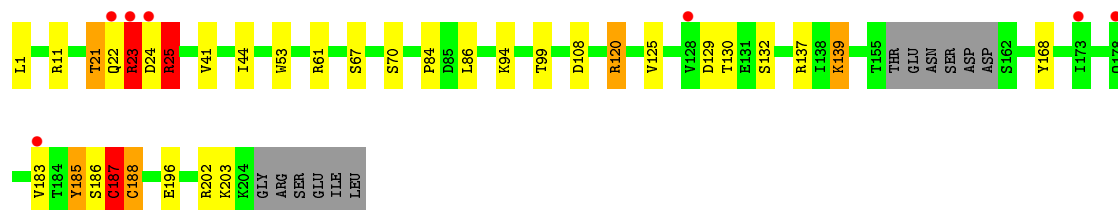


• Molecule 1: Acetylcholine-binding protein



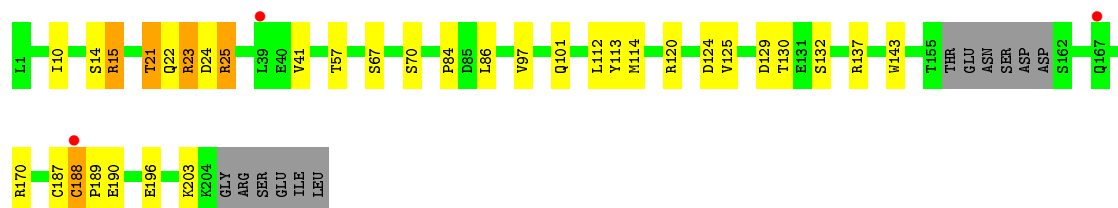
- Molecule 1: Acetylcholine-binding protein

Chain N: 3% 78% 12% •• 6%



- Molecule 1: Acetylcholine-binding protein

Chain O: 1% 78% 14% • 6%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.73Å 140.38Å 119.55Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	28.24 – 2.68 28.24 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.24-2.68) 98.1 (28.24-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.68Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.207 , 0.240 0.208 , 0.240	Depositor DCC
R_{free} test set	5278 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtrriage
Anisotropy	0.296	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.069 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.064 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.075 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.064 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.104 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24523	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, CL, NSE, 1PE, SO4, ACT

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	0.64	4/1621 (0.2%)	0.91	10/2211 (0.5%)
1	B	0.64	3/1621 (0.2%)	0.83	8/2211 (0.4%)
1	C	0.60	4/1621 (0.2%)	0.81	10/2211 (0.5%)
1	D	0.84	8/1613 (0.5%)	1.45	16/2200 (0.7%)
1	E	0.68	5/1621 (0.3%)	0.85	7/2211 (0.3%)
1	F	0.76	7/1645 (0.4%)	0.94	8/2244 (0.4%)
1	G	0.72	4/1629 (0.2%)	1.01	4/2222 (0.2%)
1	H	0.81	8/1621 (0.5%)	0.93	15/2211 (0.7%)
1	I	0.70	6/1602 (0.4%)	0.79	10/2183 (0.5%)
1	J	0.67	7/1621 (0.4%)	0.84	9/2211 (0.4%)
1	K	0.55	3/1605 (0.2%)	0.81	7/2188 (0.3%)
1	L	0.76	2/1629 (0.1%)	0.81	9/2222 (0.4%)
1	M	0.80	7/1602 (0.4%)	0.85	10/2183 (0.5%)
1	N	0.77	6/1621 (0.4%)	1.17	13/2211 (0.6%)
1	O	0.59	3/1621 (0.2%)	0.79	7/2211 (0.3%)
All	All	0.71	77/24293 (0.3%)	0.93	143/33130 (0.4%)

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	A	0	1
1	D	0	1
1	F	0	4
1	G	0	2
1	M	0	1
1	N	0	2
1	O	0	1
All	All	0	12

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	131	GLU	CD-OE1	-18.59	1.05	1.25
1	H	131	GLU	CD-OE1	-16.84	1.07	1.25
1	N	25	ARG	CZ-NH1	-16.34	1.11	1.33
1	G	23	ARG	CZ-NH1	-14.01	1.14	1.33
1	D	131	GLU	CD-OE1	-13.45	1.10	1.25
1	M	25	ARG	CZ-NH2	-12.53	1.16	1.33
1	D	11	ARG	CZ-NH1	-12.22	1.17	1.33
1	D	23	ARG	CZ-NH1	-11.46	1.18	1.33
1	E	23	ARG	CG-CD	-11.04	1.24	1.51
1	N	25	ARG	CG-CD	-10.93	1.24	1.51
1	D	25	ARG	CG-CD	-10.65	1.25	1.51
1	M	25	ARG	CB-CG	-10.55	1.24	1.52
1	J	23	ARG	CG-CD	-10.19	1.26	1.51
1	F	23	ARG	CZ-NH1	-10.13	1.19	1.33
1	M	131	GLU	CB-CG	-10.12	1.32	1.52
1	H	131	GLU	CB-CG	-9.58	1.33	1.52
1	L	23	ARG	CG-CD	-9.55	1.28	1.51
1	I	23	ARG	CB-CG	-9.37	1.27	1.52
1	O	23	ARG	CG-CD	-9.24	1.28	1.51
1	I	131	GLU	CB-CG	-9.06	1.34	1.52
1	B	23	ARG	CG-CD	-8.87	1.29	1.51
1	F	23	ARG	CG-CD	-8.71	1.30	1.51
1	I	131	GLU	CD-OE1	-8.65	1.16	1.25
1	A	23	ARG	CG-CD	-8.64	1.30	1.51
1	F	25	ARG	CB-CG	-8.07	1.30	1.52
1	F	187	CYS	CB-SG	-7.90	1.68	1.82
1	G	23	ARG	CB-CG	-7.81	1.31	1.52
1	B	25	ARG	CB-CG	-7.63	1.31	1.52
1	M	25	ARG	CD-NE	-7.60	1.33	1.46
1	B	25	ARG	CG-CD	-7.57	1.33	1.51
1	J	167	GLN	CB-CG	-7.57	1.32	1.52
1	N	23	ARG	CB-CG	-7.51	1.32	1.52
1	I	23	ARG	CZ-NH1	-7.51	1.23	1.33
1	D	25	ARG	CB-CG	-7.48	1.32	1.52
1	H	23	ARG	CB-CG	-7.35	1.32	1.52
1	D	23	ARG	CD-NE	-7.33	1.33	1.46
1	J	23	ARG	CB-CG	-7.18	1.33	1.52
1	H	23	ARG	CZ-NH1	-7.16	1.23	1.33
1	H	23	ARG	CG-CD	-7.13	1.34	1.51
1	G	25	ARG	CB-CG	-7.12	1.33	1.52
1	A	131	GLU	CB-CG	-7.11	1.38	1.52
1	M	25	ARG	CG-CD	-7.00	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	25	ARG	CZ-NH1	-6.92	1.24	1.33
1	I	23	ARG	CG-CD	-6.71	1.35	1.51
1	E	23	ARG	CB-CG	-6.70	1.34	1.52
1	C	23	ARG	CB-CG	-6.70	1.34	1.52
1	H	25	ARG	CG-CD	-6.44	1.35	1.51
1	D	23	ARG	CB-CG	-6.28	1.35	1.52
1	M	23	ARG	CG-CD	-6.26	1.36	1.51
1	H	25	ARG	CB-CG	-6.23	1.35	1.52
1	H	131	GLU	CG-CD	-6.17	1.42	1.51
1	E	25	ARG	CB-CG	-6.17	1.35	1.52
1	E	25	ARG	CG-CD	-6.16	1.36	1.51
1	C	187	CYS	CB-SG	-6.12	1.71	1.82
1	M	25	ARG	NE-CZ	-6.12	1.25	1.33
1	N	25	ARG	CB-CG	-5.98	1.36	1.52
1	F	23	ARG	CB-CG	-5.97	1.36	1.52
1	J	25	ARG	CG-CD	-5.94	1.37	1.51
1	D	131	GLU	CB-CG	-5.92	1.41	1.52
1	O	25	ARG	CB-CG	-5.83	1.36	1.52
1	N	23	ARG	CG-CD	-5.82	1.37	1.51
1	I	25	ARG	CG-CD	-5.80	1.37	1.51
1	O	25	ARG	CG-CD	-5.75	1.37	1.51
1	C	25	ARG	CB-CG	-5.65	1.37	1.52
1	A	148	ARG	CG-CD	-5.64	1.37	1.51
1	J	22	GLN	CD-OE1	-5.59	1.11	1.24
1	F	25	ARG	CG-CD	-5.54	1.38	1.51
1	K	25	ARG	CB-CG	-5.53	1.37	1.52
1	A	131	GLU	CD-OE1	-5.53	1.19	1.25
1	F	131	GLU	CB-CG	-5.53	1.41	1.52
1	G	23	ARG	CG-CD	-5.44	1.38	1.51
1	N	139	LYS	CB-CG	-5.34	1.38	1.52
1	E	131	GLU	CB-CG	-5.32	1.42	1.52
1	J	22	GLN	CB-CG	-5.20	1.38	1.52
1	K	131	GLU	CB-CG	-5.19	1.42	1.52
1	J	131	GLU	CD-OE1	-5.15	1.20	1.25
1	C	23	ARG	CG-CD	-5.15	1.39	1.51

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	ARG	NE-CZ-NH2	32.15	136.38	120.30
1	N	25	ARG	NE-CZ-NH2	28.76	134.68	120.30
1	D	11	ARG	NE-CZ-NH2	26.92	133.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	23	ARG	NE-CZ-NH2	24.77	132.69	120.30
1	D	11	ARG	NE-CZ-NH1	-23.80	108.40	120.30
1	G	23	ARG	NE-CZ-NH1	-23.38	108.61	120.30
1	N	25	ARG	NE-CZ-NH1	-22.79	108.91	120.30
1	D	23	ARG	NE-CZ-NH1	-22.74	108.93	120.30
1	F	23	ARG	NE-CZ-NH2	20.58	130.59	120.30
1	D	25	ARG	CG-CD-NE	16.20	145.81	111.80
1	H	131	GLU	CA-CB-CG	15.88	148.34	113.40
1	F	23	ARG	NE-CZ-NH1	-13.91	113.35	120.30
1	K	25	ARG	NE-CZ-NH1	-13.73	113.43	120.30
1	K	25	ARG	NE-CZ-NH2	13.67	127.13	120.30
1	M	25	ARG	NE-CZ-NH2	-13.17	113.71	120.30
1	A	148	ARG	CG-CD-NE	12.78	138.63	111.80
1	I	23	ARG	NE-CZ-NH2	12.26	126.43	120.30
1	B	23	ARG	NE-CZ-NH2	12.25	126.42	120.30
1	A	23	ARG	NE-CZ-NH1	-12.07	114.26	120.30
1	L	131	GLU	CG-CD-OE2	11.55	141.41	118.30
1	A	148	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	A	148	ARG	CB-CG-CD	-11.53	81.63	111.60
1	B	25	ARG	NE-CZ-NH1	-11.39	114.61	120.30
1	L	131	GLU	OE1-CD-OE2	-11.32	109.72	123.30
1	E	23	ARG	NE-CZ-NH2	11.21	125.91	120.30
1	B	23	ARG	NE-CZ-NH1	-11.19	114.70	120.30
1	D	25	ARG	NE-CZ-NH1	-11.15	114.73	120.30
1	H	23	ARG	NE-CZ-NH2	10.83	125.72	120.30
1	O	23	ARG	NE-CZ-NH2	10.78	125.69	120.30
1	J	23	ARG	NE-CZ-NH2	10.71	125.65	120.30
1	O	23	ARG	NE-CZ-NH1	-10.54	115.03	120.30
1	N	120	ARG	NE-CZ-NH1	-10.43	115.09	120.30
1	E	23	ARG	NE-CZ-NH1	-10.12	115.24	120.30
1	E	148	ARG	CB-CG-CD	-10.04	85.49	111.60
1	O	25	ARG	NE-CZ-NH1	-9.84	115.38	120.30
1	M	203	LYS	CG-CD-CE	9.79	141.27	111.90
1	I	23	ARG	NE-CZ-NH1	-9.75	115.43	120.30
1	J	120	ARG	CG-CD-NE	9.72	132.20	111.80
1	L	23	ARG	NE-CZ-NH2	9.63	125.12	120.30
1	A	148	ARG	CD-NE-CZ	9.57	137.00	123.60
1	N	139	LYS	CG-CD-CE	9.57	140.61	111.90
1	A	23	ARG	NE-CZ-NH2	9.51	125.05	120.30
1	D	120	ARG	CG-CD-NE	9.37	131.48	111.80
1	D	25	ARG	NE-CZ-NH2	9.31	124.96	120.30
1	C	23	ARG	NE-CZ-NH2	9.29	124.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	ARG	CD-NE-CZ	-9.23	110.67	123.60
1	H	131	GLU	CB-CA-C	-9.06	92.28	110.40
1	H	25	ARG	NE-CZ-NH1	-8.99	115.81	120.30
1	F	25	ARG	CG-CD-NE	8.83	130.34	111.80
1	N	23	ARG	CG-CD-NE	8.68	130.02	111.80
1	J	164	TYR	CB-CG-CD2	-8.65	115.81	121.00
1	B	25	ARG	CG-CD-NE	8.63	129.93	111.80
1	E	25	ARG	NE-CZ-NH1	-8.57	116.01	120.30
1	H	120	ARG	CG-CD-NE	8.49	129.64	111.80
1	E	120	ARG	CG-CD-NE	8.46	129.57	111.80
1	J	22	GLN	CA-CB-CG	8.40	131.89	113.40
1	C	11	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	C	25	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	H	179	LYS	CD-CE-NZ	8.34	130.89	111.70
1	M	203	LYS	CB-CG-CD	-8.23	90.19	111.60
1	D	131	GLU	CG-CD-OE2	8.14	134.57	118.30
1	C	25	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	K	203	LYS	CG-CD-CE	8.08	136.15	111.90
1	J	25	ARG	CG-CD-NE	7.96	128.52	111.80
1	M	23	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	D	23	ARG	CD-NE-CZ	7.88	134.63	123.60
1	H	24	ASP	CB-CG-OD1	-7.85	111.23	118.30
1	G	25	ARG	CG-CD-NE	7.80	128.18	111.80
1	J	23	ARG	NE-CZ-NH1	-7.79	116.41	120.30
1	F	186	SER	CA-CB-OG	7.78	132.19	111.20
1	I	131	GLU	CG-CD-OE2	7.72	133.74	118.30
1	D	131	GLU	OE1-CD-OE2	-7.57	114.22	123.30
1	F	185	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	B	25	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	D	23	ARG	NH1-CZ-NH2	-7.32	111.34	119.40
1	M	120	ARG	CB-CG-CD	7.29	130.56	111.60
1	N	120	ARG	CG-CD-NE	7.27	127.08	111.80
1	I	203	LYS	CD-CE-NZ	7.20	128.27	111.70
1	H	23	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	K	203	LYS	CB-CG-CD	-7.03	93.33	111.60
1	L	23	ARG	NE-CZ-NH1	-6.99	116.80	120.30
1	L	23	ARG	CD-NE-CZ	-6.89	113.95	123.60
1	B	25	ARG	CD-NE-CZ	-6.86	114.00	123.60
1	F	23	ARG	NH1-CZ-NH2	-6.81	111.91	119.40
1	C	11	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	D	120	ARG	CB-CG-CD	6.78	129.22	111.60
1	J	164	TYR	CB-CG-CD1	6.77	125.06	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	139	LYS	CB-CG-CD	6.74	129.12	111.60
1	K	120	ARG	CG-CD-NE	6.72	125.90	111.80
1	M	203	LYS	CD-CE-NZ	6.67	127.05	111.70
1	M	25	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	N	23	ARG	CB-CG-CD	6.65	128.88	111.60
1	H	131	GLU	CG-CD-OE2	6.62	131.54	118.30
1	I	23	ARG	CB-CA-C	-6.49	97.41	110.40
1	M	11	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	A	25	ARG	CB-CG-CD	-6.43	94.87	111.60
1	E	11	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	M	23	ARG	CA-CB-CG	6.26	127.17	113.40
1	N	11	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	J	120	ARG	CB-CG-CD	6.25	127.86	111.60
1	I	203	LYS	CG-CD-CE	6.17	130.41	111.90
1	H	120	ARG	CB-CG-CD	6.16	127.60	111.60
1	B	190	GLU	CA-CB-CG	-6.14	99.89	113.40
1	H	25	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	L	25	ARG	CB-CG-CD	-6.11	95.71	111.60
1	I	25	ARG	CB-CG-CD	-6.11	95.72	111.60
1	N	25	ARG	CA-CB-CG	6.10	126.82	113.40
1	C	23	ARG	CA-CB-CG	6.01	126.61	113.40
1	L	131	GLU	CA-CB-CG	5.89	126.37	113.40
1	K	11	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	O	25	ARG	CB-CG-CD	-5.83	96.43	111.60
1	H	131	GLU	CG-CD-OE1	-5.79	106.72	118.30
1	M	131	GLU	CA-CB-CG	5.79	126.13	113.40
1	H	120	ARG	CA-CB-CG	5.75	126.06	113.40
1	H	131	GLU	N-CA-CB	5.75	120.95	110.60
1	C	23	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	D	25	ARG	CB-CG-CD	5.75	126.54	111.60
1	F	23	ARG	CG-CD-NE	5.73	123.83	111.80
1	L	120	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	N	23	ARG	CD-NE-CZ	5.64	131.50	123.60
1	N	25	ARG	CB-CA-C	-5.62	99.15	110.40
1	C	120	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	23	ARG	CD-NE-CZ	-5.59	115.78	123.60
1	A	22	GLN	N-CA-C	-5.58	95.92	111.00
1	H	25	ARG	CG-CD-NE	5.56	123.48	111.80
1	G	23	ARG	CB-CA-C	-5.55	99.30	110.40
1	C	25	ARG	CD-NE-CZ	5.52	131.33	123.60
1	K	11	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	E	25	ARG	NE-CZ-NH2	5.47	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	25	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	C	23	ARG	CB-CA-C	-5.39	99.62	110.40
1	N	23	ARG	CA-CB-CG	5.38	125.23	113.40
1	O	120	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	I	185	TYR	CB-CG-CD2	-5.29	117.82	121.00
1	D	120	ARG	CA-CB-CG	5.24	124.94	113.40
1	A	25	ARG	CG-CD-NE	5.24	122.81	111.80
1	O	23	ARG	CD-NE-CZ	-5.20	116.32	123.60
1	L	131	GLU	CG-CD-OE1	-5.11	108.09	118.30
1	I	131	GLU	CG-CD-OE1	-5.08	108.14	118.30
1	B	23	ARG	CD-NE-CZ	-5.05	116.53	123.60
1	F	162	SER	C-N-CA	-5.04	109.11	121.70
1	J	11	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	I	120	ARG	NE-CZ-NH1	-5.03	117.79	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ARG	Sidechain
1	D	23	ARG	Sidechain
1	F	185	TYR	Sidechain
1	F	23	ARG	Sidechain
1	F	25	ARG	Sidechain
1	F	40	GLU	Sidechain
1	G	25	ARG	Sidechain
1	G	69	HIS	Sidechain
1	M	25	ARG	Sidechain
1	N	120	ARG	Sidechain
1	N	23	ARG	Sidechain
1	O	170	ARG	Sidechain

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	1586	0	1545	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1586	0	1545	28	0
1	C	1586	0	1545	22	0
1	D	1578	0	1530	18	0
1	E	1586	0	1545	35	0
1	F	1607	0	1564	34	0
1	G	1591	0	1557	29	0
1	H	1586	0	1545	21	0
1	I	1568	0	1532	26	0
1	J	1586	0	1545	25	0
1	K	1571	0	1530	20	0
1	L	1591	0	1549	21	0
1	M	1566	0	1535	30	0
1	N	1586	0	1545	21	0
1	O	1586	0	1545	20	0
2	A	16	0	22	0	0
2	B	16	0	22	2	0
2	C	16	0	22	1	0
2	D	16	0	22	3	0
2	E	16	0	22	2	0
2	G	16	0	22	1	0
2	H	16	0	22	3	0
2	I	16	0	22	5	0
3	D	14	0	13	0	0
3	G	14	0	12	0	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
4	E	25	0	0	1	0
4	F	10	0	0	0	0
4	G	15	0	0	0	0
4	I	5	0	0	0	0
4	J	5	0	0	1	0
4	M	5	0	0	0	0
5	A	8	0	6	0	0
5	D	4	0	3	0	0
5	F	16	0	12	1	0
5	G	12	0	9	0	0
5	J	4	0	3	0	0
5	O	4	0	3	0	0
6	A	19	0	8	2	0
6	B	19	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	19	0	8	1	0
6	I	19	0	8	1	0
6	K	19	0	8	2	0
6	M	19	0	8	2	0
7	A	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	N	1	0	0	0	0
8	J	6	0	8	0	0
9	A	28	0	0	1	0
9	B	19	0	0	0	0
9	C	22	0	0	1	0
9	D	27	0	0	2	0
9	E	23	0	0	1	0
9	F	31	0	0	0	0
9	G	28	0	0	0	0
9	H	26	0	0	1	0
9	I	21	0	0	0	0
9	J	21	0	0	1	0
9	K	26	0	0	2	0
9	L	24	0	0	0	0
9	M	21	0	0	1	0
9	N	5	0	0	0	0
9	O	13	0	0	0	0
All	All	24523	0	23450	332	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 7.

All (332) 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:E:148:ARG:CZ	1:M:25:ARG:HH22	1.57	1.18
1:E:148:ARG:CZ	1:M:25:ARG:NH2	2.21	1.02
1:A:153:ASP:OD1	1:F:179:LYS:NZ	1.93	1.01
1:E:65:TRP:HB3	2:E:302:1PE:H261	1.43	0.98
1:D:23:ARG:HG3	1:D:23:ARG:O	1.67	0.93
1:E:148:ARG:HD3	1:M:25:ARG:CZ	2.04	0.88
1:E:148:ARG:HD3	1:M:25:ARG:NH2	1.93	0.84
1:J:30:SER:HB2	1:J:57:THR:HG22	1.61	0.82
1:I:65:TRP:HB3	2:I:302:1PE:H151	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:ASN:HD22	2:E:302:1PE:H162	1.44	0.82
1:H:15:ARG:NH2	1:I:4:ALA:O	2.13	0.81
1:H:22:GLN:O	1:H:23:ARG:HB3	1.81	0.80
1:F:23:ARG:HG3	1:F:25:ARG:HD2	1.63	0.80
1:E:148:ARG:NE	1:M:25:ARG:HH22	1.78	0.80
1:E:148:ARG:NE	1:M:25:ARG:NH2	2.31	0.77
1:K:170:ARG:HH21	1:K:203:LYS:HE2	1.50	0.77
1:F:160:ASP:HB3	1:F:163:GLU:HB2	1.67	0.77
1:C:22:GLN:O	1:C:23:ARG:HB2	1.82	0.77
1:L:23:ARG:HB3	1:L:25:ARG:HG3	1.66	0.77
1:M:170:ARG:HH21	1:M:203:LYS:HE2	1.50	0.76
1:G:91:ALA:HB1	1:G:119:GLN:HE21	1.51	0.75
1:N:22:GLN:O	1:N:23:ARG:HB3	1.86	0.74
1:E:148:ARG:CD	1:M:25:ARG:NH2	2.50	0.74
1:F:23:ARG:HH11	1:F:23:ARG:HG2	1.52	0.74
1:G:23:ARG:HB2	1:G:25:ARG:HD2	1.69	0.73
1:H:130:THR:HG22	1:H:132:SER:H	1.53	0.73
1:M:130:THR:HG22	1:M:132:SER:H	1.55	0.72
1:D:130:THR:HG22	1:D:132:SER:H	1.55	0.71
1:E:148:ARG:NH1	1:M:25:ARG:NH2	2.38	0.71
1:L:61:ARG:NH1	1:L:108:ASP:O	2.24	0.71
1:G:15:ARG:NH2	1:G:17:ASP:OD2	2.23	0.70
1:M:22:GLN:O	1:M:23:ARG:HB3	1.89	0.70
1:D:148:ARG:NH1	9:D:407:HOH:O	2.25	0.69
1:I:1:LEU:HD11	2:I:302:1PE:H161	1.75	0.69
1:A:23:ARG:HB3	1:A:25:ARG:HG3	1.75	0.68
1:B:130:THR:HG22	1:B:132:SER:H	1.58	0.67
1:C:202:ARG:NH2	9:C:412:HOH:O	2.17	0.67
1:G:22:GLN:O	1:G:23:ARG:HB2	1.94	0.67
1:I:130:THR:HG22	1:I:132:SER:H	1.58	0.67
1:E:148:ARG:CD	1:M:25:ARG:CZ	2.72	0.67
1:O:130:THR:HG22	1:O:132:SER:H	1.58	0.67
1:F:130:THR:HG22	1:F:132:SER:H	1.60	0.67
1:A:181:ASN:HA	1:F:182:SER:O	1.94	0.67
1:F:22:GLN:O	1:F:23:ARG:HB3	1.94	0.67
1:K:130:THR:HG22	1:K:132:SER:H	1.61	0.66
1:K:15:ARG:NH2	1:L:4:ALA:O	2.28	0.66
6:M:301:NSE:H5	1:N:53:TRP:CH2	2.30	0.66
1:F:183:VAL:CG1	1:F:185:TYR:HE1	2.08	0.66
1:G:124:ASP:HB2	1:H:168:TYR:CE1	2.31	0.65
1:O:187:CYS:SG	1:O:188:CYS:N	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:THR:HG22	1:G:132:SER:H	1.61	0.65
1:J:130:THR:HG22	1:J:132:SER:H	1.62	0.65
1:C:130:THR:HG22	1:C:132:SER:H	1.61	0.65
1:M:170:ARG:NH2	1:M:203:LYS:HE2	2.11	0.65
1:C:65:TRP:HB3	2:C:301:1PE:H261	1.78	0.65
1:F:187:CYS:SG	1:F:188:CYS:N	2.70	0.64
1:N:130:THR:HG22	1:N:132:SER:H	1.61	0.64
1:H:61:ARG:NH2	9:H:403:HOH:O	2.29	0.64
1:L:130:THR:HG22	1:L:132:SER:H	1.62	0.64
1:F:23:ARG:CG	1:F:25:ARG:HD2	2.28	0.64
1:B:129:ASP:OD1	1:B:203:LYS:HE3	1.98	0.64
1:A:130:THR:HG22	1:A:132:SER:H	1.63	0.63
1:O:23:ARG:HB3	1:O:25:ARG:HG3	1.80	0.63
1:J:25:ARG:HH11	1:J:25:ARG:HG2	1.62	0.63
1:A:22:GLN:O	1:A:23:ARG:HB3	1.99	0.62
1:O:22:GLN:O	1:O:23:ARG:HB3	2.00	0.62
1:K:22:GLN:O	1:K:25:ARG:HG3	2.00	0.62
1:O:129:ASP:OD1	1:O:203:LYS:HE3	1.98	0.62
1:D:168:TYR:CE1	1:C:124:ASP:HB2	2.35	0.62
1:I:14:SER:O	1:I:16:PRO:HD3	2.00	0.62
1:L:23:ARG:O	1:L:24:ASP:HB2	2.00	0.62
1:K:4:ALA:O	1:O:15:ARG:NH1	2.32	0.62
6:M:301:NSE:H5	1:N:53:TRP:CZ3	2.35	0.62
1:B:22:GLN:O	1:B:23:ARG:HB3	2.00	0.61
6:K:301:NSE:H8	1:L:104:ARG:HB2	1.81	0.61
1:C:187:CYS:SG	1:C:188:CYS:N	2.74	0.60
1:A:181:ASN:OD1	1:F:182:SER:HB3	2.01	0.60
1:L:22:GLN:O	1:L:23:ARG:HB3	2.01	0.60
1:N:23:ARG:O	1:N:24:ASP:HB2	2.01	0.60
1:D:162:SER:O	9:D:413:HOH:O	2.17	0.60
1:A:15:ARG:NH2	1:A:17:ASP:OD2	2.35	0.59
1:L:94:LYS:HE3	1:M:97:VAL:O	2.01	0.59
1:G:44:ILE:HG22	1:H:170:ARG:HD2	1.84	0.59
1:G:23:ARG:O	1:G:24:ASP:HB2	2.03	0.59
1:D:170:ARG:HD2	1:C:44:ILE:HG22	1.84	0.59
1:F:160:ASP:OD1	1:L:189:PRO:HB3	2.03	0.58
1:B:137:ARG:NH1	4:B:303:SO4:O2	2.33	0.58
1:E:21:THR:HG22	1:E:25:ARG:O	2.04	0.58
1:L:21:THR:HG22	1:L:25:ARG:O	2.03	0.58
1:L:10:ILE:O	1:L:14:SER:HB3	2.03	0.58
1:N:21:THR:HG22	1:N:25:ARG:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:ARG:CB	1:G:25:ARG:HD2	2.35	0.57
1:E:148:ARG:CD	1:M:25:ARG:NH1	2.67	0.57
1:M:124:ASP:HB2	1:N:168:TYR:CE1	2.40	0.56
1:L:187:CYS:SG	1:L:188:CYS:N	2.78	0.56
1:B:23:ARG:O	1:B:24:ASP:HB2	2.05	0.56
1:B:187:CYS:SG	1:B:188:CYS:N	2.79	0.56
1:G:91:ALA:HB1	1:G:119:GLN:NE2	2.19	0.56
1:A:21:THR:HG22	1:A:25:ARG:O	2.05	0.56
1:B:23:ARG:HB3	1:B:25:ARG:HG3	1.87	0.56
1:G:60:ASP:OD1	1:G:62:THR:HB	2.06	0.56
1:F:183:VAL:CG1	1:F:185:TYR:CE1	2.89	0.55
1:D:23:ARG:O	1:D:24:ASP:HB2	2.06	0.55
1:A:23:ARG:O	1:A:24:ASP:HB2	2.08	0.54
1:H:15:ARG:HH21	1:I:4:ALA:HA	1.72	0.54
1:K:21:THR:HG22	1:K:25:ARG:O	2.08	0.54
1:E:148:ARG:CG	1:M:25:ARG:NH1	2.70	0.54
1:C:23:ARG:O	1:C:24:ASP:HB2	2.08	0.54
1:O:23:ARG:O	1:O:24:ASP:HB2	2.07	0.54
1:I:6:ILE:HG23	2:I:302:1PE:H152	1.88	0.54
1:K:170:ARG:NH2	1:K:203:LYS:HE2	2.19	0.54
1:F:14:SER:OG	1:F:80:SER:O	2.17	0.54
1:I:21:THR:HG22	1:I:25:ARG:O	2.08	0.54
1:F:183:VAL:HG12	1:F:185:TYR:CE1	2.42	0.54
1:G:21:THR:HG22	1:G:25:ARG:O	2.08	0.54
1:O:21:THR:HG22	1:O:25:ARG:O	2.07	0.54
1:E:148:ARG:HG3	1:M:25:ARG:NH1	2.22	0.54
1:C:11:ARG:O	1:C:14:SER:HB3	2.08	0.53
1:L:22:GLN:O	1:L:23:ARG:CB	2.55	0.53
6:A:301:NSE:H5	1:B:53:TRP:CZ3	2.43	0.53
1:C:14:SER:C	1:C:16:PRO:HD3	2.28	0.53
1:D:21:THR:HG22	1:D:25:ARG:O	2.07	0.53
1:K:124:ASP:HB2	1:L:168:TYR:CE1	2.43	0.53
1:I:9:ASN:ND2	2:I:302:1PE:H162	2.24	0.53
1:E:148:ARG:NH1	1:M:25:ARG:HH21	2.05	0.53
1:H:22:GLN:O	1:H:25:ARG:HG3	2.09	0.53
1:I:23:ARG:HG2	1:I:23:ARG:HH11	1.72	0.53
1:B:9:ASN:HB3	2:B:302:1PE:H151	1.90	0.52
1:G:187:CYS:C	1:G:188:CYS:SG	2.87	0.52
1:M:14:SER:HB3	9:M:401:HOH:O	2.08	0.52
1:M:23:ARG:HG2	1:M:25:ARG:HE	1.73	0.52
1:I:22:GLN:O	1:I:23:ARG:HB2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:THR:O	1:F:186:SER:HB3	2.09	0.52
6:K:301:NSE:H5	1:L:53:TRP:CH2	2.44	0.52
1:N:94:LYS:HE3	1:O:97:VAL:O	2.07	0.52
1:A:22:GLN:O	1:A:23:ARG:CB	2.57	0.52
1:I:22:GLN:O	1:I:25:ARG:HG3	2.09	0.52
1:M:143:TRP:CZ2	1:N:99:THR:HG21	2.45	0.52
1:E:124:ASP:HB2	1:A:168:TYR:CE1	2.44	0.52
1:J:21:THR:HG22	1:J:25:ARG:O	2.10	0.52
1:C:21:THR:HG22	1:C:25:ARG:O	2.10	0.52
1:F:129:ASP:OD1	1:F:203:LYS:HE3	2.10	0.52
1:H:21:THR:HG22	1:H:25:ARG:O	2.09	0.51
1:I:23:ARG:HB2	1:I:25:ARG:HG3	1.92	0.51
1:M:22:GLN:O	1:M:25:ARG:HG3	2.11	0.51
1:B:21:THR:HG22	1:B:25:ARG:O	2.10	0.51
1:F:167:GLN:NE2	5:F:306:ACT:OXT	2.44	0.51
1:C:15:ARG:NH2	1:C:17:ASP:OD2	2.43	0.51
1:H:137:ARG:HD2	1:H:196:GLU:OE1	2.10	0.51
1:D:9:ASN:HB2	2:D:301:1PE:H162	1.94	0.50
1:G:68:SER:OG	1:G:69:HIS:N	2.44	0.50
1:I:124:ASP:HB2	1:J:168:TYR:CE1	2.46	0.50
1:I:137:ARG:HD2	1:I:196:GLU:OE1	2.10	0.50
1:A:84:PRO:HB2	1:A:86:LEU:HG	1.94	0.50
1:A:137:ARG:HD2	1:A:196:GLU:OE1	2.11	0.50
1:G:13:THR:HG21	2:G:301:1PE:H142	1.93	0.50
1:F:21:THR:HG22	1:F:25:ARG:O	2.12	0.50
1:E:22:GLN:O	1:E:25:ARG:HG3	2.12	0.49
1:O:22:GLN:O	1:O:23:ARG:CB	2.60	0.49
1:H:9:ASN:HB2	2:H:301:1PE:H161	1.92	0.49
1:A:112:LEU:HD11	1:A:114:MET:HE2	1.94	0.49
1:F:183:VAL:HG12	1:F:185:TYR:HE1	1.77	0.49
1:J:190:GLU:HG3	9:J:412:HOH:O	2.12	0.49
1:I:44:ILE:HG22	1:J:170:ARG:HD2	1.95	0.49
1:L:137:ARG:HD2	1:L:196:GLU:OE1	2.13	0.49
1:G:137:ARG:HD2	1:G:196:GLU:OE1	2.13	0.49
1:A:180:LYS:O	1:F:182:SER:N	2.37	0.49
1:J:137:ARG:HD2	1:J:196:GLU:OE1	2.13	0.48
1:J:49:ASP:OD2	1:J:120:ARG:HD2	2.11	0.48
1:F:137:ARG:HD2	1:F:196:GLU:OE1	2.13	0.48
1:D:49:ASP:OD2	1:D:120:ARG:HD2	2.12	0.48
1:E:137:ARG:HD2	1:E:196:GLU:OE1	2.14	0.48
1:F:23:ARG:O	1:F:24:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ARG:HB3	1:E:25:ARG:HG3	1.94	0.48
1:E:139:LYS:HE3	4:E:307:SO4:O4	2.14	0.48
1:F:99:THR:HG21	1:J:143:TRP:CZ2	2.49	0.47
1:N:22:GLN:O	1:N:25:ARG:HG2	2.14	0.47
1:O:137:ARG:HD2	1:O:196:GLU:OE1	2.14	0.47
6:A:301:NSE:H8	1:B:104:ARG:HB2	1.96	0.47
1:B:41:VAL:HG13	1:B:125:VAL:HG11	1.97	0.47
1:E:139:LYS:NZ	9:E:414:HOH:O	2.33	0.47
1:D:22:GLN:O	1:D:23:ARG:HB3	2.14	0.47
1:I:185:TYR:CD1	1:I:185:TYR:N	2.82	0.47
1:K:99:THR:HG21	1:O:143:TRP:CZ2	2.49	0.47
1:A:66:ASN:ND2	9:A:416:HOH:O	2.46	0.47
1:H:23:ARG:O	1:H:23:ARG:HG3	2.14	0.47
1:J:146:HIS:CD2	1:J:190:GLU:HG2	2.50	0.47
1:O:10:ILE:O	1:O:14:SER:HB2	2.14	0.47
1:B:146:HIS:CE1	1:B:190:GLU:OE1	2.68	0.47
1:K:137:ARG:HD2	1:K:196:GLU:OE1	2.14	0.47
1:B:15:ARG:N	1:B:16:PRO:HD3	2.29	0.47
1:J:84:PRO:HB2	1:J:86:LEU:HG	1.96	0.47
1:B:137:ARG:HD2	1:B:196:GLU:OE1	2.14	0.47
1:D:101:GLN:OE1	1:D:113:TYR:OH	2.31	0.47
1:G:112[A]:LEU:HD11	1:G:114:MET:HE2	1.97	0.47
1:N:137:ARG:HD2	1:N:196:GLU:OE1	2.14	0.47
1:J:72:ASP:N	4:J:301:SO4:O1	2.26	0.47
1:K:84:PRO:HB2	1:K:86:LEU:HG	1.96	0.47
1:K:168:TYR:CE1	1:O:124:ASP:HB2	2.50	0.46
1:A:137:ARG:NH2	4:A:303:SO4:O1	2.36	0.46
1:L:41:VAL:HG13	1:L:125:VAL:HG11	1.97	0.46
1:O:101:GLN:OE1	1:O:113:TYR:OH	2.29	0.46
1:E:129:ASP:OD1	1:E:203:LYS:HE3	2.14	0.46
1:F:101:GLN:OE1	1:F:113:TYR:OH	2.28	0.46
1:F:41:VAL:HG13	1:F:125:VAL:HG11	1.97	0.46
1:H:49:ASP:OD2	1:H:120:ARG:HD2	2.16	0.46
1:J:146:HIS:CG	1:J:190:GLU:HG2	2.50	0.46
1:N:84:PRO:HB2	1:N:86:LEU:HG	1.96	0.46
1:A:185:TYR:HA	1:F:186:SER:HB3	1.97	0.46
1:C:137:ARG:HD2	1:C:196:GLU:OE1	2.14	0.46
2:D:301:1PE:OH2	2:D:301:1PE:H232	2.16	0.46
1:H:41:VAL:HG13	1:H:125:VAL:HG11	1.97	0.46
1:J:10:ILE:O	1:J:14:SER:HB2	2.16	0.46
1:I:185:TYR:HD1	1:I:185:TYR:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ALA:CB	1:G:119:GLN:NE2	2.79	0.46
1:L:185:TYR:CD1	1:L:185:TYR:N	2.84	0.46
1:J:23:ARG:O	1:J:24:ASP:HB2	2.14	0.46
1:A:143:TRP:CZ2	1:B:99:THR:HG21	2.50	0.45
1:E:59:SER:OG	1:E:110:GLU:OE2	2.32	0.45
1:M:41:VAL:HG13	1:M:125:VAL:HG11	1.98	0.45
1:M:137:ARG:HD2	1:M:196:GLU:OE1	2.17	0.45
1:D:137:ARG:HD2	1:D:196:GLU:OE1	2.17	0.45
1:D:41:VAL:HG13	1:D:125:VAL:HG11	1.98	0.45
1:B:22:GLN:O	1:B:25:ARG:HG3	2.17	0.45
1:B:23:ARG:HB3	1:B:25:ARG:CG	2.47	0.45
1:F:67:SER:HA	1:F:70:SER:HB2	1.98	0.45
1:G:101:GLN:OE1	1:G:113:TYR:OH	2.32	0.45
1:N:41:VAL:HG13	1:N:125:VAL:HG11	1.97	0.45
1:N:25:ARG:HH11	1:N:25:ARG:HD3	1.33	0.45
1:A:41:VAL:HG13	1:A:125:VAL:HG11	1.98	0.45
1:C:185:TYR:N	1:C:185:TYR:CD1	2.85	0.45
1:C:84:PRO:HB2	1:C:86:LEU:HG	1.99	0.45
1:K:41:VAL:HG13	1:K:125:VAL:HG11	1.97	0.45
1:O:41:VAL:HG13	1:O:125:VAL:HG11	1.99	0.45
1:E:101:GLN:OE1	1:E:113:TYR:OH	2.31	0.45
1:C:101:GLN:OE1	1:C:113:TYR:OH	2.30	0.45
1:G:99:THR:HG21	1:F:143:TRP:CZ2	2.52	0.45
1:L:183:VAL:HG12	1:L:185:TYR:CE1	2.52	0.45
1:E:22:GLN:O	1:E:23:ARG:CB	2.64	0.44
1:I:84:PRO:HB2	1:I:86:LEU:HG	1.99	0.44
1:J:25:ARG:HB3	1:J:26:PRO:HD2	1.99	0.44
1:B:185:TYR:N	1:B:185:TYR:CD1	2.85	0.44
1:B:183:VAL:HG12	1:B:185:TYR:CE1	2.52	0.44
1:D:84:PRO:HB2	1:D:86:LEU:HG	1.99	0.44
1:E:49:ASP:OD2	1:E:120:ARG:HD2	2.17	0.44
1:E:187:CYS:SG	1:E:188:CYS:N	2.90	0.44
1:O:25:ARG:HD3	1:O:25:ARG:HH11	1.40	0.44
2:D:301:1PE:H131	2:D:301:1PE:H141	1.79	0.44
1:K:193:GLU:O	9:K:408:HOH:O	2.21	0.44
1:B:68:SER:OG	1:B:69:HIS:N	2.51	0.44
1:K:139:LYS:NZ	9:K:426:HOH:O	2.39	0.44
1:A:1:LEU:HB2	1:A:70:SER:OG	2.18	0.44
1:D:67:SER:HA	1:D:70:SER:HB2	2.00	0.44
1:G:185:TYR:N	1:G:185:TYR:CD1	2.86	0.44
1:J:68:SER:OG	1:J:69:HIS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:84:PRO:HB2	1:M:86:LEU:HG	1.99	0.44
1:N:187:CYS:SG	1:N:188:CYS:N	2.91	0.44
1:A:124:ASP:HB2	1:B:168:TYR:CE1	2.52	0.43
1:H:84:PRO:HB2	1:H:86:LEU:HG	1.99	0.43
1:B:84:PRO:HB2	1:B:86:LEU:HG	1.99	0.43
1:D:99:THR:HG21	1:C:143:TRP:CZ2	2.54	0.43
1:C:41:VAL:HG13	1:C:125:VAL:HG11	2.00	0.43
1:E:67:SER:HA	1:E:70:SER:HB2	2.00	0.43
1:J:41:VAL:HG13	1:J:125:VAL:HG11	1.99	0.43
1:K:68:SER:OG	1:K:69:HIS:N	2.51	0.43
1:B:101:GLN:OE1	1:B:113:TYR:OH	2.30	0.43
1:B:22:GLN:O	1:B:23:ARG:CB	2.59	0.43
1:C:67:SER:HA	1:C:70:SER:HB2	2.00	0.43
1:E:41:VAL:HG13	1:E:125:VAL:HG11	1.99	0.43
6:I:301:NSE:H8	1:J:104:ARG:HB2	2.00	0.43
1:J:1:LEU:HB2	1:J:70:SER:OG	2.18	0.43
1:O:67:SER:HA	1:O:70:SER:HB2	2.00	0.43
1:I:41:VAL:HG13	1:I:125:VAL:HG11	2.00	0.43
1:K:1:LEU:HB2	1:K:70:SER:OG	2.18	0.43
1:M:1:LEU:HB2	1:M:70:SER:OG	2.18	0.43
1:F:1:LEU:HB2	1:F:70:SER:OG	2.19	0.43
1:H:25:ARG:HH11	1:H:25:ARG:HD3	1.39	0.43
1:J:15:ARG:HB3	1:J:15:ARG:HE	1.77	0.43
1:A:146:HIS:CE1	1:A:190:GLU:HG2	2.54	0.42
1:E:1:LEU:HB2	1:E:70:SER:OG	2.19	0.42
1:G:41:VAL:HG13	1:G:125:VAL:HG11	2.00	0.42
1:F:99:THR:HG21	1:J:143:TRP:CE2	2.54	0.42
1:H:101:GLN:OE1	1:H:113:TYR:OH	2.33	0.42
1:L:84:PRO:HB2	1:L:86:LEU:HG	2.00	0.42
1:H:67:SER:HA	1:H:70:SER:HB2	2.00	0.42
1:E:68:SER:OG	1:E:69:HIS:N	2.52	0.42
1:I:23:ARG:O	1:I:24:ASP:HB2	2.20	0.42
1:L:67:SER:HA	1:L:70:SER:HB2	2.00	0.42
1:F:84:PRO:HB2	1:F:86:LEU:HG	2.01	0.42
1:I:67:SER:HA	1:I:70:SER:HB2	2.01	0.42
1:J:67:SER:HA	1:J:70:SER:HB2	2.02	0.42
1:N:129:ASP:OD1	1:N:203:LYS:HE3	2.19	0.42
1:N:185:TYR:N	1:N:185:TYR:CD1	2.87	0.42
1:B:1:LEU:HB2	1:B:70:SER:OG	2.19	0.42
6:E:301:NSE:C2	1:A:114:MET:HB3	2.49	0.42
1:K:187:CYS:SG	1:K:188:CYS:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ARG:HD3	1:B:23:ARG:HH11	1.40	0.42
1:D:149:GLU:CD	1:E:104:ARG:HH22	2.23	0.42
2:H:301:1PE:H142	2:H:301:1PE:H151	1.81	0.42
1:M:183:VAL:HG12	1:M:185:TYR:CE1	2.55	0.42
1:O:84:PRO:HB2	1:O:86:LEU:HG	2.01	0.42
1:C:112:LEU:HD11	1:C:114:MET:HE2	2.01	0.41
1:G:67:SER:HA	1:G:70:SER:HB2	2.01	0.41
1:G:1:LEU:HB2	1:G:70:SER:OG	2.20	0.41
1:J:17:ASP:N	1:J:17:ASP:OD1	2.50	0.41
1:B:63:LEU:O	2:B:302:1PE:H262	2.20	0.41
1:C:1:LEU:HB2	1:C:70:SER:OG	2.21	0.41
1:G:168:TYR:CE1	1:F:124:ASP:HB2	2.55	0.41
1:H:143:TRP:CZ2	1:I:99:THR:HG21	2.55	0.41
1:H:1:LEU:HB2	1:H:70:SER:OG	2.20	0.41
1:M:185:TYR:N	1:M:185:TYR:CD1	2.88	0.41
1:N:183:VAL:HG12	1:N:185:TYR:CE1	2.55	0.41
1:E:84:PRO:HB2	1:E:86:LEU:HG	2.02	0.41
1:G:84:PRO:HB2	1:G:86:LEU:HG	2.03	0.41
1:K:101:GLN:OE1	1:K:113:TYR:OH	2.34	0.41
1:C:183:VAL:HG12	1:C:185:TYR:CE1	2.56	0.41
1:E:130:THR:HG22	1:E:132:SER:H	1.85	0.41
1:G:183:VAL:HG12	1:G:185:TYR:CE1	2.56	0.41
1:G:1:LEU:HA	1:G:1:LEU:HD23	1.90	0.41
1:O:112:LEU:HD11	1:O:114:MET:HE2	2.02	0.41
1:G:146:HIS:CE1	1:G:190:GLU:OE1	2.74	0.41
1:N:67:SER:HA	1:N:70:SER:HB2	2.03	0.41
1:A:68:SER:OG	1:A:69:HIS:N	2.54	0.40
1:I:183:VAL:HG12	1:I:185:TYR:CE1	2.56	0.40
1:N:1:LEU:HB2	1:N:70:SER:OG	2.21	0.40
1:I:9:ASN:HD22	2:I:302:1PE:H162	1.84	0.40
1:K:67:SER:HA	1:K:70:SER:HB2	2.03	0.40
1:N:61:ARG:NH1	1:N:108:ASP:O	2.50	0.40
1:F:23:ARG:HH11	1:F:23:ARG:CG	2.23	0.40
2:H:301:1PE:H151	2:H:301:1PE:H162	1.66	0.40
1:H:143:TRP:CE2	1:I:99:THR:HG21	2.56	0.40
1:M:67:SER:HA	1:M:70:SER:HB2	2.02	0.40

There are no symmetry-related clashes.

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	A	194/210 (92%)	187 (96%)	7 (4%)	0	100	100
1	B	194/210 (92%)	189 (97%)	5 (3%)	0	100	100
1	C	194/210 (92%)	185 (95%)	9 (5%)	0	100	100
1	D	193/210 (92%)	186 (96%)	6 (3%)	1 (0%)	29	52
1	E	194/210 (92%)	189 (97%)	5 (3%)	0	100	100
1	F	197/210 (94%)	186 (94%)	11 (6%)	0	100	100
1	G	195/210 (93%)	189 (97%)	6 (3%)	0	100	100
1	H	194/210 (92%)	187 (96%)	7 (4%)	0	100	100
1	I	189/210 (90%)	185 (98%)	4 (2%)	0	100	100
1	J	194/210 (92%)	186 (96%)	8 (4%)	0	100	100
1	K	191/210 (91%)	186 (97%)	5 (3%)	0	100	100
1	L	195/210 (93%)	189 (97%)	6 (3%)	0	100	100
1	M	189/210 (90%)	184 (97%)	5 (3%)	0	100	100
1	N	194/210 (92%)	186 (96%)	7 (4%)	1 (0%)	29	52
1	O	194/210 (92%)	185 (95%)	7 (4%)	2 (1%)	15	34
All	All	2901/3150 (92%)	2799 (96%)	98 (3%)	4 (0%)	51	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	187	CYS
1	O	189	PRO
1	N	187	CYS
1	O	190	GLU

5.3.2 Protein sidechains [i](#)

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	185/196 (94%)	179 (97%)	6 (3%)	39	65
1	B	185/196 (94%)	177 (96%)	8 (4%)	29	54
1	C	185/196 (94%)	178 (96%)	7 (4%)	33	59
1	D	184/196 (94%)	179 (97%)	5 (3%)	44	71
1	E	185/196 (94%)	176 (95%)	9 (5%)	25	49
1	F	188/196 (96%)	182 (97%)	6 (3%)	39	65
1	G	186/196 (95%)	180 (97%)	6 (3%)	39	65
1	H	185/196 (94%)	176 (95%)	9 (5%)	25	49
1	I	182/196 (93%)	178 (98%)	4 (2%)	52	77
1	J	185/196 (94%)	180 (97%)	5 (3%)	44	71
1	K	183/196 (93%)	175 (96%)	8 (4%)	28	53
1	L	186/196 (95%)	181 (97%)	5 (3%)	44	71
1	M	182/196 (93%)	177 (97%)	5 (3%)	44	71
1	N	185/196 (94%)	176 (95%)	9 (5%)	25	49
1	O	185/196 (94%)	181 (98%)	4 (2%)	52	77
All	All	2771/2940 (94%)	2675 (96%)	96 (4%)	36	62

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	21	THR
1	G	25	ARG
1	G	69	HIS
1	G	120	ARG
1	G	187	CYS
1	G	188	CYS
1	D	21	THR
1	D	23	ARG
1	D	57	THR
1	D	132	SER

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Mol	Chain	Res	Type
1	D	187	CYS
1	E	21	THR
1	E	23	ARG
1	E	57	THR
1	E	68	SER
1	E	120	ARG
1	E	132	SER
1	E	184	THR
1	E	186	SER
1	E	188	CYS
1	A	21	THR
1	A	57	THR
1	A	59	SER
1	A	148	ARG
1	A	184	THR
1	A	188	CYS
1	B	21	THR
1	B	25	ARG
1	B	59	SER
1	B	69	HIS
1	B	185	TYR
1	B	186	SER
1	B	187	CYS
1	B	188	CYS
1	C	21	THR
1	C	25	ARG
1	C	129	ASP
1	C	185	TYR
1	C	186	SER
1	C	187	CYS
1	C	188	CYS
1	F	21	THR
1	F	25	ARG
1	F	57	THR
1	F	185	TYR
1	F	187	CYS
1	F	188	CYS
1	H	21	THR
1	H	23	ARG
1	H	57	THR
1	H	61	ARG
1	H	120	ARG

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Mol	Chain	Res	Type
1	H	179	LYS
1	H	182	SER
1	H	184	THR
1	H	188	CYS
1	I	21	THR
1	I	25	ARG
1	I	61	ARG
1	I	185	TYR
1	J	14	SER
1	J	21	THR
1	J	25	ARG
1	J	57	THR
1	J	188	CYS
1	K	11	ARG
1	K	21	THR
1	K	25	ARG
1	K	57	THR
1	K	69	HIS
1	K	184	THR
1	K	186	SER
1	K	188	CYS
1	L	21	THR
1	L	57	THR
1	L	186	SER
1	L	187	CYS
1	L	188	CYS
1	M	23	ARG
1	M	25	ARG
1	M	59	SER
1	M	69	HIS
1	M	120	ARG
1	N	21	THR
1	N	25	ARG
1	N	44	ILE
1	N	139	LYS
1	N	185	TYR
1	N	186	SER
1	N	187	CYS
1	N	188	CYS
1	N	202	ARG
1	O	15	ARG
1	O	21	THR

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Mol	Chain	Res	Type
1	O	57	THR
1	O	188	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	119	GLN
1	D	167	GLN
1	E	9	ASN
1	C	9	ASN
1	I	9	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 53 ligands modelled in this entry, 4 are monoatomic - leaving 49 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	SO4	F	302	-	4,4,4	0.16	0	6,6,6	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NSE	E	301	-	17,21,21	0.89	1 (5%)	23,28,28	1.15	1 (4%)
4	SO4	I	303	-	4,4,4	0.16	0	6,6,6	0.08	0
2	1PE	E	302	-	15,15,15	0.73	0	14,14,14	2.00	4 (28%)
2	1PE	H	301	-	15,15,15	0.82	0	14,14,14	1.30	2 (14%)
4	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.24	0
5	ACT	F	305	-	1,3,3	0.89	0	0,3,3	0.00	-
6	NSE	I	301	-	17,21,21	0.88	0	23,28,28	1.65	5 (21%)
5	ACT	F	306	-	1,3,3	0.76	0	0,3,3	0.00	-
2	1PE	C	301	-	15,15,15	1.02	0	14,14,14	1.37	3 (21%)
5	ACT	G	307	-	1,3,3	1.63	0	0,3,3	0.00	-
4	SO4	E	304	-	4,4,4	0.19	0	6,6,6	0.33	0
6	NSE	A	301	-	17,21,21	0.74	0	23,28,28	1.97	5 (21%)
4	SO4	E	307	-	4,4,4	0.17	0	6,6,6	0.20	0
2	1PE	G	301	-	15,15,15	0.60	0	14,14,14	1.36	2 (14%)
8	GOL	J	303	-	5,5,5	0.34	0	5,5,5	0.45	0
4	SO4	E	306	-	4,4,4	0.19	0	6,6,6	0.20	0
4	SO4	D	305	-	4,4,4	0.13	0	6,6,6	0.15	0
4	SO4	E	305	-	4,4,4	0.17	0	6,6,6	0.06	0
6	NSE	K	301	-	17,21,21	0.78	0	23,28,28	1.96	6 (26%)
5	ACT	O	301	-	1,3,3	1.04	0	0,3,3	0.00	-
5	ACT	G	306	-	1,3,3	1.51	0	0,3,3	0.00	-
4	SO4	A	304	-	4,4,4	0.18	0	6,6,6	0.10	0
5	ACT	F	304	-	1,3,3	1.44	0	0,3,3	0.00	-
5	ACT	A	305	-	1,3,3	1.62	0	0,3,3	0.00	-
4	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.20	0
4	SO4	D	303	-	4,4,4	0.27	0	6,6,6	0.23	0
5	ACT	J	302	-	1,3,3	2.40	1 (100%)	0,3,3	0.00	-
3	NAG	G	302	1	14,14,15	4.14	7 (50%)	17,19,21	3.90	12 (70%)
3	NAG	D	302	1	14,14,15	2.07	2 (14%)	17,19,21	2.02	5 (29%)
4	SO4	B	304	-	4,4,4	0.20	0	6,6,6	0.25	0
5	ACT	A	307	-	1,3,3	1.25	0	0,3,3	0.00	-
4	SO4	G	305	-	4,4,4	0.20	0	6,6,6	0.23	0
5	ACT	F	303	-	1,3,3	1.03	0	0,3,3	0.00	-
5	ACT	D	304	-	1,3,3	1.10	0	0,3,3	0.00	-
4	SO4	G	304	-	4,4,4	0.13	0	6,6,6	0.18	0
4	SO4	E	303	-	4,4,4	0.13	0	6,6,6	0.27	0
5	ACT	G	308	-	1,3,3	0.98	0	0,3,3	0.00	-
4	SO4	G	303	-	4,4,4	0.19	0	6,6,6	0.14	0
2	1PE	B	302	-	15,15,15	0.76	0	14,14,14	1.93	4 (28%)
2	1PE	A	302	-	15,15,15	0.77	0	14,14,14	1.17	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	302	-	4,4,4	0.15	0	6,6,6	0.11	0
6	NSE	M	301	-	17,21,21	0.77	0	23,28,28	1.12	2 (8%)
2	1PE	I	302	-	15,15,15	0.88	0	14,14,14	1.11	2 (14%)
6	NSE	B	301	-	17,21,21	0.84	0	23,28,28	1.24	2 (8%)
4	SO4	F	301	-	4,4,4	0.11	0	6,6,6	0.26	0
4	SO4	M	302	-	4,4,4	0.13	0	6,6,6	0.13	0
2	1PE	D	301	-	15,15,15	0.83	0	14,14,14	1.16	1 (7%)
4	SO4	J	301	-	4,4,4	0.13	0	6,6,6	0.21	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
6	NSE	E	301	-	-	1/8/10/10	0/3/3/3
3	NAG	G	302	1	-	2/6/23/26	0/1/1/1
6	NSE	A	301	-	-	2/8/10/10	0/3/3/3
2	1PE	E	302	-	-	4/13/13/13	-
6	NSE	M	301	-	-	0/8/10/10	0/3/3/3
2	1PE	H	301	-	-	3/13/13/13	-
6	NSE	K	301	-	-	1/8/10/10	0/3/3/3
2	1PE	A	302	-	-	3/13/13/13	-
6	NSE	I	301	-	-	2/8/10/10	0/3/3/3
3	NAG	D	302	1	-	2/6/23/26	0/1/1/1
2	1PE	G	301	-	-	1/13/13/13	-
2	1PE	B	302	-	-	5/13/13/13	-
8	GOL	J	303	-	-	3/4/4/4	-
2	1PE	C	301	-	-	5/13/13/13	-
6	NSE	B	301	-	-	1/8/10/10	0/3/3/3
2	1PE	I	302	-	-	3/13/13/13	-
2	1PE	D	301	-	-	1/13/13/13	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	NAG	C1-C2	-9.97	1.37	1.52
3	G	302	NAG	C8-C7	8.20	1.67	1.50
3	G	302	NAG	O7-C7	-5.90	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	NAG	C1-C2	5.26	1.60	1.52
3	D	302	NAG	C2-N2	4.85	1.54	1.46
3	G	302	NAG	C2-N2	-3.77	1.39	1.46
3	G	302	NAG	C7-N2	2.74	1.43	1.34
6	E	301	NSE	C11-N2	2.41	1.38	1.35
5	J	302	ACT	CH3-C	2.40	1.51	1.48
3	G	302	NAG	C3-C2	-2.32	1.47	1.52
3	G	302	NAG	C4-C3	-2.25	1.46	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	302	NAG	C1-O5-C5	7.30	122.08	112.19
3	G	302	NAG	C2-N2-C7	6.66	132.39	122.90
6	A	301	NSE	C9-C11-N3	6.25	127.25	119.12
3	G	302	NAG	O7-C7-N2	-6.17	110.61	121.95
3	D	302	NAG	O5-C1-C2	-5.48	102.63	111.29
6	K	301	NSE	C9-C11-N3	5.39	126.13	119.12
3	G	302	NAG	O5-C1-C2	-4.94	103.49	111.29
6	I	301	NSE	C9-C11-N3	4.45	124.91	119.12
3	D	302	NAG	C1-O5-C5	4.24	117.93	112.19
3	G	302	NAG	O5-C5-C6	4.23	113.84	107.20
3	G	302	NAG	O5-C5-C4	3.94	120.42	110.83
2	E	302	1PE	C26-OH6-C15	3.93	130.33	113.29
2	E	302	1PE	OH6-C26-C16	3.87	127.08	110.07
3	G	302	NAG	O3-C3-C4	-3.84	101.47	110.35
6	A	301	NSE	C9-C11-N2	-3.84	118.92	123.71
2	B	302	1PE	OH3-C23-C13	3.80	127.53	110.39
6	E	301	NSE	C8-C7-N2	3.77	128.62	123.56
6	K	301	NSE	C5-C8-C7	-3.69	114.66	120.06
3	G	302	NAG	C6-C5-C4	3.60	121.43	113.00
2	E	302	1PE	C25-OH5-C14	-3.58	97.76	113.29
2	B	302	1PE	OH6-C26-C16	3.22	124.23	110.07
6	I	301	NSE	C9-C11-N2	-3.22	119.69	123.71
6	B	301	NSE	C9-C11-N3	3.13	123.20	119.12
3	G	302	NAG	C1-C2-N2	-3.03	105.31	110.49
2	G	301	1PE	OH3-C23-C13	-3.02	96.78	110.39
6	A	301	NSE	C5-C8-C7	-2.99	115.69	120.06
2	A	302	1PE	OH3-C23-C13	-2.94	97.15	110.39
6	K	301	NSE	C9-C11-N2	-2.92	120.07	123.71
6	I	301	NSE	C10-C9-C11	-2.90	117.47	121.31
2	D	301	1PE	OH6-C15-C25	-2.81	97.73	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	302	NAG	O6-C6-C5	2.79	120.88	111.29
2	B	302	1PE	C23-OH3-C22	2.72	125.05	113.29
6	K	301	NSE	C11-N2-C7	2.71	103.32	101.13
6	K	301	NSE	C6-C8-C7	2.70	124.56	120.44
2	C	301	1PE	OH6-C15-C25	-2.70	98.24	110.39
6	M	301	NSE	C9-C11-N3	2.67	122.60	119.12
2	I	302	1PE	OH4-C24-C14	-2.65	98.47	110.39
6	A	301	NSE	C11-N2-C7	2.57	103.21	101.13
2	C	301	1PE	OH3-C23-C13	2.57	121.98	110.39
2	B	302	1PE	OH3-C22-C12	2.56	121.31	110.07
2	I	302	1PE	OH6-C15-C25	2.52	121.77	110.39
3	G	302	NAG	C3-C4-C5	-2.48	105.82	110.24
6	I	301	NSE	C6-C8-C5	2.43	121.60	118.16
6	M	301	NSE	C8-C7-N2	2.42	126.81	123.56
2	H	301	1PE	OH3-C22-C12	2.40	120.63	110.07
2	H	301	1PE	OH4-C13-C23	2.39	121.17	110.39
6	K	301	NSE	C5-C3-C4	-2.34	116.42	119.54
3	D	302	NAG	C4-C3-C2	-2.33	107.61	111.02
6	B	301	NSE	C8-C7-N2	2.32	126.67	123.56
3	D	302	NAG	O5-C5-C4	-2.24	105.39	110.83
3	D	302	NAG	C1-C2-N2	-2.23	106.69	110.49
2	C	301	1PE	OH6-C26-C16	-2.19	100.44	110.07
2	G	301	1PE	OH6-C15-C25	2.18	120.23	110.39
2	A	302	1PE	OH6-C26-C16	2.18	119.62	110.07
3	G	302	NAG	O4-C4-C3	-2.15	105.38	110.35
6	A	301	NSE	C6-C8-C5	2.13	121.17	118.16
2	E	302	1PE	OH4-C24-C14	-2.03	101.25	110.39
6	I	301	NSE	C5-C8-C7	-2.00	117.13	120.06

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	NSE	N3-C11-C9-C12
3	G	302	NAG	O7-C7-N2-C2
3	G	302	NAG	O5-C5-C6-O6
3	D	302	NAG	O5-C5-C6-O6
2	E	302	1PE	C14-C24-OH4-C13
3	D	302	NAG	C4-C5-C6-O6
2	B	302	1PE	C15-C25-OH5-C14
8	J	303	GOL	O1-C1-C2-C3
8	J	303	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	E	302	1PE	C25-C15-OH6-C26
2	A	302	1PE	C15-C25-OH5-C14
2	B	302	1PE	C16-C26-OH6-C15
2	I	302	1PE	C13-C23-OH3-C22
2	H	301	1PE	C16-C26-OH6-C15
6	A	301	NSE	N2-C11-C9-C12
2	I	302	1PE	C25-C15-OH6-C26
8	J	303	GOL	O2-C2-C3-O3
6	I	301	NSE	N2-C7-C8-C6
2	C	301	1PE	C13-C23-OH3-C22
2	G	301	1PE	C25-C15-OH6-C26
2	A	302	1PE	C16-C26-OH6-C15
2	B	302	1PE	C12-C22-OH3-C23
2	C	301	1PE	C12-C22-OH3-C23
2	C	301	1PE	C23-C13-OH4-C24
6	E	301	NSE	N2-C7-C8-C6
6	I	301	NSE	N2-C7-C8-C5
6	K	301	NSE	N2-C7-C8-C6
6	B	301	NSE	N2-C7-C8-C6
2	E	302	1PE	C24-C14-OH5-C25
2	B	302	1PE	C13-C23-OH3-C22
2	H	301	1PE	OH6-C15-C25-OH5
2	B	302	1PE	OH6-C15-C25-OH5
2	D	301	1PE	OH4-C13-C23-OH3
2	A	302	1PE	OH6-C15-C25-OH5
2	C	301	1PE	OH4-C13-C23-OH3
2	I	302	1PE	OH4-C13-C23-OH3
2	H	301	1PE	C15-C25-OH5-C14
2	E	302	1PE	OH5-C14-C24-OH4
2	C	301	1PE	C14-C24-OH4-C13

There are no ring outliers.

17 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	301	NSE	1	0
2	E	302	1PE	2	0
2	H	301	1PE	3	0
4	A	303	SO4	1	0
6	I	301	NSE	1	0
5	F	306	ACT	1	0
2	C	301	1PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	NSE	2	0
4	E	307	SO4	1	0
2	G	301	1PE	1	0
6	K	301	NSE	2	0
4	B	303	SO4	1	0
2	B	302	1PE	2	0
6	M	301	NSE	2	0
2	I	302	1PE	5	0
2	D	301	1PE	3	0
4	J	301	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	198/210 (94%)	-0.12	0 100 100	28, 45, 79, 97	0
1	B	198/210 (94%)	-0.07	5 (2%) 57 57	33, 51, 87, 102	0
1	C	198/210 (94%)	0.03	3 (1%) 73 74	34, 51, 82, 101	0
1	D	197/210 (93%)	-0.06	1 (0%) 91 92	30, 47, 76, 99	0
1	E	198/210 (94%)	-0.05	4 (2%) 65 65	29, 47, 81, 99	0
1	F	200/210 (95%)	0.00	5 (2%) 57 57	26, 43, 78, 95	0
1	G	198/210 (94%)	-0.04	2 (1%) 82 82	27, 46, 79, 102	0
1	H	198/210 (94%)	0.01	2 (1%) 82 82	29, 50, 82, 103	0
1	I	195/210 (92%)	0.15	5 (2%) 56 55	37, 56, 84, 106	0
1	J	198/210 (94%)	0.05	2 (1%) 82 82	32, 50, 74, 96	0
1	K	197/210 (93%)	0.09	1 (0%) 91 92	31, 54, 78, 88	0
1	L	198/210 (94%)	-0.02	2 (1%) 82 82	32, 48, 77, 99	0
1	M	194/210 (92%)	0.10	6 (3%) 49 48	33, 57, 80, 107	0
1	N	198/210 (94%)	0.27	7 (3%) 44 43	38, 64, 89, 112	0
1	O	198/210 (94%)	0.14	3 (1%) 73 74	41, 58, 83, 98	0
All	All	2963/3150 (94%)	0.03	48 (1%) 72 73	26, 51, 83, 112	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	185	TYR	5.6
1	O	39	LEU	5.1
1	N	23	ARG	5.1
1	J	1	LEU	4.6
1	B	186	SER	4.5
1	E	23	ARG	4.1
1	N	183	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	189	PRO	3.7
1	F	67	SER	3.5
1	M	23	ARG	3.5
1	O	188	CYS	3.3
1	B	24	ASP	3.2
1	G	186	SER	3.2
1	C	188	CYS	3.1
1	H	185	TYR	3.1
1	M	185	TYR	3.0
1	E	24	ASP	2.9
1	B	187	CYS	2.9
1	F	53	TRP	2.8
1	N	24	ASP	2.8
1	M	22	GLN	2.7
1	C	184	THR	2.7
1	J	178	GLN	2.7
1	B	188	CYS	2.7
1	N	22	GLN	2.6
1	O	167	GLN	2.6
1	M	24	ASP	2.5
1	N	128	VAL	2.5
1	I	69	HIS	2.4
1	D	23	ARG	2.4
1	C	130	THR	2.3
1	G	190	GLU	2.3
1	L	164	TYR	2.3
1	E	22	GLN	2.2
1	B	185	TYR	2.2
1	N	178	GLN	2.2
1	E	185	TYR	2.2
1	F	186	SER	2.2
1	K	205	GLY	2.2
1	L	186	SER	2.2
1	N	173	ILE	2.1
1	I	178	GLN	2.1
1	M	25	ARG	2.1
1	I	23	ARG	2.1
1	I	190	GLU	2.1
1	F	23	ARG	2.1
1	H	179	LYS	2.1
1	M	130	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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, 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
8	GOL	J	303	6/6	0.66	0.25	64,75,83,86	0
4	SO4	J	301	5/5	0.68	0.23	88,90,97,112	0
3	NAG	G	302	14/15	0.70	0.34	93,103,106,109	0
3	NAG	D	302	14/15	0.77	0.19	80,85,91,92	0
5	ACT	G	306	4/4	0.78	0.23	48,52,60,62	0
6	NSE	I	301	19/19	0.78	0.33	60,70,78,80	0
4	SO4	F	302	5/5	0.79	0.42	64,69,75,106	0
5	ACT	F	305	4/4	0.82	0.22	51,60,67,69	0
5	ACT	A	307	4/4	0.83	0.15	43,66,70,71	0
4	SO4	C	302	5/5	0.83	0.25	84,85,107,110	0
4	SO4	A	304	5/5	0.83	0.29	78,80,93,104	0
4	SO4	M	302	5/5	0.84	0.43	80,82,96,100	0
6	NSE	B	301	19/19	0.85	0.33	54,67,78,78	0
4	SO4	D	305	5/5	0.85	0.34	75,85,105,110	0
5	ACT	J	302	4/4	0.85	0.20	34,35,41,55	0
4	SO4	D	303	5/5	0.86	0.39	56,61,72,92	0
4	SO4	G	304	5/5	0.86	0.19	87,91,106,110	0
4	SO4	E	304	5/5	0.86	0.23	64,67,85,94	0
2	1PE	E	302	16/16	0.87	0.31	46,55,63,64	0
4	SO4	E	306	5/5	0.87	0.24	82,85,104,121	0
6	NSE	M	301	19/19	0.87	0.42	61,74,79,80	0
5	ACT	A	305	4/4	0.88	0.20	47,60,61,61	0
2	1PE	I	302	16/16	0.88	0.23	46,59,67,69	0
5	ACT	G	308	4/4	0.88	0.23	44,44,58,59	0
2	1PE	B	302	16/16	0.88	0.31	47,57,64,69	0
6	NSE	E	301	19/19	0.88	0.25	45,57,74,75	0
5	ACT	F	303	4/4	0.89	0.13	59,62,64,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	F	304	4/4	0.89	0.22	36,51,56,68	0
6	NSE	K	301	19/19	0.89	0.32	51,58,68,68	0
4	SO4	E	307	5/5	0.89	0.18	76,82,96,96	0
2	1PE	D	301	16/16	0.89	0.23	47,55,67,70	0
6	NSE	A	301	19/19	0.89	0.34	50,58,68,69	0
5	ACT	D	304	4/4	0.90	0.14	62,63,63,72	0
4	SO4	B	303	5/5	0.91	0.12	86,87,91,101	0
5	ACT	G	307	4/4	0.92	0.13	58,61,70,73	0
7	CL	L	301	1/1	0.92	0.20	60,60,60,60	0
7	CL	A	306	1/1	0.92	0.18	86,86,86,86	0
2	1PE	C	301	16/16	0.93	0.16	49,57,61,63	0
4	SO4	B	304	5/5	0.93	0.30	54,61,89,90	0
4	SO4	G	305	5/5	0.94	0.36	64,81,87,93	0
2	1PE	H	301	16/16	0.94	0.24	38,46,58,62	0
4	SO4	F	301	5/5	0.94	0.18	67,71,76,78	0
2	1PE	A	302	16/16	0.94	0.18	36,48,56,62	0
2	1PE	G	301	16/16	0.94	0.22	33,34,35,35	16
4	SO4	A	303	5/5	0.94	0.13	71,75,77,79	0
7	CL	K	302	1/1	0.95	0.08	69,69,69,69	0
5	ACT	F	306	4/4	0.95	0.11	45,52,57,58	0
5	ACT	O	301	4/4	0.95	0.20	37,43,45,49	0
4	SO4	I	303	5/5	0.95	0.08	95,97,105,111	0
4	SO4	G	303	5/5	0.95	0.14	63,64,79,83	0
7	CL	N	301	1/1	0.97	0.10	54,54,54,54	0
4	SO4	E	305	5/5	0.97	0.11	79,79,90,94	0
4	SO4	E	303	5/5	0.98	0.08	58,60,66,74	0

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

There are no such residues in this entry.