



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 PM GMT

PDB ID : 4LOQ  
Title : Structural basis of autoactivation of p38 alpha induced by TAB1 (Tetragonal crystal form with bound sulphate)  
Authors : Chaikuad, A.; DeNicola, G.F.; Yue, W.W.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Marber, M.S.; Knapp, S.; Structural Genomics Consortium (SGC)  
Deposited on : 2013-07-13  
Resolution : 2.32 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

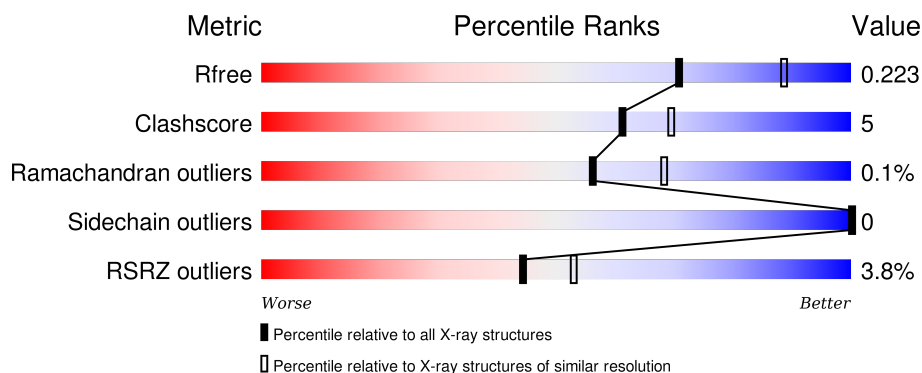
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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.



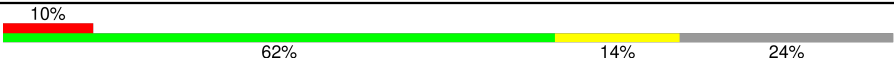
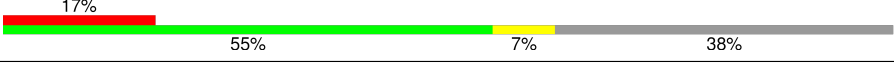
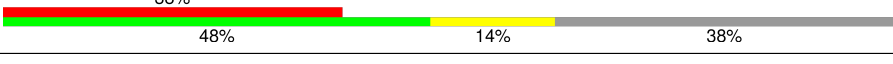
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	361	<div> <div>87%</div> <div>11%</div> <div>•</div> </div>
1	B	361	<div> <div>3%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>
1	C	361	<div> <div>2%</div> <div>82%</div> <div>11%</div> <div>7%</div> </div>
1	D	361	<div> <div>4%</div> <div>88%</div> <div>9%</div> <div>•</div> </div>
2	K	29	<div> <div>3%</div> <div>66%</div> <div>10%</div> <div>24%</div> </div>

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Mol	Chain	Length	Quality of chain
2	L	29	
2	M	29	
2	N	29	

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
5	EDO	B	406	-	-	-	X
5	EDO	D	404	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12478 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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	5	0
			2849	1823	491	522	13			
1	B	351	Total	C	N	O	S	0	8	0
			2870	1837	491	529	13			
1	C	337	Total	C	N	O	S	0	4	0
			2706	1732	463	499	12			
1	D	351	Total	C	N	O	S	0	3	0
			2829	1810	484	522	13			

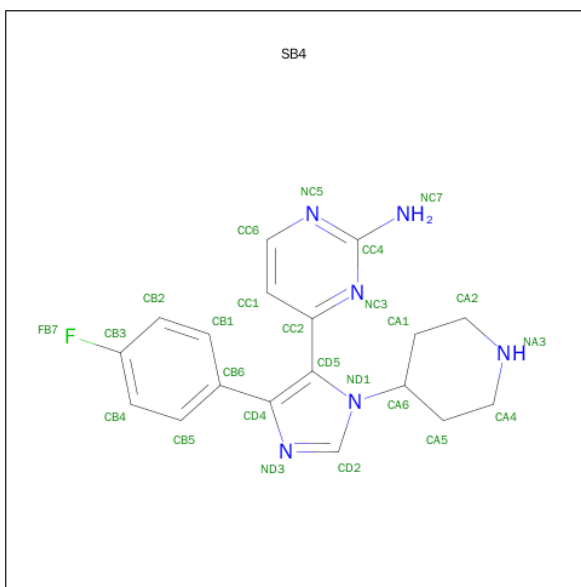
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP P47811
B	0	GLY	-	EXPRESSION TAG	UNP P47811
C	0	GLY	-	EXPRESSION TAG	UNP P47811
D	0	GLY	-	EXPRESSION TAG	UNP P47811

- Molecule 2 is a protein called TGF-beta-activated kinase 1 and MAP3K7-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	18	Total	C	N	O	S	0	0	0
			134	89	18	26	1			
2	L	22	Total	C	N	O	S	0	0	0
			165	106	26	32	1			
2	K	22	Total	C	N	O	S	0	0	0
			165	106	26	32	1			
2	N	18	Total	C	N	O	S	0	0	0
			134	89	18	26	1			

- Molecule 3 is 4-(4-FLUOROPHENYL)-1-(4-PIPERIDINYL)-5-(2-AMINO-4-PYRIMIDINYL)-IMIDAZOLE (three-letter code: SB4) (formula: C<sub>18</sub>H<sub>19</sub>FN<sub>6</sub>).



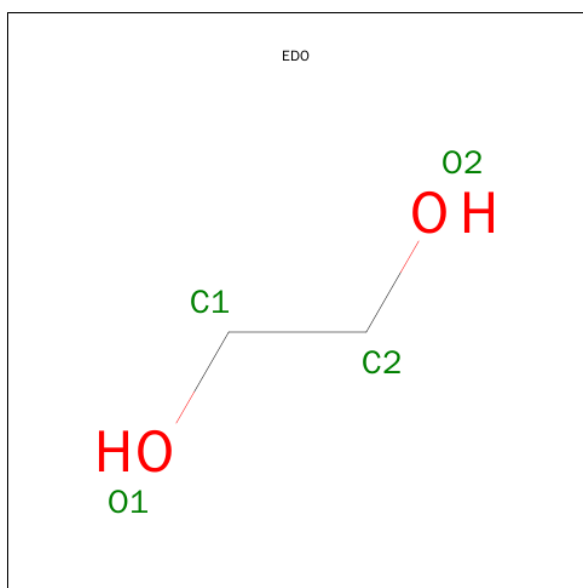
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			25	18	1	6		
3	B	1	Total	C	F	N	0	0
			25	18	1	6		
3	C	1	Total	C	F	N	0	0
			25	18	1	6		
3	D	1	Total	C	F	N	0	0
			25	18	1	6		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

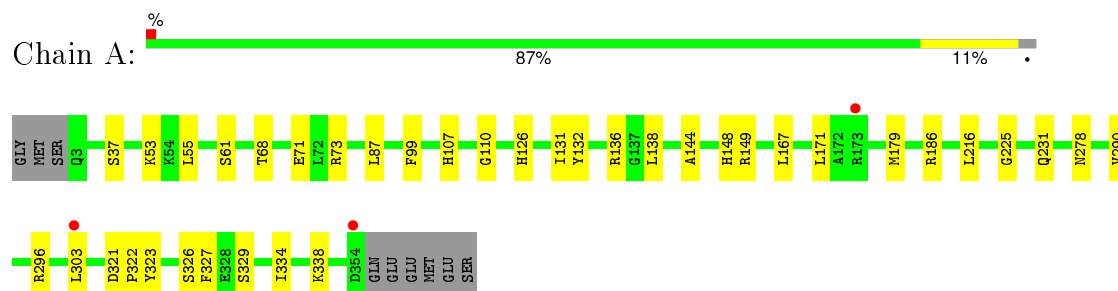
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	131	Total	O	0	0
			131	131		
6	B	90	Total	O	0	0
			90	90		
6	C	107	Total	O	0	0
			107	107		
6	D	107	Total	O	0	0
			107	107		
6	M	6	Total	O	0	0
			6	6		
6	L	5	Total	O	0	0
			5	5		
6	K	9	Total	O	0	0
			9	9		
6	N	3	Total	O	0	0
			3	3		

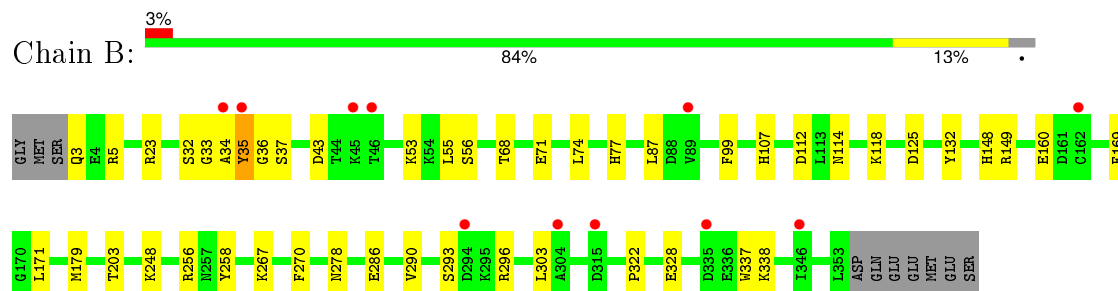
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

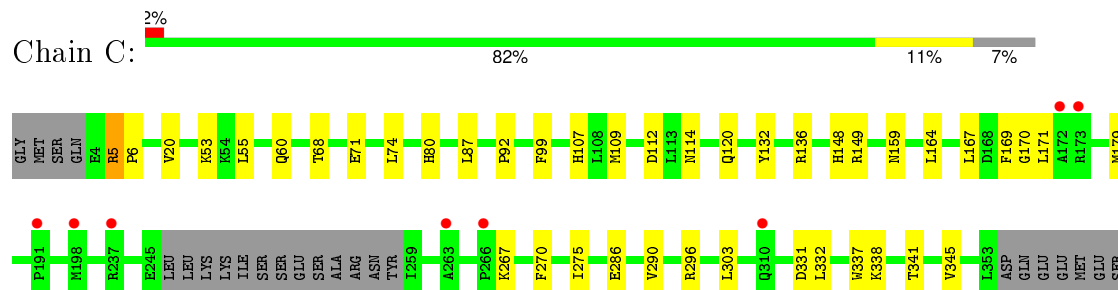
- Molecule 1: Mitogen-activated protein kinase 14



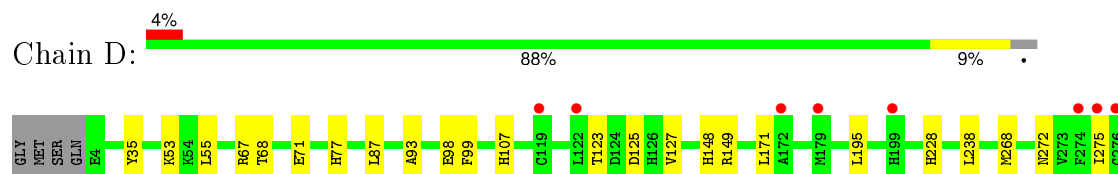
- Molecule 1: Mitogen-activated protein kinase 14



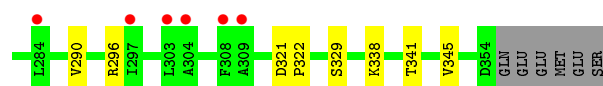
- Molecule 1: Mitogen-activated protein kinase 14



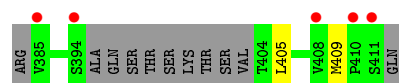
- Molecule 1: Mitogen-activated protein kinase 14



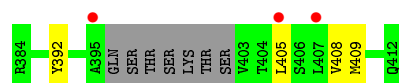




- Molecule 2: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1



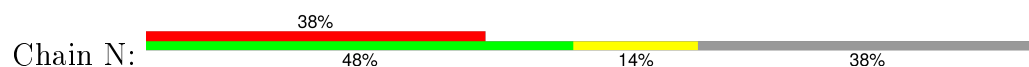
- Molecule 2: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1



- Molecule 2: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1



- Molecule 2: TGF-beta-activated kinase 1 and MAP3K7-binding protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.10Å 87.10Å 228.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.78 – 2.32 42.78 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.78-2.32) 98.6 (42.78-2.32)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.192 , 0.236 0.192 , 0.223	Depositor DCC
$R_{free}$ test set	3627 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 19.2	EDS
Estimated twinning fraction	0.708 for H, K, L 0.292 for K, H, -L 0.276 for h,-k,-l	Xtriage
Reported twinning fraction	0.708 for H, K, L 0.292 for K, H, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 72157 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12478	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: EDO, SB4, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.76	0/2932	0.77	0/3982
1	B	0.63	1/2944 (0.0%)	0.69	0/3997
1	C	0.71	1/2782 (0.0%)	0.73	1/3781 (0.0%)
1	D	0.67	0/2905	0.72	0/3946
2	K	0.64	0/168	0.82	0/228
2	L	0.62	0/168	0.80	0/228
2	M	0.71	0/137	0.78	0/188
2	N	0.48	0/137	0.61	0/188
All	All	0.69	2/12173 (0.0%)	0.73	1/16538 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	TRP	CD2-CE2	5.44	1.47	1.41
1	C	337	TRP	CD2-CE2	5.39	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	ARG	NE-CZ-NH2	5.53	123.06	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	35[B]	TYR	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2849	0	2821	31	1
1	B	2870	0	2846	38	1
1	C	2706	0	2658	35	0
1	D	2829	0	2797	25	0
2	K	165	0	164	3	0
2	L	165	0	164	6	0
2	M	134	0	136	2	0
2	N	134	0	136	5	0
3	A	25	0	19	1	0
3	B	25	0	19	1	0
3	C	25	0	19	1	0
3	D	25	0	19	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	4	0	6	0	0
5	B	16	0	24	1	0
5	C	4	0	6	1	0
5	D	4	0	6	0	0
6	A	131	0	0	3	0
6	B	90	0	0	1	0
6	C	107	0	0	7	0
6	D	107	0	0	2	0
6	K	9	0	0	1	0
6	L	5	0	0	0	0
6	M	6	0	0	0	0
6	N	3	0	0	0	0
All	All	12478	0	11840	131	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (131) 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:C:179:MET:SD	6:C:541:HOH:O	2.49	0.71
1:C:270:PHE:CD2	1:C:286[A]:GLU:HG3	2.26	0.70
1:C:331:ASP:O	1:C:332:LEU:HD23	1.92	0.68
1:D:195:LEU:HB2	6:D:551:HOH:O	1.95	0.67
1:A:99:PHE:O	1:A:338:LYS:HE3	1.93	0.67
1:B:33[B]:GLY:CA	1:B:179:MET:SD	2.83	0.67
1:D:238:LEU:HA	1:D:268:MET:HE3	1.77	0.66
1:C:5:ARG:NH1	1:C:92:PRO:O	2.29	0.66
1:B:87:LEU:HD21	1:B:107:HIS:NE2	2.13	0.64
1:C:275:ILE:O	2:K:388:VAL:HG22	1.99	0.63
1:A:171:LEU:N	1:A:171:LEU:HD12	2.13	0.63
1:B:33[B]:GLY:HA3	1:B:179:MET:SD	2.38	0.63
1:B:99:PHE:O	1:B:338:LYS:CE	2.47	0.62
1:A:87:LEU:HD21	1:A:107:HIS:NE2	2.14	0.62
1:A:87:LEU:HD11	1:A:107:HIS:CD2	2.35	0.62
1:C:148:HIS:O	1:C:149:ARG:HB2	2.01	0.61
1:A:167:LEU:HD11	3:A:401:SB4:H52	1.83	0.61
1:C:341:THR:O	1:C:345:VAL:HG23	2.01	0.60
1:B:35[B]:TYR:CE1	1:B:36[B]:GLY:O	2.54	0.60
1:A:99:PHE:O	1:A:338:LYS:CE	2.49	0.60
1:D:87:LEU:HD21	1:D:107:HIS:NE2	2.17	0.59
1:B:125:ASP:HB3	2:L:405:LEU:HD23	1.85	0.58
1:A:61:SER:HA	1:A:334:ILE:HD11	1.86	0.58
1:C:267:LYS:HZ1	1:C:286[B]:GLU:CD	2.09	0.56
1:B:74:LEU:HD21	1:B:169:PHE:CD1	2.40	0.56
1:C:87:LEU:HD21	1:C:107:HIS:NE2	2.21	0.56
1:A:329[B]:SER:OG	1:D:329[B]:SER:OG	2.22	0.56
1:D:55:LEU:CD1	1:D:68:THR:HG23	2.35	0.56
2:N:390:VAL:O	2:N:390:VAL:HG12	2.07	0.55
1:B:160:GLU:HA	2:L:409:MET:HE1	1.89	0.55
1:B:55:LEU:CD1	1:B:68:THR:HG23	2.36	0.55
1:B:35[B]:TYR:CD1	1:B:36[B]:GLY:O	2.60	0.55
1:A:55:LEU:CD1	1:A:68:THR:HG23	2.37	0.54
1:A:148:HIS:O	1:A:149:ARG:HB2	2.08	0.54
1:C:74:LEU:HD21	1:C:169:PHE:CD1	2.43	0.54
1:D:272:ASN:O	2:N:385:VAL:HG22	2.07	0.54
1:C:55:LEU:CD1	1:C:68:THR:HG23	2.37	0.53
1:B:33[A]:GLY:N	1:B:36[A]:GLY:O	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34[B]:ALA:HB1	1:B:56:SER:CB	2.39	0.53
1:D:99:PHE:O	1:D:338:LYS:CE	2.57	0.53
1:B:248:LYS:HG3	1:B:256:ARG:CZ	2.39	0.52
1:C:60:GLN:NE2	6:C:574:HOH:O	2.38	0.52
1:D:148:HIS:O	1:D:149:ARG:HB2	2.10	0.52
1:A:171:LEU:N	1:A:171:LEU:CD1	2.72	0.51
1:B:99:PHE:O	1:B:338:LYS:HE3	2.10	0.51
1:A:278:ASN:ND2	6:A:538:HOH:O	2.37	0.51
1:A:110:GLY:HA3	2:M:409:MET:SD	2.51	0.51
1:C:331:ASP:C	1:C:332:LEU:HD23	2.31	0.51
1:B:53:LYS:NZ	1:B:71:GLU:OE2	2.43	0.50
1:C:53:LYS:NZ	1:C:71:GLU:OE2	2.44	0.50
1:A:186[B]:ARG:NH1	6:A:609:HOH:O	2.44	0.50
1:C:87:LEU:HD11	1:C:107:HIS:CD2	2.46	0.50
1:A:132:TYR:CE1	1:A:303:LEU:HD22	2.46	0.49
1:A:131:ILE:HD11	1:A:216:LEU:HD12	1.94	0.49
1:B:112:ASP:OD1	1:B:114:ASN:HB3	2.11	0.49
1:A:73:ARG:HB3	1:A:323:TYR:OH	2.12	0.49
1:A:53:LYS:NZ	1:A:71:GLU:OE2	2.45	0.49
1:A:136:ARG:HA	1:A:303:LEU:HD11	1.95	0.48
1:A:290:VAL:HG22	1:A:296:ARG:HG3	1.94	0.48
1:B:35[B]:TYR:N	1:B:35[B]:TYR:CD2	2.78	0.48
1:C:99:PHE:O	1:C:338:LYS:HE3	2.13	0.48
1:B:87:LEU:HD11	1:B:107:HIS:CD2	2.49	0.48
1:B:148:HIS:O	1:B:149:ARG:HB2	2.14	0.47
1:C:120:GLN:NE2	2:K:408:VAL:O	2.37	0.47
1:D:53:LYS:NZ	1:D:71:GLU:OE2	2.48	0.47
1:A:329[A]:SER:HA	1:D:329[A]:SER:HA	1.96	0.47
1:C:132:TYR:CE1	1:C:303:LEU:HD22	2.49	0.47
1:C:171:LEU:N	1:C:171:LEU:HD12	2.29	0.47
1:C:109:MET:HA	1:C:159[B]:ASN:OD1	2.15	0.47
1:C:20:VAL:HG22	6:C:568:HOH:O	2.15	0.47
1:B:290:VAL:HG22	1:B:296:ARG:HG3	1.98	0.46
5:C:404:EDO:H22	6:C:548:HOH:O	2.16	0.46
1:D:125:ASP:HB3	2:N:405:LEU:HD21	1.98	0.45
3:B:401:SB4:NC3	3:B:401:SB4:H6	2.32	0.45
1:A:55:LEU:HD12	1:A:68:THR:HG23	1.97	0.45
1:C:167:LEU:HD11	3:C:401:SB4:H52	1.99	0.45
1:D:123:THR:HA	2:N:390:VAL:HB	1.98	0.45
1:A:326:SER:OG	1:A:327:PHE:N	2.49	0.45
1:D:290:VAL:HG22	1:D:296:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:TYR:HB2	1:D:67:ARG:CZ	2.46	0.45
1:C:267:LYS:NZ	1:C:286[B]:GLU:OE2	2.48	0.45
1:B:32[B]:SER:HA	1:B:37:SER:HB2	1.98	0.45
1:C:80:HIS:HA	6:C:580:HOH:O	2.17	0.45
1:B:171:LEU:HD12	1:B:171:LEU:N	2.32	0.45
1:B:55:LEU:HD12	1:B:68:THR:HG23	2.00	0.44
1:B:33[B]:GLY:HA2	1:B:179:MET:SD	2.56	0.44
2:L:408:VAL:CG1	2:L:409:MET:N	2.81	0.44
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.83	0.44
1:B:33[A]:GLY:O	1:B:36[A]:GLY:O	2.35	0.44
1:D:171:LEU:N	1:D:171:LEU:HD12	2.33	0.44
1:D:99:PHE:O	1:D:338:LYS:HE2	2.18	0.43
1:C:148:HIS:O	1:C:149:ARG:CB	2.66	0.43
1:B:34[B]:ALA:HB1	1:B:56:SER:OG	2.18	0.43
1:C:112:ASP:OD1	1:C:114:ASN:HB3	2.18	0.43
1:C:164:LEU:C	1:C:164:LEU:HD23	2.39	0.43
1:B:160:GLU:HB3	2:L:409:MET:HE3	2.01	0.43
1:C:55:LEU:HD12	1:C:68:THR:HG23	2.01	0.43
1:B:267:LYS:HZ1	1:B:286[B]:GLU:CD	2.22	0.43
1:B:118:LYS:HZ1	5:B:406:EDO:C2	2.32	0.42
1:C:290:VAL:HG22	1:C:296:ARG:HG3	2.01	0.42
1:A:126:HIS:HA	2:M:405:LEU:HD13	2.00	0.42
1:A:329[B]:SER:HA	1:D:329[B]:SER:HA	2.00	0.42
1:B:77:HIS:CE1	1:B:322:PRO:O	2.72	0.42
1:A:179:MET:HG3	6:C:539:HOH:O	2.20	0.42
1:B:132:TYR:CE1	1:B:303:LEU:HD22	2.54	0.42
1:A:37:SER:HB2	6:A:521:HOH:O	2.18	0.42
2:K:384:ARG:NH2	6:K:504:HOH:O	2.46	0.42
1:C:5:ARG:HA	1:C:6:PRO:HD3	1.81	0.42
1:C:149:ARG:HD2	1:C:170:GLY:O	2.19	0.42
1:C:136:ARG:HA	1:C:303:LEU:HD11	2.00	0.42
1:C:270:PHE:CG	1:C:286[A]:GLU:HG3	2.53	0.42
1:B:160:GLU:CA	2:L:409:MET:HE1	2.50	0.42
1:D:275:ILE:O	2:N:388:VAL:HG13	2.20	0.42
1:D:228:HIS:ND1	1:D:228:HIS:O	2.52	0.42
1:A:144:ALA:HA	1:A:322:PRO:HA	2.01	0.42
1:B:23:ARG:HH21	1:B:43:ASP:CG	2.21	0.42
1:B:107:HIS:CD2	6:B:554:HOH:O	2.72	0.41
1:B:278:ASN:HA	2:L:392:TYR:CD2	2.55	0.41
1:D:93:ALA:HB1	1:D:98:GLU:HG3	2.02	0.41
1:D:321:ASP:HB3	1:D:322:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:THR:OG1	1:B:293:SER:HB2	2.20	0.41
1:C:267:LYS:HE3	6:C:607:HOH:O	2.21	0.41
1:A:87:LEU:HD21	1:A:107:HIS:CE1	2.55	0.41
1:D:87:LEU:HD11	1:D:107:HIS:CD2	2.56	0.41
1:B:3:GLN:C	1:B:5:ARG:H	2.23	0.41
1:D:341:THR:O	1:D:345:VAL:HG23	2.21	0.41
1:C:270:PHE:CD2	1:C:286[B]:GLU:HG2	2.55	0.41
1:A:225:GLY:HA3	1:A:231:GLN:OE1	2.21	0.41
1:D:123:THR:O	1:D:127:VAL:HG23	2.22	0.40
1:B:270:PHE:CD2	1:B:286[A]:GLU:HG3	2.57	0.40
1:D:77:HIS:HB2	6:D:553:HOH:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ASP:OD2	1:B:258:TYR:OH[3_555]	2.16	0.04

## 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	355/361 (98%)	340 (96%)	15 (4%)	0	100	100
1	B	357/361 (99%)	333 (93%)	23 (6%)	1 (0%)	46	56
1	C	337/361 (93%)	320 (95%)	17 (5%)	0	100	100
1	D	352/361 (98%)	343 (97%)	9 (3%)	0	100	100
2	K	18/29 (62%)	17 (94%)	1 (6%)	0	100	100
2	L	18/29 (62%)	16 (89%)	2 (11%)	0	100	100
2	M	14/29 (48%)	14 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	14/29 (48%)	12 (86%)	2 (14%)	0	100	100
All	All	1465/1560 (94%)	1395 (95%)	69 (5%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	328	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/319 (97%)	309 (100%)	0	100	100
1	B	311/319 (98%)	311 (100%)	0	100	100
1	C	291/319 (91%)	291 (100%)	0	100	100
1	D	307/319 (96%)	307 (100%)	0	100	100
2	K	20/28 (71%)	20 (100%)	0	100	100
2	L	20/28 (71%)	20 (100%)	0	100	100
2	M	18/28 (64%)	18 (100%)	0	100	100
2	N	18/28 (64%)	18 (100%)	0	100	100
All	All	1294/1388 (93%)	1294 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	SB4	A	401	-	24,28,28	4.12	5 (20%)	29,39,39	3.88	11 (37%)
4	SO4	A	402	-	4,4,4	0.63	0	6,6,6	0.45	0
4	SO4	A	403	-	4,4,4	0.98	0	6,6,6	1.01	0
5	EDO	A	404	-	3,3,3	0.75	0	2,2,2	0.28	0
3	SB4	B	401	-	24,28,28	3.14	6 (25%)	29,39,39	2.98	16 (55%)
4	SO4	B	402	-	4,4,4	0.58	0	6,6,6	0.57	0
4	SO4	B	403	-	4,4,4	1.01	0	6,6,6	0.59	0
5	EDO	B	404	-	3,3,3	0.63	0	2,2,2	0.54	0
5	EDO	B	405	-	3,3,3	0.71	0	2,2,2	0.28	0
5	EDO	B	406	-	3,3,3	0.37	0	2,2,2	0.84	0
5	EDO	B	407	-	3,3,3	0.71	0	2,2,2	0.09	0
3	SB4	C	401	-	24,28,28	3.62	5 (20%)	29,39,39	3.69	16 (55%)
4	SO4	C	402	-	4,4,4	0.20	0	6,6,6	1.88	1 (16%)
4	SO4	C	403	-	4,4,4	0.86	0	6,6,6	0.30	0
5	EDO	C	404	-	3,3,3	0.48	0	2,2,2	0.71	0
3	SB4	D	401	-	24,28,28	3.44	5 (20%)	29,39,39	2.89	14 (48%)
4	SO4	D	402	-	4,4,4	0.69	0	6,6,6	0.68	0
4	SO4	D	403	-	4,4,4	0.61	0	6,6,6	0.70	0
5	EDO	D	404	-	3,3,3	0.86	0	2,2,2	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
3	SB4	A	401	-	-	0/5/20/20	0/4/4/4
4	SO4	A	402	-	-	0/0/0/0	0/0/0/0
4	SO4	A	403	-	-	0/0/0/0	0/0/0/0
5	EDO	A	404	-	-	0/1/1/1	0/0/0/0
3	SB4	B	401	-	-	0/5/20/20	0/4/4/4
4	SO4	B	402	-	-	0/0/0/0	0/0/0/0
4	SO4	B	403	-	-	0/0/0/0	0/0/0/0
5	EDO	B	404	-	-	0/1/1/1	0/0/0/0
5	EDO	B	405	-	-	0/1/1/1	0/0/0/0
5	EDO	B	406	-	-	0/1/1/1	0/0/0/0
5	EDO	B	407	-	-	0/1/1/1	0/0/0/0
3	SB4	C	401	-	-	0/5/20/20	0/4/4/4
4	SO4	C	402	-	-	0/0/0/0	0/0/0/0
4	SO4	C	403	-	-	0/0/0/0	0/0/0/0
5	EDO	C	404	-	-	0/1/1/1	0/0/0/0
3	SB4	D	401	-	-	0/5/20/20	0/4/4/4
4	SO4	D	402	-	-	0/0/0/0	0/0/0/0
4	SO4	D	403	-	-	0/0/0/0	0/0/0/0
5	EDO	D	404	-	-	0/1/1/1	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	SB4	CB6-CD4	-14.04	1.33	1.49
3	A	401	SB4	FB7-CB3	-13.66	1.05	1.36
3	C	401	SB4	CB6-CD4	-13.64	1.34	1.49
3	A	401	SB4	CB6-CD4	-13.57	1.34	1.49
3	B	401	SB4	CB6-CD4	-13.40	1.34	1.49
3	C	401	SB4	FB7-CB3	-9.46	1.14	1.36
3	D	401	SB4	FB7-CB3	-6.51	1.21	1.36
3	D	401	SB4	CD5-CD4	-4.36	1.33	1.43
3	B	401	SB4	CD5-CD4	-4.28	1.33	1.43
3	A	401	SB4	CD5-CD4	-3.87	1.34	1.43
3	C	401	SB4	CD5-CD4	-3.17	1.36	1.43
3	C	401	SB4	CC4-NC5	-2.30	1.32	1.35
3	A	401	SB4	CA1-CA2	-2.09	1.44	1.52
3	B	401	SB4	CA1-CA2	-2.02	1.45	1.52
3	B	401	SB4	CB2-CB3	2.00	1.41	1.37
3	B	401	SB4	CC6-NC5	2.12	1.39	1.34
3	D	401	SB4	CC6-NC5	2.28	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	SB4	CA6-ND1	2.30	1.52	1.49
3	B	401	SB4	FB7-CB3	3.02	1.43	1.36
3	A	401	SB4	CC6-NC5	3.08	1.41	1.34
3	C	401	SB4	CC6-NC5	3.20	1.41	1.34

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	SB4	CA2-CA1-CA6	-7.52	104.47	110.41
3	A	401	SB4	NC5-CC4-NC3	-5.66	119.87	125.78
3	D	401	SB4	CA2-CA1-CA6	-4.77	106.64	110.41
3	B	401	SB4	NC5-CC4-NC3	-4.59	120.99	125.78
3	B	401	SB4	CB5-CB6-CD4	-4.30	113.89	120.60
4	C	402	SO4	O2-S-O1	-4.27	95.96	109.50
3	C	401	SB4	NC5-CC4-NC3	-4.23	121.37	125.78
3	D	401	SB4	CC1-CC6-NC5	-4.22	119.08	123.90
3	C	401	SB4	CC1-CC2-NC3	-4.17	116.26	122.01
3	D	401	SB4	CA1-CA2-NA3	-4.07	103.55	110.46
3	A	401	SB4	CB5-CB6-CD4	-3.91	114.49	120.60
3	A	401	SB4	CC1-CC2-NC3	-3.88	116.66	122.01
3	D	401	SB4	CA4-CA5-CA6	-3.87	107.35	110.41
3	C	401	SB4	CC1-CC6-NC5	-3.87	119.49	123.90
3	C	401	SB4	CA5-CA6-ND1	-3.72	104.31	110.76
3	C	401	SB4	CA1-CA2-NA3	-3.44	104.61	110.46
3	A	401	SB4	CA5-CA4-NA3	-3.22	105.00	110.46
3	D	401	SB4	CC1-CC2-NC3	-3.21	117.57	122.01
3	B	401	SB4	CA5-CA4-NA3	-2.83	105.65	110.46
3	B	401	SB4	CC1-CC6-NC5	-2.66	120.86	123.90
3	C	401	SB4	CB5-CB6-CD4	-2.56	116.60	120.60
3	C	401	SB4	CA5-CA6-CA1	-2.55	105.23	110.13
3	D	401	SB4	NC5-CC4-NC3	-2.47	123.21	125.78
3	A	401	SB4	CA2-CA1-CA6	-2.43	108.49	110.41
3	D	401	SB4	CB4-CB3-CB2	-2.29	119.57	122.87
3	A	401	SB4	CC1-CC2-CD5	-2.09	116.76	120.92
3	D	401	SB4	CA5-CA4-NA3	-2.07	106.95	110.46
3	A	401	SB4	CC1-CC6-NC5	-2.06	121.55	123.90
3	B	401	SB4	CC1-CC2-NC3	-2.06	119.17	122.01
3	B	401	SB4	CB4-CB3-CB2	-2.03	119.94	122.87
3	D	401	SB4	NC7-CC4-NC5	2.28	119.44	117.39
3	C	401	SB4	CD5-ND1-CA6	2.39	130.92	126.12
3	D	401	SB4	CB1-CB2-CB3	2.45	120.99	118.35
3	B	401	SB4	FB7-CB3-CB2	2.55	122.77	118.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	SB4	NC7-CC4-NC3	2.68	121.64	117.20
3	C	401	SB4	CC6-NC5-CC4	2.74	118.78	116.32
3	B	401	SB4	CB1-CB2-CB3	2.74	121.31	118.35
3	C	401	SB4	CA4-CA5-CA6	2.79	112.61	110.41
3	B	401	SB4	CA2-CA1-CA6	2.80	112.62	110.41
3	B	401	SB4	CC6-NC5-CC4	2.93	118.95	116.32
3	D	401	SB4	CD5-CC2-NC3	2.93	121.91	116.50
3	C	401	SB4	CA1-CA6-ND1	3.20	116.31	110.76
3	A	401	SB4	CB1-CB6-CD4	3.21	125.61	120.60
3	C	401	SB4	CD5-CC2-NC3	3.21	122.43	116.50
3	D	401	SB4	CD5-ND1-CA6	3.30	132.75	126.12
3	B	401	SB4	CD5-CC2-NC3	3.31	122.60	116.50
3	C	401	SB4	CC6-CC1-CC2	3.40	120.52	117.26
3	A	401	SB4	NC7-CC4-NC3	3.60	123.16	117.20
3	B	401	SB4	NC7-CC4-NC3	3.63	123.21	117.20
3	D	401	SB4	CC6-CC1-CC2	3.84	120.93	117.26
3	B	401	SB4	CA4-CA5-CA6	3.87	113.46	110.41
3	B	401	SB4	CB1-CB6-CD4	4.33	127.36	120.60
3	B	401	SB4	CA5-CA6-CA1	4.33	118.47	110.13
3	A	401	SB4	CD5-CC2-NC3	5.38	126.43	116.50
3	B	401	SB4	CC2-NC3-CC4	8.16	120.77	116.34
3	D	401	SB4	CC2-NC3-CC4	8.74	121.08	116.34
3	C	401	SB4	CC2-NC3-CC4	13.25	123.52	116.34
3	A	401	SB4	CC2-NC3-CC4	16.53	125.30	116.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	SB4	1	0
3	B	401	SB4	1	0
5	B	406	EDO	1	0
3	C	401	SB4	1	0
5	C	404	EDO	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	352/361 (97%)	-0.04	3 (0%) 85 89	26, 39, 55, 72	0
1	B	351/361 (97%)	0.26	11 (3%) 52 61	28, 52, 69, 93	0
1	C	337/361 (93%)	0.03	8 (2%) 62 71	26, 44, 67, 96	0
1	D	351/361 (97%)	0.27	14 (3%) 42 50	28, 47, 75, 98	0
2	K	22/29 (75%)	0.32	1 (4%) 37 46	40, 47, 73, 92	0
2	L	22/29 (75%)	0.67	3 (13%) 4 6	43, 55, 72, 74	0
2	M	18/29 (62%)	1.01	5 (27%) 1 1	45, 49, 65, 73	0
2	N	18/29 (62%)	2.59	11 (61%) 0 0	68, 79, 99, 101	0
All	All	1471/1560 (94%)	0.18	56 (3%) 44 53	26, 46, 72, 101	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	411	SER	5.8
1	D	303	LEU	5.7
2	N	410	PRO	5.5
1	D	304	ALA	4.7
1	B	45	LYS	4.5
2	N	392	TYR	4.5
1	D	308	PHE	4.4
2	M	411	SER	4.3
2	N	407	LEU	4.3
2	L	405	LEU	4.1
1	C	172	ALA	4.0
2	N	408	VAL	3.9
2	N	386	TYR	3.8
1	C	237	ARG	3.8
1	C	198	MET	3.8
1	B	346	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
2	N	405	LEU	3.6
1	B	46	THR	3.5
1	D	275	ILE	3.5
2	M	408	VAL	3.5
2	M	410	PRO	3.5
2	N	385	VAL	3.4
1	D	309	ALA	3.2
1	D	172	ALA	3.1
1	C	266	PRO	3.1
2	N	409	MET	3.0
1	B	34[A]	ALA	3.0
2	M	394	SER	3.0
1	C	173	ARG	2.9
1	C	310	GLN	2.8
2	N	406	SER	2.8
1	D	276	GLY	2.8
1	B	315	ASP	2.7
1	D	284	LEU	2.6
2	K	386	TYR	2.6
1	D	179	MET	2.6
1	D	274	PHE	2.5
1	B	304	ALA	2.5
1	C	263	ALA	2.4
1	D	199	HIS	2.4
2	L	395	ALA	2.3
1	D	297	ILE	2.3
1	C	191	PRO	2.2
1	A	354	ASP	2.2
1	B	89	VAL	2.2
2	M	385	VAL	2.2
1	B	294	ASP	2.2
2	L	407	LEU	2.1
1	D	122	LEU	2.1
2	N	404	THR	2.1
1	B	162	CYS	2.1
1	A	173	ARG	2.1
1	D	119	CYS	2.0
1	B	335	ASP	2.0
1	A	303	LEU	2.0
1	B	35[A]	TYR	2.0



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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	D	404	4/4	0.77	0.19	3.35	47,48,49,50	0
5	EDO	B	406	4/4	0.93	0.16	2.22	42,44,45,46	0
3	SB4	D	401	25/25	0.94	0.14	0.21	31,37,42,44	0
3	SB4	C	401	25/25	0.95	0.12	-0.12	33,37,42,46	0
4	SO4	A	402	5/5	0.99	0.10	-0.54	37,43,46,49	0
4	SO4	B	402	5/5	0.97	0.12	-0.58	38,42,50,62	0
4	SO4	C	402	5/5	0.99	0.12	-0.67	34,42,45,49	0
3	SB4	B	401	25/25	0.94	0.13	-0.70	40,48,52,54	0
4	SO4	D	402	5/5	0.99	0.11	-1.05	33,35,41,41	0
3	SB4	A	401	25/25	0.96	0.10	-1.10	24,27,40,43	0
5	EDO	C	404	4/4	0.95	0.09	-1.43	37,39,41,43	0
5	EDO	B	405	4/4	0.83	0.18	-	38,48,53,57	0
5	EDO	B	407	4/4	0.80	0.14	-	53,54,57,58	0
4	SO4	B	403	5/5	0.95	0.11	-	43,44,52,53	0
4	SO4	A	403	5/5	0.95	0.11	-	38,42,47,49	0
4	SO4	D	403	5/5	0.97	0.11	-	38,39,46,50	0
5	EDO	A	404	4/4	0.90	0.15	-	44,46,48,52	0
5	EDO	B	404	4/4	0.83	0.12	-	44,48,49,51	0
4	SO4	C	403	5/5	0.96	0.09	-	39,45,49,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.