



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:31 AM GMT

PDB ID : 3MAA  
Title : Complex of GS-Alpha with the Catalytic Domains of Mammalian Adenylyl Cyclase: Complex with Adenosine 5-O-(l-Thiophosphate) and Low Ca Concentration  
Authors : Mou, T.-C.; Sprang, S.R.  
Deposited on : 2010-03-23  
Resolution : 3.00 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

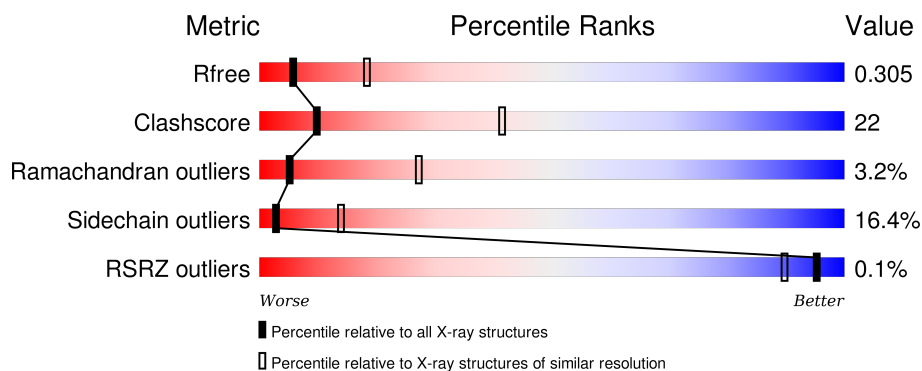
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	225	
2	B	212	
3	C	394	

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	FKP	A	101	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5744 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 Adenylate cyclase type 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1484	933	260	274	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	MET	-	EXPRESSION TAG	UNP P30803
A	357	HIS	-	EXPRESSION TAG	UNP P30803
A	358	HIS	-	EXPRESSION TAG	UNP P30803
A	359	HIS	-	EXPRESSION TAG	UNP P30803
A	360	HIS	-	EXPRESSION TAG	UNP P30803
A	361	HIS	-	EXPRESSION TAG	UNP P30803
A	362	HIS	-	EXPRESSION TAG	UNP P30803
A	476	MET	VAL	ENGINEERED	UNP P30803

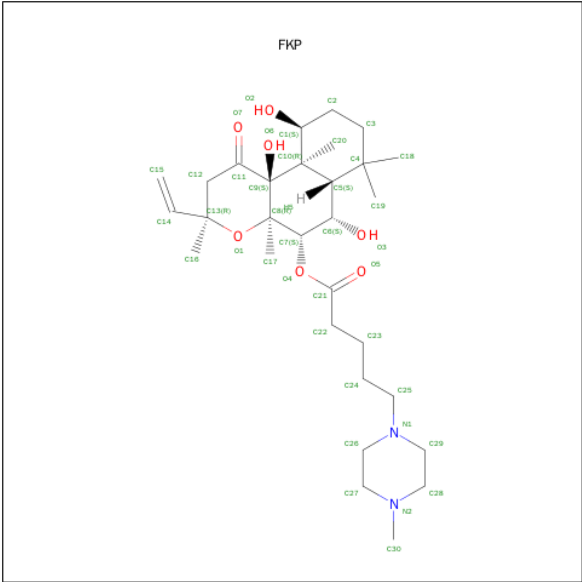
- Molecule 2 is a protein called Adenylate cyclase type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1459	930	241	278	10			

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	328	Total	C	N	O	S	0	0	0
			2684	1701	467	504	12			

- Molecule 4 is METHYLPIPERAZINOFORSKOLIN (three-letter code: FKP) (formula:  $C_{30}H_{50}N_2O_7$ ).

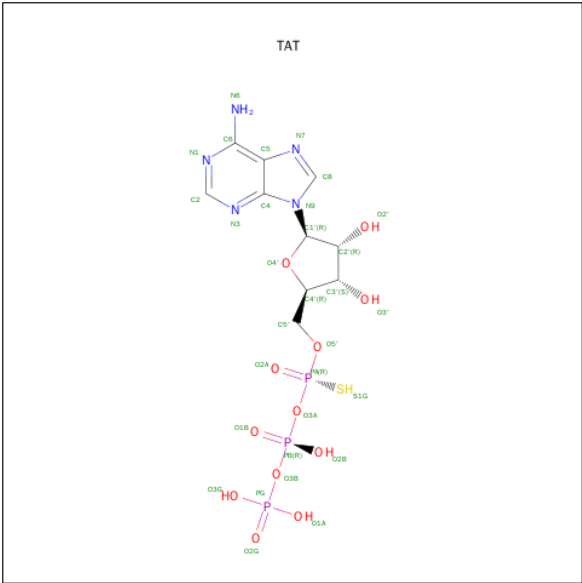


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			39	30	2	7		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-RP-ALPHA-THIO-TRIPHOSPHATE (three-letter code: TAT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).

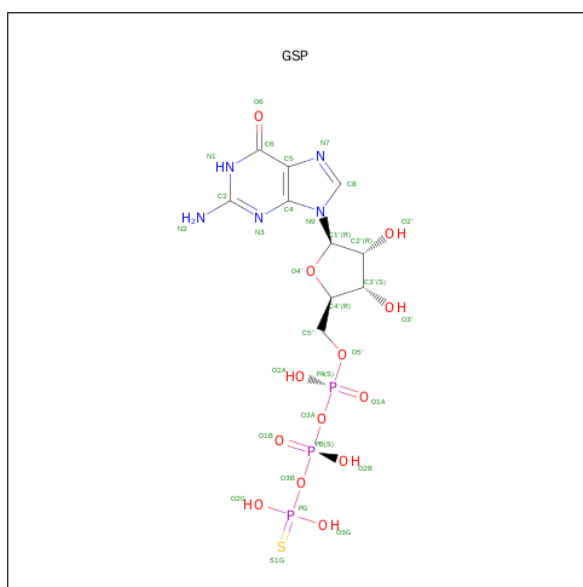


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	S	
			31	10	5	12	3	1	
									0
									0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg		
			1	1	0	0

- Molecule 8 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	S	
			32	10	5	13	3	1	
									0
									0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Cl		
			1	1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	O		
			2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	5	Total	O	0	0
			5	5		
10	C	5	Total	O	0	0
			5	5		





K307	R228
I308	D229
E309	E230
D310	R231
GLN	R232
TYR	K233
GLU	W234
LEU	
LEU	C237
	V241
	I244
	I245
	F246
	V247
	S250
	T355
	Y253
	N254
	M255
	V256
	I257
	R258
	E259
	D260
	N261
	Q262
	T263
	T264
	R265
	L270
	N271
	L272
	F273
	W277
	R280
	T284
	I285
	S286
	V287
	I288
	L291
	N292
	K293
	Q294
	D295
	L296
	L297
	Y301
	K305
	S306

MET

HIS

LEU

ARG

GLN

TYR

GLU

LEU

LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.74Å 133.72Å 70.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 24.71 – 2.95	Depositor EDS
% Data completeness (in resolution range)	82.7 (25.00-3.00) 82.0 (24.71-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.94Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.239 , 0.309 0.237 , 0.305	Depositor DCC
$R_{free}$ test set	964 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.923	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 10.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 20016 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	5744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TAT, GSP, MG, CL, CA, FKP

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	0.51	0/1512	0.70	1/2038 (0.0%)
2	B	0.56	0/1484	0.72	0/2003
3	C	0.57	0/2740	0.72	0/3708
All	All	0.55	0/5736	0.72	1/7749 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	LEU	CA-CB-CG	5.16	127.18	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1484	0	1454	59	0
2	B	1459	0	1459	67	0
3	C	2684	0	2631	126	0
4	A	39	0	50	5	0
5	A	1	0	0	0	0
6	B	31	0	14	0	0
7	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	32	0	12	5	0
9	C	1	0	0	1	0
10	A	2	0	0	0	0
10	B	5	0	0	2	0
10	C	5	0	0	3	0
All	All	5744	0	5620	252	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 22.

All (252) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1045:THR:HG22	2:B:1049:LEU:HD11	1.36	1.05
2:B:1045:THR:HG22	2:B:1049:LEU:CD1	1.94	0.97
3:C:307:LYS:HB3	3:C:309:GLU:OE2	1.66	0.95
3:C:95:ILE:HG23	3:C:178:PHE:CE2	2.04	0.93
2:B:1045:THR:CG2	2:B:1049:LEU:HD11	2.04	0.87
3:C:166:SER:HA	3:C:169:TYR:CE2	2.10	0.85
4:A:101:FKP:H173	4:A:101:FKP:H201	1.60	0.84
3:C:95:ILE:HG23	3:C:178:PHE:HE2	1.44	0.82
2:B:1049:LEU:O	2:B:1054:TYR:HB2	1.83	0.79
1:A:530:LYS:HD2	1:A:531:ALA:H	1.48	0.76
2:B:891:SER:HB2	10:B:16:HOH:O	1.85	0.76
2:B:991:PHE:O	3:C:232:ARG:HA	1.86	0.75
3:C:166:SER:HA	3:C:169:TYR:HE2	1.51	0.75
3:C:230:GLU:HG3	10:C:401:HOH:O	1.88	0.74
2:B:1059:ARG:HB2	2:B:1074:PHE:CE2	2.23	0.74
2:B:884:CYS:HG	2:B:966:TYR:HE1	1.36	0.73
2:B:880:GLN:HE22	2:B:882:TYR:HE1	1.37	0.73
1:A:527:HIS:NE2	1:A:561:THR:HB	2.04	0.72
1:A:486:GLY:HA2	1:A:527:HIS:HB3	1.72	0.72
2:B:905:ASN:O	2:B:907:GLU:N	2.23	0.72
3:C:371:ASN:O	3:C:375:VAL:HG22	1.90	0.72
1:A:467:ILE:HA	1:A:470:ILE:HG22	1.71	0.72
2:B:972:MET:O	2:B:975:PHE:HB3	1.90	0.72
1:A:505:ASP:HB3	1:A:507:TRP:CZ2	2.27	0.70
3:C:284:THR:O	3:C:357:HIS:HB3	1.90	0.70
3:C:44:LEU:HD22	3:C:237:CYS:HB3	1.75	0.67
1:A:546:CYS:O	1:A:549:GLU:HG2	1.95	0.67
3:C:131:ILE:O	3:C:134:VAL:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:ALA:O	3:C:106:ILE:HG13	1.94	0.67
1:A:542:VAL:HB	1:A:563:LEU:O	1.96	0.65
3:C:143:PRO:HB2	3:C:145:GLU:OE2	1.96	0.65
1:A:521:GLY:HA2	1:A:527:HIS:HD1	1.61	0.65
3:C:321:PRO:O	3:C:324:ALA:HB2	1.96	0.65
1:A:530:LYS:CD	1:A:531:ALA:H	2.11	0.63
3:C:343:ASP:O	3:C:347:ARG:HG3	1.97	0.63
3:C:295:ASP:OD1	3:C:295:ASP:N	2.31	0.62
1:A:388:ASP:HB3	1:A:389:ASN:ND2	2.14	0.62
2:B:1067:LYS:O	2:B:1067:LYS:HG3	2.00	0.62
3:C:166:SER:OG	3:C:171:LEU:HD23	2.00	0.62
1:A:434:ARG:HG2	1:A:435:ILE:N	2.16	0.61
2:B:925:LEU:HD12	2:B:979:LEU:HD23	1.82	0.61
1:A:423:PHE:HB3	1:A:442:TYR:CE1	2.36	0.61
1:A:456:ALA:O	1:A:460:VAL:HG23	2.00	0.61
2:B:885:VAL:O	2:B:1002:HIS:HA	1.99	0.61
3:C:42:ARG:HD3	3:C:42:ARG:H	1.66	0.61
2:B:884:CYS:SG	2:B:966:TYR:HE1	2.23	0.60
1:A:379:PHE:CE2	2:B:913:ARG:HG2	2.37	0.60
2:B:1030:MET:HE3	2:B:1042:THR:HG23	1.83	0.60
1:A:388:ASP:HB3	1:A:389:ASN:HD22	1.66	0.60
3:C:99:LEU:HD11	3:C:179:LEU:HD23	1.84	0.59
4:A:101:FKP:H202	4:A:101:FKP:H193	1.84	0.59
1:A:388:ASP:C	1:A:389:ASN:HD22	2.06	0.59
1:A:547:GLY:HA2	1:A:550:ARG:HH11	1.68	0.58
3:C:55:THR:HA	3:C:58:LYS:HD2	1.85	0.58
1:A:543:GLU:HB2	1:A:544:PRO:HD2	1.85	0.58
1:A:528:ILE:HD12	1:A:529:THR:O	2.04	0.58
3:C:151:LYS:O	3:C:155:GLU:HG2	2.03	0.57
3:C:254:ASN:OD1	3:C:255:MET:HG3	2.04	0.57
3:C:207:ILE:HD11	3:C:224:VAL:HG12	1.87	0.57
2:B:890:ALA:HB1	2:B:996:LEU:HD11	1.86	0.57
2:B:1044:GLU:H	2:B:1044:GLU:CD	2.08	0.57
3:C:123:GLU:O	3:C:126:PHE:HD2	1.88	0.56
1:A:408:THR:O	1:A:410:GLN:N	2.38	0.56
2:B:1040:GLN:HA	2:B:1073:TYR:O	2.05	0.56
2:B:1000:ILE:CG2	2:B:1001:ASN:N	2.69	0.56
3:C:55:THR:O	3:C:58:LYS:HB2	2.05	0.56
3:C:132:LEU:HB3	3:C:135:MET:HE3	1.87	0.56
3:C:291:LEU:HD22	3:C:341:ILE:HG22	1.87	0.56
3:C:100:LYS:O	3:C:104:GLU:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:891:SER:CB	10:B:16:HOH:O	2.49	0.55
3:C:187:GLN:O	3:C:190:TYR:HB3	2.06	0.55
3:C:330:GLU:OE2	3:C:335:THR:HG23	2.07	0.55
3:C:253:TYR:CE1	3:C:308:ILE:HG12	2.41	0.55
1:A:479:VAL:HG13	1:A:481:VAL:HG22	1.88	0.55
2:B:1045:THR:HG22	2:B:1049:LEU:HD12	1.82	0.55
2:B:1030:MET:HE3	2:B:1042:THR:CG2	2.35	0.55
3:C:327:GLU:O	3:C:330:GLU:HB3	2.07	0.55
3:C:44:LEU:HD22	3:C:237:CYS:CB	2.37	0.54
2:B:1000:ILE:HG22	2:B:1001:ASN:N	2.21	0.54
2:B:948:THR:HB	2:B:968:HIS:HB2	1.88	0.54
1:A:467:ILE:HA	1:A:470:ILE:CG2	2.38	0.54
2:B:1075:VAL:HG12	2:B:1076:ASN:N	2.23	0.53
2:B:891:SER:HB3	2:B:943:THR:HG23	1.90	0.53
2:B:918:ILE:HG12	2:B:986:ILE:HG13	1.88	0.53
3:C:291:LEU:CD2	3:C:341:ILE:HG22	2.39	0.53
3:C:181:LYS:O	3:C:185:ILE:HG13	2.09	0.53
3:C:326:PRO:HB3	3:C:335:THR:HG21	1.89	0.53
3:C:201:ARG:HB2	8:C:395:GSP:O3'	2.09	0.53
3:C:195:GLN:HA	3:C:195:GLN:NE2	2.24	0.53
3:C:368:ASP:O	3:C:370:GLU:N	2.42	0.52
1:A:435:ILE:HG12	1:A:444:CYS:HA	1.91	0.52
3:C:94:ASP:HB3	3:C:200:CYS:SG	2.49	0.52
3:C:241:VAL:HG13	3:C:285:ILE:HG13	1.92	0.52
3:C:225:GLY:HA3	3:C:230:GLU:HB3	1.92	0.52
3:C:365:CYS:SG	3:C:368:ASP:HB2	2.50	0.52
1:A:427:ALA:HA	1:A:462:MET:CE	2.39	0.52
3:C:309:GLU:O	3:C:313:PRO:HA	2.09	0.52
2:B:886:CYS:HA	2:B:1001:ASN:O	2.10	0.51
1:A:386:LYS:O	1:A:387:HIS:CD2	2.64	0.51
3:C:99:LEU:CD1	3:C:179:LEU:HD23	2.40	0.51
3:C:257:ILE:HG22	3:C:265:ARG:CG	2.41	0.51
1:A:423:PHE:HA	1:A:426:LEU:HD12	1.93	0.51
3:C:107:VAL:O	3:C:108:ALA:C	2.49	0.50
3:C:293:LYS:HG2	8:C:395:GSP:C6	2.46	0.50
2:B:884:CYS:O	2:B:968:HIS:NE2	2.36	0.50
1:A:493:HIS:O	1:A:506:VAL:HA	2.11	0.50
3:C:199:ARG:HA	8:C:395:GSP:O2'	2.12	0.50
1:A:434:ARG:HG3	1:A:442:TYR:CE2	2.47	0.50
3:C:307:LYS:HB2	3:C:310:ASP:OD2	2.12	0.49
3:C:277:TRP:CE2	3:C:349:SER:HA	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:VAL:O	3:C:114:VAL:HG13	2.12	0.49
1:A:512:THR:HG22	1:A:516:HIS:HD2	1.77	0.49
2:B:897:GLU:O	2:B:899:TYR:N	2.45	0.49
3:C:257:ILE:HG22	3:C:265:ARG:HG3	1.94	0.49
2:B:988:LYS:HB2	2:B:988:LYS:NZ	2.26	0.49
2:B:1030:MET:HA	2:B:1040:GLN:NE2	2.28	0.49
3:C:207:ILE:HG12	3:C:223:ASP:O	2.12	0.49
2:B:1047:LEU:O	2:B:1050:GLN:HB2	2.13	0.49
3:C:100:LYS:HE2	3:C:134:VAL:HG23	1.95	0.48
1:A:517:MET:HE2	1:A:527:HIS:CD2	2.49	0.48
1:A:452:ARG:HE	1:A:454:ASP:HB2	1.77	0.48
3:C:320:THR:HA	3:C:321:PRO:HD3	1.76	0.48
3:C:182:ILE:O	3:C:185:ILE:N	2.45	0.48
1:A:382:ILE:H	1:A:382:ILE:HG13	1.46	0.48
3:C:106:ILE:HG23	3:C:169:TYR:OH	2.13	0.48
3:C:173:ASP:OD2	3:C:173:ASP:N	2.42	0.48
1:A:470:ILE:O	1:A:470:ILE:HG13	2.13	0.47
3:C:130:TYR:O	3:C:133:SER:OG	2.29	0.47
3:C:142:PHE:N	3:C:143:PRO:HD3	2.29	0.47
2:B:1045:THR:O	2:B:1049:LEU:HD12	2.15	0.47
3:C:232:ARG:HB3	3:C:232:ARG:CZ	2.44	0.47
3:C:253:TYR:CZ	3:C:308:ILE:HG12	2.49	0.47
1:A:427:ALA:HA	1:A:462:MET:HE2	1.96	0.47
3:C:366:ALA:HB3	8:C:395:GSP:N7	2.30	0.47
3:C:325:THR:HG23	3:C:339:TYR:OH	2.14	0.47
3:C:277:TRP:CD1	3:C:348:ILE:HG22	2.50	0.47
3:C:206:GLY:O	3:C:207:ILE:HG13	2.15	0.47
2:B:1030:MET:HE1	2:B:1072:THR:HG22	1.97	0.47
3:C:288:ILE:HG23	3:C:360:TYR:HB2	1.97	0.47
3:C:272:LEU:HD12	3:C:272:LEU:O	2.15	0.47
2:B:974:GLU:HA	2:B:974:GLU:OE2	2.15	0.46
9:C:397:CL:CL	10:C:398:HOH:O	2.58	0.46
4:A:101:FKP:C17	4:A:101:FKP:H201	2.37	0.46
1:A:391:SER:OG	1:A:456:ALA:HA	2.16	0.46
3:C:53:LYS:C	3:C:55:THR:H	2.18	0.46
2:B:1060:GLY:O	2:B:1071:LYS:HA	2.15	0.46
3:C:137:VAL:CG1	3:C:138:PRO:HD2	2.46	0.46
1:A:488:HIS:ND1	1:A:529:THR:HG21	2.30	0.46
2:B:1055:THR:HB	2:B:1076:ASN:ND2	2.30	0.46
1:A:417:ASN:HA	2:B:1010:ILE:HD12	1.98	0.46
1:A:506:VAL:C	1:A:507:TRP:CG	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:TYR:N	1:A:383:TYR:CD2	2.84	0.46
1:A:436:LYS:HE3	1:A:503:GLN:OE1	2.16	0.45
2:B:888:MET:HG3	2:B:1000:ILE:CG1	2.47	0.45
2:B:892:ILE:O	2:B:892:ILE:HG22	2.15	0.45
1:A:415:THR:O	1:A:418:GLU:HB3	2.15	0.45
1:A:500:ARG:O	2:B:936:LYS:NZ	2.45	0.45
1:A:554:LEU:O	1:A:555:LYS:C	2.55	0.45
1:A:414:MET:O	1:A:418:GLU:HB2	2.16	0.45
1:A:383:TYR:HB2	1:A:496:VAL:HG22	1.99	0.45
3:C:322:GLU:C	3:C:324:ALA:H	2.21	0.45
1:A:417:ASN:HA	2:B:1010:ILE:CD1	2.46	0.45
3:C:164:GLU:HB3	3:C:305:LYS:NZ	2.31	0.45
3:C:175:ALA:O	3:C:176:GLN:C	2.54	0.45
4:A:101:FKP:H171	4:A:101:FKP:H163	1.99	0.45
2:B:902:SER:O	2:B:905:ASN:O	2.35	0.44
3:C:270:LEU:O	3:C:273:PHE:HB3	2.17	0.44
3:C:364:THR:HG22	3:C:375:VAL:HG21	1.99	0.44
3:C:215:ASP:OD2	3:C:380:ARG:NH2	2.51	0.44
2:B:891:SER:CB	2:B:943:THR:HG23	2.47	0.44
2:B:1030:MET:CE	2:B:1042:THR:HG22	2.47	0.44
2:B:1000:ILE:HB	2:B:1041:VAL:HG12	1.98	0.44
3:C:265:ARG:NH1	10:C:400:HOH:O	2.50	0.44
2:B:911:CYS:O	2:B:914:LEU:N	2.44	0.44
2:B:1062:ILE:O	2:B:1069:ASP:HA	2.18	0.44
2:B:1022:ASN:C	2:B:1022:ASN:HD22	2.19	0.44
3:C:44:LEU:HA	3:C:222:PHE:HB2	1.99	0.44
1:A:537:ASN:O	1:A:538:GLY:C	2.56	0.44
3:C:207:ILE:HG12	3:C:224:VAL:HA	1.99	0.44
3:C:292:ASN:HA	3:C:364:THR:O	2.18	0.44
3:C:143:PRO:HA	3:C:144:PRO:HD3	1.89	0.44
3:C:121:ASN:HA	3:C:122:PRO:HD2	1.72	0.44
3:C:244:ILE:CG2	3:C:287:VAL:HG13	2.48	0.44
3:C:109:ALA:HA	3:C:112:ASN:HB2	2.00	0.43
3:C:87:GLU:C	3:C:89:ALA:H	2.21	0.43
3:C:353:GLY:O	3:C:356:ARG:HB3	2.18	0.43
2:B:1030:MET:CE	2:B:1042:THR:CG2	2.96	0.43
3:C:260:ASP:OD1	3:C:261:ASN:N	2.52	0.43
2:B:950:LEU:H	2:B:950:LEU:HD12	1.82	0.43
3:C:125:GLN:O	3:C:128:VAL:HB	2.18	0.43
3:C:257:ILE:HG12	3:C:258:ARG:N	2.32	0.43
3:C:127:ARG:O	3:C:130:TYR:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:257:ILE:HD12	3:C:263:THR:HB	2.01	0.43
3:C:228:ARG:HB2	3:C:259:GLU:HG2	2.00	0.43
3:C:297:LEU:O	3:C:301:VAL:HG23	2.18	0.43
2:B:925:LEU:O	2:B:928:LYS:HB2	2.18	0.43
3:C:53:LYS:C	3:C:55:THR:N	2.73	0.43
3:C:114:VAL:O	3:C:114:VAL:CG1	2.66	0.43
2:B:1039:ILE:O	2:B:1074:PHE:HA	2.19	0.42
3:C:99:LEU:O	3:C:100:LYS:C	2.57	0.42
1:A:423:PHE:HB3	1:A:442:TYR:HE1	1.84	0.42
2:B:927:SER:O	2:B:928:LYS:C	2.57	0.42
3:C:46:LEU:HB2	3:C:246:PHE:HD1	1.85	0.42
3:C:349:SER:HB2	3:C:359:CYS:HB2	2.02	0.42
3:C:131:ILE:HD13	3:C:131:ILE:HA	1.92	0.42
3:C:154:TRP:CE2	3:C:179:LEU:HB3	2.54	0.42
3:C:257:ILE:HG22	3:C:265:ARG:HA	2.01	0.42
3:C:137:VAL:HG13	3:C:138:PRO:HD2	2.02	0.42
3:C:199:ARG:HG2	3:C:367:VAL:HG11	2.01	0.42
3:C:323:ASP:O	3:C:325:THR:HG22	2.19	0.42
3:C:130:TYR:O	3:C:134:VAL:HG13	2.19	0.42
2:B:979:LEU:O	2:B:983:LEU:N	2.43	0.42
3:C:339:TYR:O	3:C:342:ARG:HB3	2.20	0.42
3:C:56:ILE:O	3:C:57:VAL:C	2.58	0.42
3:C:346:LEU:O	3:C:350:THR:HB	2.20	0.42
2:B:1075:VAL:CG1	2:B:1076:ASN:N	2.83	0.42
1:A:430:ASN:O	1:A:431:HIS:HB2	2.20	0.42
1:A:517:MET:CE	1:A:527:HIS:CD2	3.03	0.42
3:C:293:LYS:HA	8:C:395:GSP:O6	2.20	0.42
3:C:46:LEU:O	3:C:247:VAL:HG23	2.19	0.42
4:A:101:FKP:H1	4:A:101:FKP:O7	2.19	0.41
3:C:368:ASP:O	3:C:371:ASN:N	2.50	0.41
3:C:257:ILE:O	3:C:261:ASN:HA	2.19	0.41
2:B:1030:MET:HA	2:B:1040:GLN:HE21	1.83	0.41
1:A:485:VAL:HG21	1:A:526:ILE:HG12	2.02	0.41
3:C:377:ASN:C	3:C:379:CYS:H	2.24	0.41
3:C:188:ASP:N	3:C:188:ASP:OD1	2.50	0.41
3:C:231:ARG:HG2	3:C:234:TRP:CZ2	2.55	0.41
1:A:457:HIS:HD2	1:A:540:TYR:HE1	1.67	0.41
1:A:530:LYS:HG3	1:A:530:LYS:H	1.64	0.41
2:B:891:SER:O	2:B:996:LEU:HD12	2.21	0.41
3:C:368:ASP:O	3:C:369:THR:C	2.57	0.41
1:A:418:GLU:HB3	1:A:419:LEU:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:ARG:HG2	3:C:160:ARG:HH11	1.86	0.41
2:B:992:ASN:ND2	3:C:232:ARG:HB2	2.36	0.41
3:C:343:ASP:HA	3:C:346:LEU:HB2	2.03	0.41
3:C:325:THR:OG1	3:C:325:THR:O	2.36	0.41
2:B:923:ASP:OD1	2:B:944:TYR:OH	2.24	0.41
1:A:549:GLU:H	1:A:549:GLU:HG2	1.76	0.41
2:B:1059:ARG:HD3	2:B:1072:THR:OG1	2.20	0.41
2:B:880:GLN:NE2	2:B:880:GLN:O	2.54	0.41
1:A:507:TRP:O	1:A:508:SER:HB3	2.21	0.41
3:C:277:TRP:CZ3	3:C:357:HIS:CE1	3.09	0.41
3:C:54:SER:HB3	3:C:223:ASP:OD2	2.21	0.41
3:C:241:VAL:CG1	3:C:285:ILE:HG13	2.51	0.41
1:A:453:ALA:C	1:A:455:HIS:H	2.23	0.41
2:B:1007:ALA:HB1	2:B:1017:TYR:HE1	1.86	0.41
2:B:891:SER:HB3	2:B:943:THR:OG1	2.21	0.40
1:A:466:MET:O	1:A:470:ILE:HG22	2.21	0.40
3:C:277:TRP:CZ2	3:C:349:SER:O	2.75	0.40
3:C:134:VAL:O	3:C:137:VAL:HG23	2.21	0.40
1:A:552:ALA:O	1:A:554:LEU:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	188/225 (84%)	156 (83%)	26 (14%)	6 (3%)	5	27
2	B	184/212 (87%)	153 (83%)	26 (14%)	5 (3%)	6	32
3	C	324/394 (82%)	264 (82%)	49 (15%)	11 (3%)	5	25
All	All	696/831 (84%)	573 (82%)	101 (14%)	22 (3%)	5	27

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	ALA
3	C	48	ALA
3	C	122	PRO
3	C	138	PRO
3	C	175	ALA
1	A	413	VAL
1	A	538	GLY
1	A	552	ALA
1	A	553	TYR
2	B	898	PHE
2	B	906	LYS
2	B	1011	GLY
3	C	378	ASP
1	A	418	GLU
3	C	88	LYS
3	C	381	ASP
2	B	1023	THR
2	B	1032	SER
3	C	250	SER
3	C	313	PRO
3	C	367	VAL
3	C	128	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	159/189 (84%)	131 (82%)	28 (18%)	2	12
2	B	161/184 (88%)	134 (83%)	27 (17%)	2	13
3	C	295/351 (84%)	249 (84%)	46 (16%)	3	16
All	All	615/724 (85%)	514 (84%)	101 (16%)	3	14

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	ILE

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Mol	Chain	Res	Type
1	A	383	TYR
1	A	385	GLN
1	A	388	ASP
1	A	389	ASN
1	A	401	THR
1	A	402	SER
1	A	408	THR
1	A	411	GLU
1	A	415	THR
1	A	422	ARG
1	A	424	ASP
1	A	433	LEU
1	A	434	ARG
1	A	440	ASP
1	A	450	GLU
1	A	454	ASP
1	A	467	ILE
1	A	480	ASN
1	A	481	VAL
1	A	485	VAL
1	A	491	ARG
1	A	508	SER
1	A	518	GLU
1	A	528	ILE
1	A	530	LYS
1	A	534	SER
1	A	537	ASN
2	B	880	GLN
2	B	891	SER
2	B	894	ASP
2	B	896	LYS
2	B	924	ASP
2	B	928	LYS
2	B	937	ILE
2	B	938	LYS
2	B	940	ILE
2	B	950	LEU
2	B	964	ARG
2	B	972	MET
2	B	988	LYS
2	B	997	ARG
2	B	1001	ASN

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Mol	Chain	Res	Type
2	B	1005	VAL
2	B	1014	LYS
2	B	1017	TYR
2	B	1022	ASN
2	B	1029	ARG
2	B	1048	ILE
2	B	1055	THR
2	B	1059	ARG
2	B	1062	ILE
2	B	1070	LEU
2	B	1076	ASN
2	B	1077	THR
3	C	40	THR
3	C	42	ARG
3	C	45	LEU
3	C	87	GLU
3	C	111	SER
3	C	132	LEU
3	C	133	SER
3	C	139	ASP
3	C	145	GLU
3	C	169	TYR
3	C	173	ASP
3	C	184	VAL
3	C	186	LYS
3	C	190	TYR
3	C	195	GLN
3	C	204	THR
3	C	207	ILE
3	C	216	LYS
3	C	221	MET
3	C	228	ARG
3	C	229	ASP
3	C	257	ILE
3	C	262	GLN
3	C	271	ASN
3	C	272	LEU
3	C	280	ARG
3	C	286	SER
3	C	291	LEU
3	C	295	ASP
3	C	307	LYS

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Mol	Chain	Res	Type
3	C	308	ILE
3	C	309	GLU
3	C	320	THR
3	C	323	ASP
3	C	325	THR
3	C	330	GLU
3	C	335	THR
3	C	357	HIS
3	C	365	CYS
3	C	370	GLU
3	C	371	ASN
3	C	375	VAL
3	C	380	ARG
3	C	382	ILE
3	C	383	ILE
3	C	384	GLN

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

Mol	Chain	Res	Type
1	A	385	GLN
1	A	389	ASN
1	A	480	ASN
2	B	880	GLN
2	B	905	ASN
2	B	989	HIS
2	B	1001	ASN
2	B	1022	ASN
2	B	1050	GLN
3	C	64	HIS
3	C	213	GLN
3	C	239	ASN
3	C	371	ASN
3	C	377	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	FKP	A	101	-	37,42,42	0.90	1 (2%)	49,68,68	1.46	6 (12%)
6	TAT	B	1	5	22,33,33	1.44	4 (18%)	29,52,52	2.16	5 (17%)
8	GSP	C	395	7	25,34,34	2.15	2 (8%)	31,54,54	2.17	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FKP	A	101	-	-	0/14/97/97	0/4/4/4
6	TAT	B	1	5	-	0/13/38/38	0/3/3/3
8	GSP	C	395	7	-	0/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	395	GSP	PG-S1G	-9.69	1.71	1.90
8	C	395	GSP	C6-N1	2.15	1.37	1.33
6	B	1	TAT	PG-O3G	2.29	1.62	1.54
6	B	1	TAT	PG-O1A	2.48	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1	TAT	PA-O5'	3.29	1.63	1.58
4	A	101	FKP	O4-C21	3.63	1.45	1.34
6	B	1	TAT	O4'-C1'	3.68	1.45	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1	TAT	N3-C2-N1	-8.96	122.04	128.89
8	C	395	GSP	PB-O3B-PG	-6.77	109.98	132.67
8	C	395	GSP	PA-O3A-PB	-4.88	119.01	132.73
6	B	1	TAT	C4'-O4'-C1'	-4.49	104.78	109.72
8	C	395	GSP	N3-C2-N1	-4.10	121.20	127.44
8	C	395	GSP	O3A-PA-O5'	-3.77	92.94	102.94
6	B	1	TAT	C4-C5-N7	-3.21	106.53	109.48
8	C	395	GSP	C4-C5-N7	-3.21	106.53	109.48
8	C	395	GSP	C5-C6-N1	-2.65	119.96	123.59
4	A	101	FKP	C7-O4-C21	-2.46	112.97	118.37
4	A	101	FKP	C13-C14-C15	-2.33	117.24	129.04
6	B	1	TAT	PB-O3B-PG	-2.33	124.85	132.67
8	C	395	GSP	C6-N1-C2	2.04	118.78	115.94
6	B	1	TAT	O4'-C1'-N9	2.16	112.61	108.10
4	A	101	FKP	C3-C4-C5	3.36	113.10	107.73
4	A	101	FKP	O1-C13-C12	3.47	115.32	111.23
4	A	101	FKP	O4-C21-C22	4.11	120.46	111.53
4	A	101	FKP	C13-O1-C8	4.40	124.65	120.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	101	FKP	5	0
8	C	395	GSP	5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	190/225 (84%)	-0.54	0 <span>100</span> <span>100</span>	17, 39, 66, 75	0
2	B	188/212 (88%)	-0.62	1 (0%) <span>91</span> <span>76</span>	17, 23, 54, 73	0
3	C	328/394 (83%)	-0.68	0 <span>100</span> <span>100</span>	17, 26, 47, 78	0
All	All	706/831 (84%)	-0.63	1 (0%) <span>95</span> <span>90</span>	17, 28, 58, 78	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1065	LYS	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 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
4	FKP	A	101	39/39	0.94	0.23	<span>3.46</span>	36,50,93,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	TAT	B	1	31/31	0.82	0.30	1.28	68,77,107,108	0
9	CL	C	397	1/1	0.98	0.19	0.96	50,50,50,50	0
8	GSP	C	395	32/32	0.95	0.15	0.18	17,22,66,73	0
7	MG	C	396	1/1	0.71	0.20	-	45,45,45,45	0
5	CA	A	581	1/1	0.84	0.15	-	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.