



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2018 – 03:07 PM EST

PDB ID : 2GVD  
Title : Complex Of Gs- With The Catalytic Domains Of Mammalian Adenylyl Cyclase: Complex With TNP-ATP and Mn  
Authors : Mou, T.-C.; Sprang, S.R.  
Deposited on : 2006-05-02  
Resolution : 2.90 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

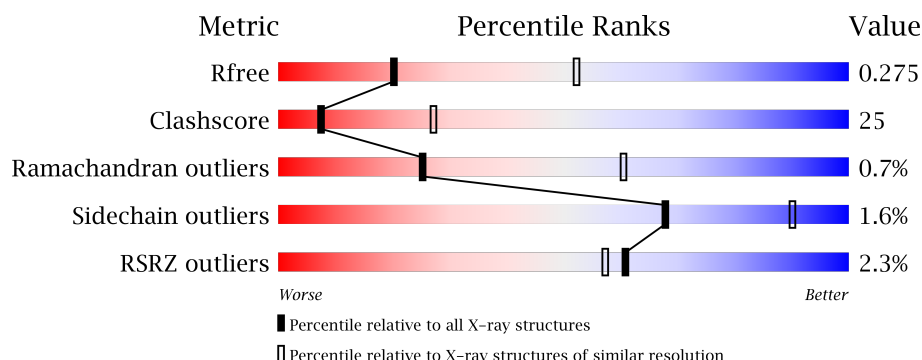
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	<div> <div>6%</div> <div> <div>41%</div> <div>41%</div> <div>•</div> <div>16%</div> </div> </div>
2	B	212	<div> <div>52%</div> <div>36%</div> <div>•</div> <div>11%</div> </div>
3	C	394	<div> <div>%</div> <div>48%</div> <div>32%</div> <div>•</div> <div>18%</div> </div>

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	FKP	A	583	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5758 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	476	MET	VAL	ENGINEERED	UNP P30803
A	356	MET	-	INITIATING METHIONINE	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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	189	Total	C	N	O	S	0	0	0
			1467	936	242	279	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	322	Total	C	N	O	S	0	0	0
			2635	1673	456	494	12			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

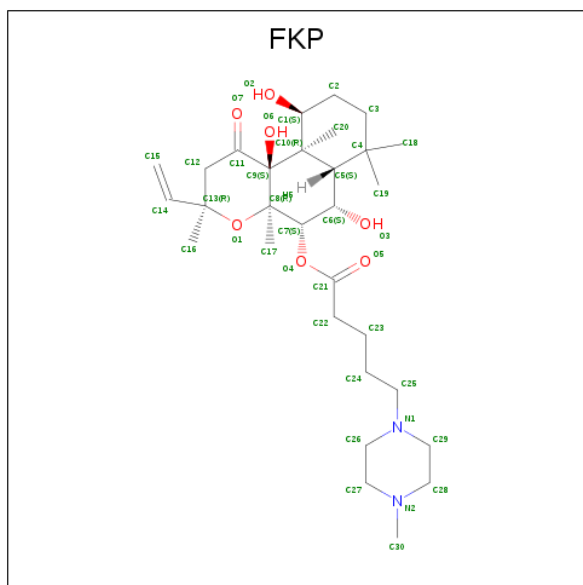
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

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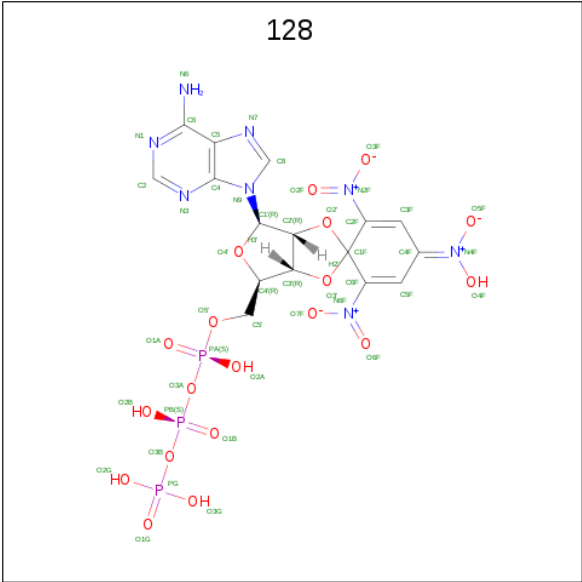
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mn	0	0
			1	1		

- Molecule 5 is METHYLPIPERAZINOFORSKOLIN (three-letter code: FKP) (formula:  $C_{30}H_{50}N_2O_7$ ).



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

- Molecule 6 is SPIRO(2,4,6-TRINITROBENZENE[1,2A]-2O',3O'-METHYLENE-ADENIN E-TRIPHOSPHATE (three-letter code: 128) (formula:  $C_{16}H_{17}N_8O_{19}P_3$ ).

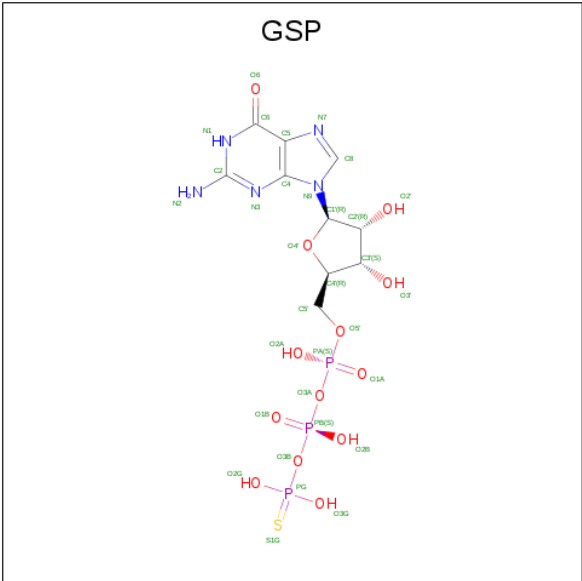


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			46	16	8	19	3		

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

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

- 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).



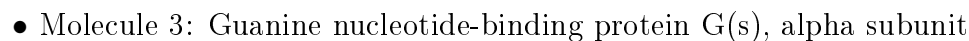
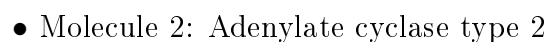
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

- Molecule 9 is water.

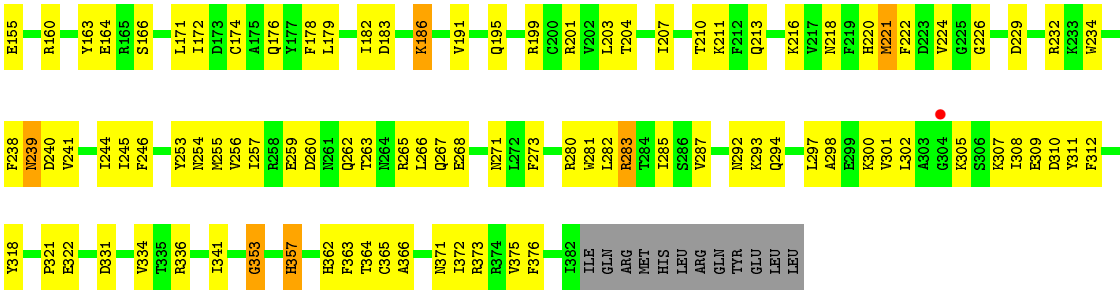
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	11	Total	O	0	0
			11	11		
9	B	15	Total	O	0	0
			15	15		
9	C	25	Total	O	0	0
			25	25		



- Molecule 1: Adenylate cyclase type 5







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.20 Å   133.40 Å   70.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	14.96 – 2.90 45.32 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.5 (14.96-2.90) 73.3 (45.32-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.81 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.245   ,   0.279 0.244   ,   0.275	Depositor DCC
$R_{free}$ test set	925 reflections (4.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.900	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5758	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: FKP, GSP, MN, 128, CL

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	0.40	0/1512	0.49	0/2038
2	B	0.47	0/1492	0.51	0/2014
3	C	0.46	0/2691	0.51	0/3643
All	All	0.44	0/5695	0.51	0/7695

There are no bond length outliers.

There are no bond angle outliers.

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	1452	95	0
2	B	1467	0	1470	64	0
3	C	2635	0	2582	123	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	A	39	0	50	4	0
6	A	46	0	13	3	0
7	C	1	0	0	0	0
8	C	32	0	12	3	0
9	A	11	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	15	0	0	2	0
9	C	25	0	0	4	0
All	All	5758	0	5579	278	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 25.

All (278) 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:A:503:GLN:HA	9:A:45:HOH:O	1.50	1.10
1:A:508:SER:HB3	1:A:511:VAL:HG23	1.51	0.93
1:A:541:GLU:HG3	1:A:565:LEU:HD12	1.55	0.88
3:C:207:ILE:HG12	3:C:224:VAL:HG12	1.55	0.88
1:A:452:ARG:HG2	1:A:454:ASP:H	1.41	0.85
2:B:907:GLU:HG2	9:B:28:HOH:O	1.75	0.84
3:C:282:LEU:HA	3:C:285:ILE:HD13	1.58	0.84
1:A:424:ASP:HB3	2:B:1013:GLN:HG2	1.65	0.77
3:C:254:ASN:HD21	3:C:300:LYS:HD3	1.50	0.77
6:A:584:128:H2'	2:B:1025:ASN:HD22	1.47	0.77
3:C:255:MET:HB2	3:C:265:ARG:HD2	1.65	0.76
2:B:1062:ILE:HD13	2:B:1063:ASN:N	2.02	0.75
3:C:257:ILE:HG12	3:C:259:GLU:HG2	1.69	0.74
1:A:401:THR:HA	1:A:404:ALA:HB3	1.68	0.74
5:A:583:FKP:H173	5:A:583:FKP:H201	1.67	0.74
3:C:210:THR:HB	3:C:221:MET:HB3	1.67	0.73
1:A:528:ILE:HD13	1:A:528:ILE:H	1.52	0.73
3:C:257:ILE:HD12	3:C:268:GLU:HG2	1.70	0.72
1:A:452:ARG:HB2	1:A:452:ARG:HH11	1.53	0.72
1:A:403:LEU:HD23	1:A:403:LEU:H	1.54	0.71
1:A:499:LEU:HA	1:A:502:TRP:HE1	1.53	0.71
6:A:584:128:N3	9:A:68:HOH:O	2.24	0.71
2:B:906:LYS:HB2	2:B:909:LEU:HB3	1.73	0.71
2:B:890:ALA:HB1	2:B:996:LEU:HD11	1.74	0.69
1:A:479:VAL:HG12	1:A:480:ASN:H	1.58	0.69
1:A:452:ARG:NH1	1:A:452:ARG:HB2	2.07	0.69
3:C:365:CYS:H	3:C:371:ASN:ND2	1.91	0.69
2:B:905:ASN:HB2	2:B:910:GLU:HB2	1.73	0.69
3:C:372:ILE:HD12	3:C:373:ARG:N	2.08	0.68
1:A:422:ARG:HA	1:A:425:LYS:HE3	1.75	0.68
1:A:452:ARG:HD3	1:A:454:ASP:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:948:THR:HG22	2:B:968:HIS:HB2	1.75	0.67
3:C:88:LYS:O	3:C:92:VAL:HG23	1.95	0.66
5:A:583:FKP:H202	5:A:583:FKP:H193	1.76	0.66
1:A:379:PHE:CZ	3:C:281:TRP:HB3	2.31	0.65
1:A:460:VAL:O	1:A:464:MET:HG2	1.97	0.65
1:A:484:ARG:HH21	1:A:519:ALA:HA	1.62	0.65
3:C:364:THR:HA	3:C:371:ASN:HD21	1.62	0.65
2:B:1029:ARG:HG3	2:B:1064:VAL:HG13	1.80	0.64
1:A:474:ARG:NH2	1:A:482:ASN:HD21	1.95	0.63
2:B:1033:THR:HG22	2:B:1059:ARG:HH22	1.64	0.63
3:C:244:ILE:HB	3:C:287:VAL:HG22	1.81	0.63
1:A:470:ILE:HG21	1:A:483:MET:HG2	1.80	0.63
2:B:1021:GLY:O	2:B:1024:VAL:HG22	1.99	0.63
1:A:526:ILE:HD12	1:A:526:ILE:N	2.14	0.62
1:A:404:ALA:HA	1:A:412:LEU:HD11	1.81	0.62
1:A:506:VAL:HG23	1:A:511:VAL:HG11	1.82	0.62
3:C:119:LEU:HD12	3:C:119:LEU:H	1.63	0.62
1:A:467:ILE:O	1:A:470:ILE:HG22	1.99	0.62
1:A:398:GLU:OE1	1:A:523:ALA:HB2	2.00	0.62
3:C:166:SER:HB2	3:C:171:LEU:HD23	1.80	0.61
1:A:479:VAL:HG12	1:A:480:ASN:N	2.14	0.61
2:B:990:SER:O	2:B:991:PHE:HB2	2.00	0.61
1:A:378:MET:HE1	3:C:283:ARG:HG2	1.82	0.60
3:C:61:ARG:O	3:C:65:VAL:HB	2.01	0.60
2:B:1026:VAL:HG21	2:B:1067:LYS:HZ2	1.67	0.60
1:A:378:MET:CE	3:C:283:ARG:H	2.15	0.60
2:B:1044:GLU:H	2:B:1044:GLU:CD	2.04	0.60
3:C:183:ASP:HA	3:C:186:LYS:HD3	1.84	0.60
1:A:435:ILE:HD11	1:A:445:VAL:HB	1.84	0.59
1:A:530:LYS:H	1:A:530:LYS:HD3	1.67	0.59
2:B:918:ILE:HG12	2:B:986:ILE:HD13	1.82	0.59
1:A:536:LEU:HD21	1:A:540:TYR:HB2	1.84	0.59
1:A:378:MET:HE1	3:C:283:ARG:H	1.66	0.59
1:A:477:THR:OG1	1:A:478:GLY:N	2.35	0.59
1:A:497:LEU:HD23	1:A:507:TRP:CH2	2.38	0.59
3:C:107:VAL:HG23	3:C:108:ALA:N	2.18	0.59
3:C:163:TYR:OH	3:C:176:GLN:HB2	2.03	0.58
1:A:437:ILE:HG12	1:A:442:TYR:HD1	1.68	0.58
2:B:879:HIS:N	9:B:13:HOH:O	2.37	0.58
1:A:470:ILE:HD12	1:A:483:MET:SD	2.44	0.58
2:B:1001:ASN:ND2	2:B:1002:HIS:H	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:297:LEU:O	3:C:301:VAL:HG23	2.04	0.58
3:C:109:ALA:O	3:C:113:LEU:HG	2.04	0.57
3:C:341:ILE:HB	9:C:398:HOH:O	2.04	0.57
3:C:364:THR:HG22	3:C:375:VAL:HG11	1.85	0.57
3:C:59:GLN:HG3	3:C:372:ILE:HG12	1.86	0.57
2:B:984:ASP:HA	2:B:987:ASN:HD22	1.69	0.57
1:A:392:ILE:HD11	1:A:492:VAL:CG1	2.35	0.57
1:A:452:ARG:CB	1:A:452:ARG:HH11	2.17	0.57
1:A:408:THR:HB	9:A:11:HOH:O	2.03	0.57
3:C:336:ARG:CZ	9:C:422:HOH:O	2.53	0.56
3:C:255:MET:CB	3:C:265:ARG:HD2	2.33	0.56
3:C:365:CYS:H	3:C:371:ASN:HD22	1.51	0.56
1:A:454:ASP:OD2	1:A:457:HIS:HB2	2.05	0.56
3:C:88:LYS:HG2	3:C:90:THR:HG22	1.87	0.56
1:A:393:LEU:C	1:A:393:LEU:HD23	2.25	0.56
3:C:119:LEU:HD21	3:C:128:VAL:HG21	1.88	0.55
2:B:1045:THR:O	2:B:1049:LEU:HG	2.06	0.55
3:C:307:LYS:HB2	3:C:310:ASP:OD2	2.07	0.55
2:B:879:HIS:HB2	2:B:1007:ALA:O	2.06	0.55
3:C:99:LEU:HD11	3:C:182:ILE:CD1	2.37	0.55
3:C:44:LEU:HA	3:C:222:PHE:HB2	1.88	0.55
3:C:366:ALA:HB3	8:C:395:GSP:N7	2.22	0.55
2:B:887:VAL:HG21	2:B:1024:VAL:HG12	1.89	0.55
3:C:119:LEU:HD12	3:C:119:LEU:N	2.22	0.54
3:C:100:LYS:O	3:C:104:GLU:HG2	2.07	0.54
1:A:422:ARG:HH21	1:A:425:LYS:HD2	1.72	0.54
2:B:914:LEU:O	2:B:918:ILE:HG13	2.08	0.54
1:A:456:ALA:O	1:A:460:VAL:HG23	2.07	0.54
3:C:353:GLY:HA3	3:C:357:HIS:NE2	2.23	0.54
1:A:392:ILE:HD11	1:A:492:VAL:HG11	1.89	0.54
3:C:372:ILE:HA	3:C:375:VAL:HG22	1.89	0.54
3:C:245:ILE:HA	9:C:404:HOH:O	2.07	0.53
2:B:1007:ALA:HB1	2:B:1017:TYR:OH	2.08	0.53
3:C:179:LEU:O	3:C:182:ILE:HG12	2.08	0.53
1:A:551:ASN:HD22	1:A:552:ALA:N	2.05	0.53
3:C:179:LEU:HA	3:C:182:ILE:HD11	1.91	0.53
3:C:254:ASN:ND2	3:C:300:LYS:HD3	2.20	0.53
1:A:501:LYS:HD2	2:B:936:LYS:O	2.09	0.53
3:C:121:ASN:HB2	3:C:124:ASN:ND2	2.24	0.53
3:C:213:GLN:OE1	3:C:216:LYS:HA	2.08	0.52
3:C:253:TYR:CE1	3:C:308:ILE:HG12	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:HIS:NE2	1:A:561:THR:HB	2.24	0.52
3:C:331:ASP:HB3	3:C:334:VAL:HG23	1.92	0.52
1:A:397:ILE:HG21	1:A:400:PHE:HD1	1.75	0.52
1:A:473:VAL:HB	1:A:481:VAL:HG21	1.91	0.51
3:C:294:GLN:HG3	3:C:363:PHE:HB3	1.92	0.51
2:B:936:LYS:HD2	2:B:944:TYR:OH	2.11	0.51
1:A:542:VAL:HG12	1:A:564:ILE:HD13	1.93	0.51
2:B:966:TYR:HA	2:B:968:HIS:CE1	2.46	0.51
1:A:382:ILE:HD12	1:A:382:ILE:O	2.11	0.51
2:B:891:SER:O	2:B:996:LEU:HD12	2.11	0.51
3:C:99:LEU:HD11	3:C:179:LEU:HD23	1.93	0.51
2:B:1055:THR:OG1	2:B:1076:ASN:HB2	2.10	0.51
3:C:191:VAL:O	3:C:191:VAL:HG13	2.10	0.51
1:A:397:ILE:HD13	1:A:483:MET:SD	2.51	0.51
3:C:143:PRO:HB2	3:C:145:GLU:OE1	2.11	0.51
2:B:888:MET:HG3	2:B:1000:ILE:HG12	1.92	0.51
1:A:434:ARG:HD2	1:A:435:ILE:N	2.26	0.50
3:C:234:TRP:HB3	3:C:238:PHE:HE1	1.76	0.50
3:C:280:ARG:HA	3:C:283:ARG:NH1	2.25	0.50
2:B:1030:MET:CE	2:B:1042:THR:HG23	2.42	0.50
2:B:888:MET:HG2	2:B:889:PHE:N	2.25	0.50
3:C:257:ILE:CG1	3:C:259:GLU:HG2	2.38	0.50
3:C:54:SER:O	3:C:58:LYS:HG3	2.12	0.50
2:B:1033:THR:HG22	2:B:1059:ARG:NH2	2.26	0.50
2:B:1050:GLN:HA	2:B:1054:TYR:O	2.12	0.49
1:A:473:VAL:O	1:A:477:THR:HG23	2.12	0.49
1:A:551:ASN:HD22	1:A:552:ALA:H	1.60	0.49
1:A:516:HIS:HB3	1:A:551:ASN:OD1	2.13	0.49
3:C:172:ILE:HD12	3:C:174:CYS:SG	2.52	0.49
1:A:505:ASP:HB3	1:A:507:TRP:CZ2	2.47	0.49
2:B:886:CYS:HB2	2:B:969:ILE:HD13	1.94	0.49
1:A:434:ARG:C	1:A:434:ARG:HD2	2.33	0.49
3:C:257:ILE:HD12	3:C:268:GLU:CG	2.42	0.48
2:B:1009:VAL:HG13	2:B:1016:GLN:N	2.29	0.48
3:C:239:ASN:HD22	3:C:240:ASP:H	1.61	0.48
1:A:436:LYS:HE2	1:A:503:GLN:HB3	1.95	0.47
1:A:551:ASN:ND2	1:A:552:ALA:N	2.62	0.47
2:B:1061:ILE:CG2	2:B:1069:ASP:HB3	2.44	0.47
3:C:124:ASN:O	3:C:128:VAL:HG23	2.14	0.47
3:C:58:LYS:HA	3:C:61:ARG:NH1	2.29	0.47
1:A:470:ILE:O	1:A:470:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:ILE:HG23	3:C:104:GLU:N	2.28	0.47
1:A:426:LEU:HB3	1:A:462:MET:HE3	1.94	0.47
3:C:43:LEU:HD12	3:C:221:MET:HE3	1.96	0.47
3:C:318:TYR:OH	3:C:321:PRO:HD3	2.13	0.47
2:B:879:HIS:HB3	2:B:1008:GLY:HA3	1.96	0.47
2:B:1022:ASN:HD21	2:B:1067:LYS:NZ	2.13	0.47
3:C:285:ILE:N	3:C:285:ILE:HD12	2.30	0.47
3:C:59:GLN:CG	3:C:372:ILE:HG12	2.45	0.47
2:B:1013:GLN:HA	2:B:1013:GLN:NE2	2.30	0.47
3:C:318:TYR:O	3:C:336:ARG:NH2	2.48	0.47
3:C:254:ASN:HA	3:C:311:TYR:CE2	2.49	0.47
3:C:183:ASP:HA	3:C:186:LYS:CD	2.45	0.46
2:B:906:LYS:O	2:B:907:GLU:HB2	2.15	0.46
3:C:211:LYS:NZ	3:C:220:HIS:HE1	2.13	0.46
3:C:119:LEU:H	3:C:119:LEU:CD1	2.28	0.46
3:C:267:GLN:HG3	3:C:271:ASN:HD21	1.81	0.46
1:A:523:ALA:O	1:A:525:ARG:HG2	2.15	0.46
3:C:166:SER:CB	3:C:171:LEU:HD23	2.45	0.46
3:C:292:ASN:ND2	3:C:293:LYS:HG3	2.31	0.46
1:A:470:ILE:HD13	1:A:482:ASN:C	2.36	0.46
1:A:394:PHE:HB2	1:A:518:GLU:HB2	1.97	0.46
2:B:894:ASP:O	2:B:897:GLU:HG2	2.15	0.46
3:C:246:PHE:CE2	3:C:273:PHE:HB2	2.50	0.46
2:B:1033:THR:HG21	2:B:1062:ILE:HG12	1.97	0.46
3:C:257:ILE:CG2	3:C:263:THR:HB	2.46	0.46
1:A:466:MET:O	1:A:469:ALA:HB3	2.15	0.45
3:C:151:LYS:HG2	3:C:155:GLU:OE2	2.16	0.45
3:C:257:ILE:CD1	3:C:259:GLU:HG2	2.46	0.45
1:A:437:ILE:HG12	1:A:442:TYR:CD1	2.49	0.45
3:C:203:LEU:HD23	3:C:204:THR:N	2.30	0.45
3:C:266:LEU:HD23	3:C:312:PHE:CZ	2.51	0.45
1:A:530:LYS:N	1:A:530:LYS:HD3	2.30	0.45
2:B:1009:VAL:HA	2:B:1016:GLN:O	2.17	0.45
1:A:408:THR:OG1	1:A:411:GLU:HG3	2.16	0.45
3:C:201:ARG:HB2	8:C:395:GSP:O3'	2.17	0.45
1:A:487:ILE:HB	1:A:528:ILE:HG22	1.97	0.45
5:A:583:FKP:H162	2:B:896:LYS:HA	1.98	0.45
2:B:951:SER:O	2:B:952:ALA:HB2	2.16	0.45
3:C:53:LYS:NZ	3:C:226:GLY:HA3	2.31	0.45
1:A:522:LYS:HE3	1:A:550:ARG:HH22	1.82	0.45
2:B:891:SER:HB3	2:B:943:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:GLN:HA	3:C:195:GLN:NE2	2.31	0.45
3:C:307:LYS:HB3	3:C:309:GLU:OE1	2.17	0.45
3:C:63:LEU:HD11	3:C:372:ILE:CD1	2.47	0.45
5:A:583:FKP:C17	5:A:583:FKP:H201	2.41	0.45
3:C:241:VAL:O	3:C:241:VAL:HG13	2.17	0.45
1:A:530:LYS:H	1:A:530:LYS:CD	2.29	0.44
3:C:121:ASN:HB2	3:C:124:ASN:HD22	1.83	0.44
3:C:256:VAL:C	3:C:265:ARG:HG3	2.38	0.44
2:B:1062:ILE:HD13	2:B:1063:ASN:H	1.77	0.44
3:C:280:ARG:HA	3:C:283:ARG:HH11	1.82	0.44
1:A:484:ARG:O	1:A:518:GLU:HG2	2.18	0.44
6:A:584:128:N6	2:B:1028:SER:OG	2.51	0.44
1:A:481:VAL:O	1:A:481:VAL:HG23	2.17	0.44
1:A:461:GLU:O	1:A:464:MET:HB2	2.18	0.43
2:B:995:LYS:HD2	2:B:1037:ASP:OD2	2.18	0.43
3:C:123:GLU:N	3:C:123:GLU:OE1	2.48	0.43
3:C:164:GLU:HB3	3:C:305:LYS:NZ	2.34	0.43
3:C:95:ILE:HG23	3:C:178:PHE:CE1	2.53	0.43
1:A:434:ARG:HH11	1:A:434:ARG:HG3	1.83	0.43
3:C:372:ILE:O	3:C:376:PHE:HB2	2.18	0.43
3:C:42:ARG:HA	3:C:220:HIS:HB2	2.01	0.43
1:A:420:PHE:HA	1:A:423:PHE:HB2	2.00	0.43
3:C:362:HIS:O	3:C:364:THR:HG23	2.19	0.43
2:B:1001:ASN:ND2	2:B:1002:HIS:N	2.66	0.43
2:B:1033:THR:HG21	2:B:1062:ILE:CG1	2.49	0.43
2:B:922:PHE:CG	2:B:979:LEU:HD22	2.54	0.43
1:A:449:PRO:HG2	1:A:450:GLU:H	1.83	0.43
1:A:513:LEU:O	1:A:517:MET:HG2	2.19	0.43
1:A:462:MET:HG3	1:A:466:MET:SD	2.58	0.43
1:A:463:GLY:O	1:A:467:ILE:HG13	2.18	0.42
1:A:433:LEU:O	1:A:444:CYS:HB2	2.19	0.42
3:C:365:CYS:N	3:C:371:ASN:ND2	2.64	0.42
1:A:493:HIS:HB2	1:A:507:TRP:O	2.20	0.42
2:B:1009:VAL:HG13	2:B:1016:GLN:O	2.19	0.42
3:C:100:LYS:HA	3:C:146:PHE:HZ	1.83	0.42
3:C:257:ILE:HG22	3:C:263:THR:HB	2.02	0.42
3:C:298:ALA:O	3:C:302:LEU:HG	2.19	0.42
2:B:1048:ILE:O	2:B:1052:LEU:HG	2.20	0.42
3:C:100:LYS:C	3:C:102:ALA:H	2.22	0.42
3:C:127:ARG:O	3:C:131:ILE:HG12	2.20	0.42
1:A:550:ARG:HH11	1:A:550:ARG:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:THR:HG23	1:A:411:GLU:OE2	2.19	0.42
1:A:526:ILE:CD1	1:A:526:ILE:N	2.82	0.42
3:C:245:ILE:HG23	9:C:404:HOH:O	2.19	0.42
3:C:372:ILE:HD12	3:C:372:ILE:C	2.39	0.42
3:C:98:ASN:O	3:C:102:ALA:HB2	2.19	0.42
1:A:434:ARG:HG3	1:A:434:ARG:NH1	2.34	0.42
2:B:964:ARG:HG3	2:B:964:ARG:HH11	1.85	0.42
1:A:425:LYS:O	1:A:429:GLU:HG3	2.20	0.41
3:C:154:TRP:CZ2	3:C:160:ARG:NH1	2.88	0.41
3:C:260:ASP:OD1	3:C:262:GLN:N	2.50	0.41
3:C:239:ASN:HD22	3:C:240:ASP:N	2.17	0.41
3:C:239:ASN:ND2	3:C:240:ASP:N	2.68	0.41
1:A:390:VAL:HG22	1:A:490:GLY:O	2.19	0.41
3:C:174:CYS:HB3	3:C:199:ARG:O	2.20	0.41
3:C:322:GLU:HA	3:C:322:GLU:OE1	2.20	0.41
3:C:58:LYS:HA	3:C:61:ARG:HH12	1.86	0.41
3:C:88:LYS:C	3:C:92:VAL:HG23	2.41	0.41
1:A:435:ILE:HD11	1:A:445:VAL:CB	2.49	0.41
2:B:915:LEU:HA	2:B:918:ILE:HD12	2.03	0.41
3:C:53:LYS:HE3	3:C:224:VAL:O	2.20	0.41
3:C:372:ILE:HA	3:C:375:VAL:CG2	2.51	0.41
3:C:99:LEU:HD21	3:C:182:ILE:HD12	2.01	0.41
3:C:107:VAL:HG23	3:C:108:ALA:H	1.84	0.41
3:C:218:ASN:HD22	3:C:218:ASN:N	2.18	0.41
1:A:491:ARG:HH21	2:B:901:GLU:HB3	1.85	0.41
1:A:485:VAL:HB	1:A:526:ILE:HA	2.01	0.41
1:A:379:PHE:N	1:A:379:PHE:CD1	2.88	0.41
1:A:386:LYS:HE3	1:A:491:ARG:HD2	2.03	0.41
2:B:918:ILE:HA	2:B:986:ILE:HD11	2.02	0.41
2:B:937:ILE:HG13	2:B:945:MET:HE2	2.03	0.41
3:C:160:ARG:O	3:C:163:TYR:HB3	2.21	0.41
3:C:293:LYS:HG2	8:C:395:GSP:C6	2.56	0.41
1:A:496:VAL:HG21	1:A:502:TRP:CE3	2.56	0.41
2:B:879:HIS:CB	2:B:1008:GLY:HA3	2.51	0.41
3:C:257:ILE:HG12	3:C:259:GLU:H	1.86	0.41
1:A:401:THR:OG1	2:B:1065:LYS:HE3	2.21	0.40
2:B:1009:VAL:HG13	2:B:1016:GLN:C	2.42	0.40
2:B:897:GLU:HG3	2:B:898:PHE:N	2.37	0.40
3:C:100:LYS:HG2	3:C:104:GLU:OE1	2.22	0.40
3:C:229:ASP:O	3:C:232:ARG:HG2	2.22	0.40
2:B:879:HIS:N	2:B:879:HIS:CD2	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:THR:CG2	3:C:366:ALA:HB1	2.51	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%)	170 (90%)	15 (8%)	3 (2%)	11	37
2	B	185/212 (87%)	174 (94%)	10 (5%)	1 (0%)	32	68
3	C	318/394 (81%)	285 (90%)	32 (10%)	1 (0%)	44	77
All	All	691/831 (83%)	629 (91%)	57 (8%)	5 (1%)	25	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	MET
1	A	378	MET
1	A	478	GLY
3	C	353	GLY
2	B	1013	GLN

### 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	159/189 (84%)	157 (99%)	2 (1%)	73	93
2	B	162/184 (88%)	159 (98%)	3 (2%)	62	88
3	C	290/351 (83%)	285 (98%)	5 (2%)	66	89
All	All	611/724 (84%)	601 (98%)	10 (2%)	68	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	528	ILE
1	A	530	LYS
2	B	879	HIS
2	B	921	ASP
2	B	1062	ILE
3	C	186	LYS
3	C	221	MET
3	C	239	ASN
3	C	283	ARG
3	C	357	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	A	430	ASN
1	A	482	ASN
1	A	509	ASN
1	A	515	ASN
1	A	551	ASN
2	B	879	HIS
2	B	992	ASN
2	B	1001	ASN
2	B	1013	GLN
2	B	1016	GLN
2	B	1022	ASN
2	B	1025	ASN
2	B	1050	GLN
2	B	1076	ASN
3	C	97	ASN
3	C	98	ASN
3	C	218	ASN
3	C	220	HIS

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Mol	Chain	Res	Type
3	C	267	GLN
3	C	271	ASN
3	C	362	HIS
3	C	371	ASN

### 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 ⓘ

Of 7 ligands modelled in this entry, 4 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	$\# Z  > 2$
5	FKP	A	583	-	37,42,42	2.27	15 (40%)	45,68,68	1.81	10 (22%)
6	128	A	584	4	34,50,50	3.23	16 (47%)	33,80,80	3.95	12 (36%)
8	GSP	C	395	4	26,34,34	2.34	6 (23%)	24,54,54	2.97	11 (45%)

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
5	FKP	A	583	-	-	0/14/97/97	0/4/4/4
6	128	A	584	4	-	0/22/80/80	0/5/5/5
8	GSP	C	395	4	-	0/17/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	584	128	PB-O2B	-10.14	1.04	1.55
6	A	584	128	PB-O1B	-8.13	1.20	1.50
8	C	395	GSP	PG-O2G	-7.70	1.28	1.55
8	C	395	GSP	C8-N7	-3.56	1.28	1.34
5	A	583	FKP	C27-C26	-3.32	1.38	1.51
6	A	584	128	C3'-C4'	-2.67	1.45	1.52
6	A	584	128	C8-N7	-2.40	1.30	1.34
6	A	584	128	PG-O3G	-2.21	1.45	1.54
5	A	583	FKP	C26-N1	2.09	1.52	1.47
5	A	583	FKP	C23-C22	2.12	1.60	1.52
6	A	584	128	PA-O1A	2.14	1.58	1.50
6	A	584	128	C2-N1	2.28	1.38	1.33
5	A	583	FKP	C25-N1	2.42	1.53	1.47
5	A	583	FKP	C29-N1	2.43	1.53	1.47
5	A	583	FKP	C20-C10	2.51	1.58	1.53
5	A	583	FKP	C22-C21	2.56	1.58	1.50
8	C	395	GSP	C6-C5	2.60	1.46	1.41
5	A	583	FKP	C3-C2	2.73	1.59	1.53
5	A	583	FKP	C5-C6	2.79	1.63	1.54
6	A	584	128	PG-O1G	2.82	1.60	1.50
6	A	584	128	C2'-C3'	2.95	1.59	1.53
8	C	395	GSP	O4'-C1'	3.34	1.45	1.41
6	A	584	128	C5'-C4'	3.41	1.62	1.51
5	A	583	FKP	C2-C1	3.41	1.57	1.52
8	C	395	GSP	C2-N1	3.44	1.41	1.35
6	A	584	128	C4-N3	3.45	1.40	1.35
5	A	583	FKP	C17-C8	3.49	1.57	1.51
6	A	584	128	C2-N3	3.66	1.38	1.32
6	A	584	128	O3'-C1F	3.69	1.53	1.42
5	A	583	FKP	C6-C7	3.86	1.61	1.53
6	A	584	128	O2'-C1F	4.17	1.54	1.42
5	A	583	FKP	C4-C5	4.19	1.62	1.56
5	A	583	FKP	C12-C11	4.48	1.57	1.51
8	C	395	GSP	C6-N1	4.56	1.41	1.33
6	A	584	128	C5F-C6F	4.77	1.51	1.37
6	A	584	128	PG-O3B	4.90	1.68	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	583	FKP	C10-C5	5.51	1.66	1.56

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	395	GSP	C5-C6-N1	-9.59	109.82	123.48
6	A	584	128	N3-C2-N1	-8.85	121.15	128.86
6	A	584	128	O3'-C1F-C6F	-6.74	101.25	110.47
5	A	583	FKP	C10-C5-C4	-6.10	111.39	116.48
6	A	584	128	O4'-C1'-C2'	-5.06	97.75	106.59
6	A	584	128	O2'-C1F-C2F	-5.04	103.57	110.47
5	A	583	FKP	C19-C4-C18	-4.97	100.28	107.88
8	C	395	GSP	N3-C2-N1	-3.81	121.90	127.46
5	A	583	FKP	C19-C4-C3	-3.07	102.56	109.00
6	A	584	128	O4'-C4'-C3'	-2.67	98.92	104.81
5	A	583	FKP	C4-C5-C6	-2.42	111.28	115.20
8	C	395	GSP	PB-O3B-PG	-2.39	124.64	132.35
5	A	583	FKP	C20-C10-C1	-2.14	104.42	107.63
8	C	395	GSP	C1'-N9-C4	-2.03	123.12	126.64
8	C	395	GSP	O3'-C3'-C4'	-2.02	105.18	111.09
5	A	583	FKP	O7-C11-C12	-2.01	117.61	121.92
8	C	395	GSP	C2-N3-C4	-2.01	112.82	115.16
5	A	583	FKP	O4-C21-C22	2.07	115.85	111.55
6	A	584	128	O2'-C1F-C6F	2.07	113.30	110.47
5	A	583	FKP	O4-C7-C6	2.13	112.20	107.90
8	C	395	GSP	O2A-PA-O1A	2.13	123.30	112.28
8	C	395	GSP	N2-C2-N1	2.26	120.85	117.24
8	C	395	GSP	C2'-C3'-C4'	2.33	107.15	102.62
6	A	584	128	C5'-C4'-C3'	2.37	122.33	114.30
6	A	584	128	C2'-C3'-C4'	2.63	110.11	103.68
6	A	584	128	O3'-C3'-C2'	2.92	108.23	103.60
5	A	583	FKP	C13-O1-C8	2.96	122.86	119.96
5	A	583	FKP	C19-C4-C5	3.42	124.29	111.89
8	C	395	GSP	C4'-O4'-C1'	3.61	113.61	109.77
6	A	584	128	O2'-C2'-C3'	4.94	111.42	103.60
6	A	584	128	O2'-C1F-O3'	6.16	114.39	105.77
8	C	395	GSP	C6-N1-C2	7.44	126.77	116.06
6	A	584	128	C4'-O4'-C1'	15.02	125.75	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	583	FKP	4	0
6	A	584	128	3	0
8	C	395	GSP	3	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 [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%)	0.28	13 (6%) 18 13	21, 56, 102, 127	0
2	B	189/212 (89%)	-0.19	1 (0%) 90 90	13, 35, 68, 106	0
3	C	322/394 (81%)	-0.20	2 (0%) 89 88	15, 38, 75, 95	0
All	All	701/831 (84%)	-0.07	16 (2%) 61 57	13, 42, 81, 127	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	MET	4.8
1	A	474	ARG	4.5
1	A	479	VAL	4.0
1	A	475	GLU	3.6
1	A	477	THR	3.1
1	A	473	VAL	3.1
1	A	478	GLY	2.7
3	C	304	GLY	2.6
3	C	39	ALA	2.4
1	A	429	GLU	2.3
2	B	966	TYR	2.3
1	A	470	ILE	2.2
1	A	472	LEU	2.2
1	A	471	SER	2.2
1	A	376	ASP	2.0
1	A	468	GLU	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( $\text{\AA}^2$ )	Q<0.9
5	FKP	A	583	39/39	0.92	0.26	3.18	18,26,77,78	0
6	128	A	584	46/46	0.88	0.25	1.01	60,70,87,92	0
8	GSP	C	395	32/32	0.97	0.16	-0.21	11,26,59,61	0
4	MN	A	582	1/1	0.99	0.15	-1.78	20,20,20,20	0
4	MN	C	396	1/1	0.91	0.12	-2.11	40,40,40,40	0
7	CL	C	397	1/1	0.96	0.07	-8.99	25,25,25,25	0
4	MN	A	581	1/1	0.95	0.17	-	56,56,56,56	0

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

There are no such residues in this entry.