



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 03:03 PM EDT

PDB ID : 3MAA
Title : Complex of GS-Alpha with the Catalytic Domains of Mammalian Adenylyl Cyclase: Complex with Adenosine 5-O-(1-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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

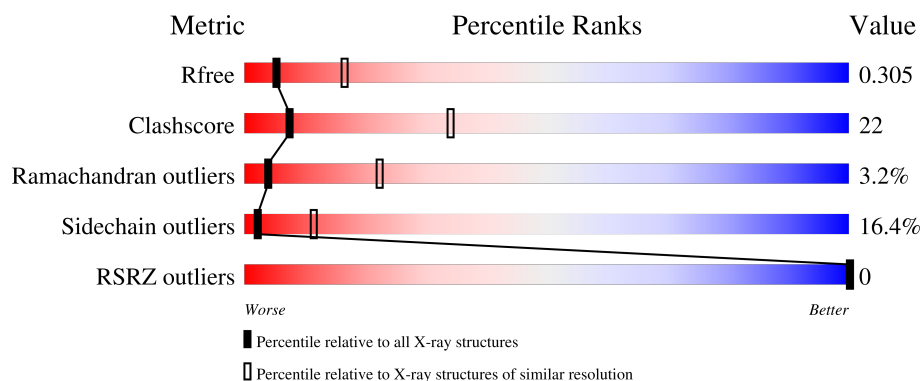
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	225	
2	B	212	
3	C	394	

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 mutation	UNP P30803

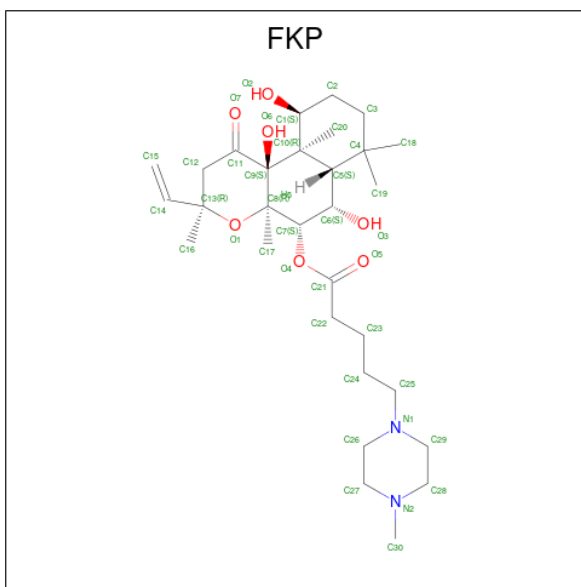
- Molecule 2 is a protein called Adenylate cyclase type 2.

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: $C_{30}H_{50}N_2O_7$).

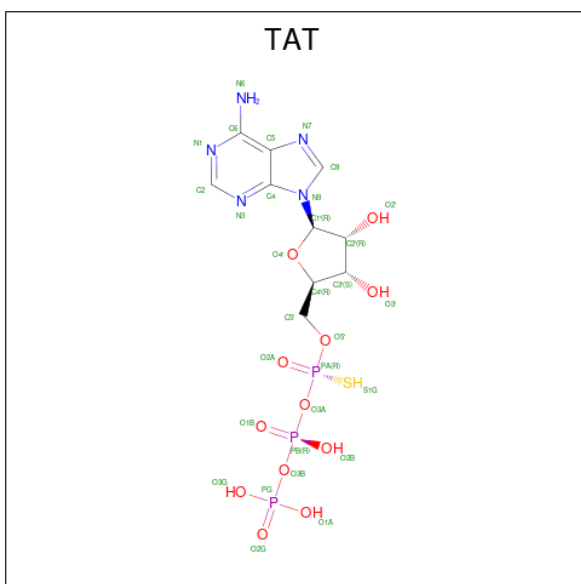


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			39	30	2	7		

- 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: $C_{10}H_{16}N_5O_{12}P_3S$).

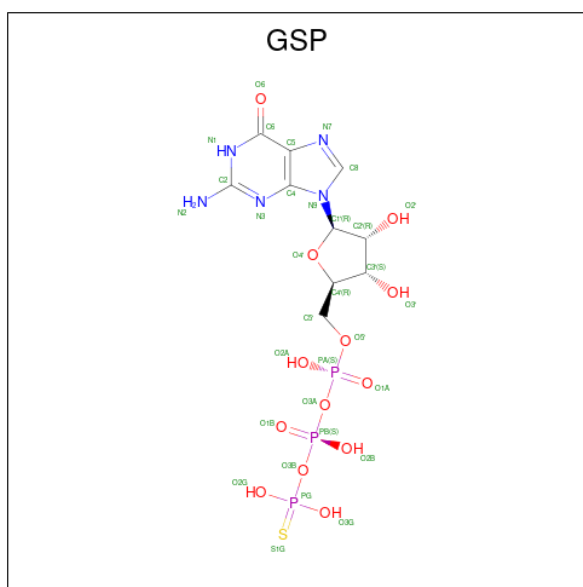


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	S	
			31	10	5	12	3	1	
									0
									0

- 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: C₁₀H₁₆N₅O₁₃P₃S).



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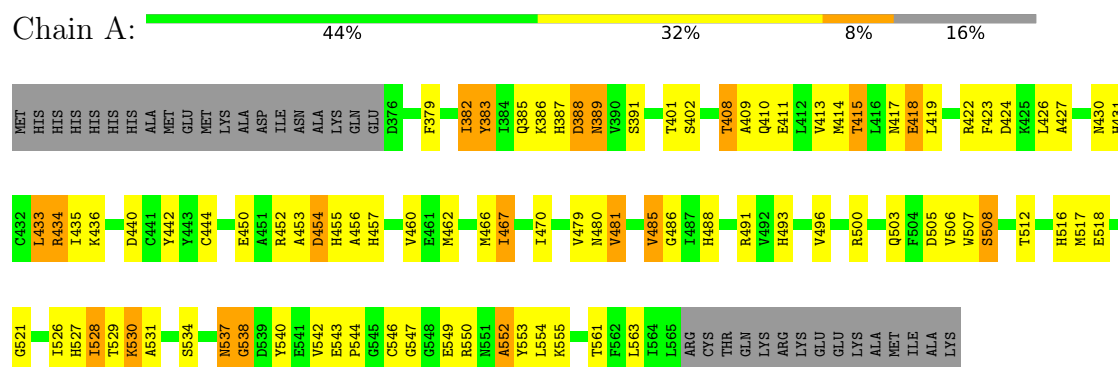
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	5	Total	O	0	0
			5	5		
10	C	5	Total	O	0	0
			5	5		

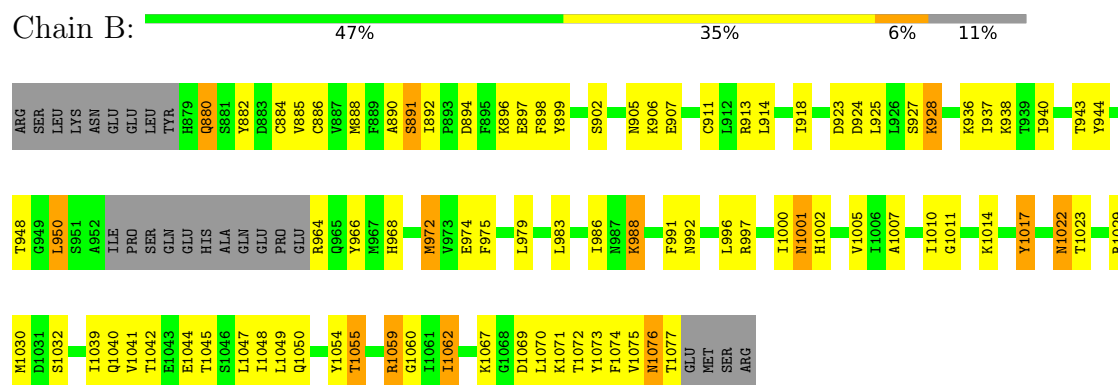
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

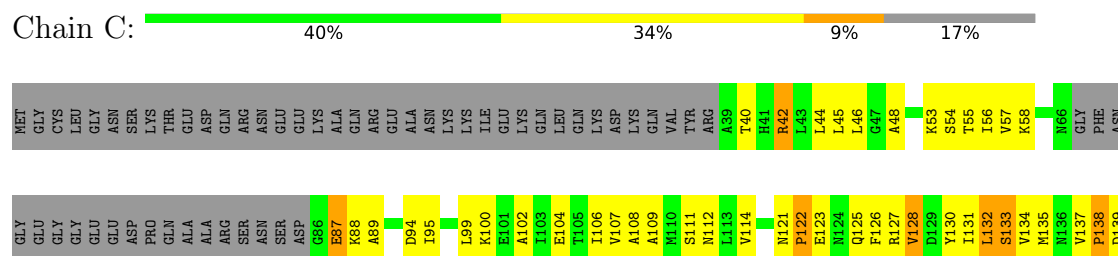
• Molecule 1: Adenylate cyclase type 5

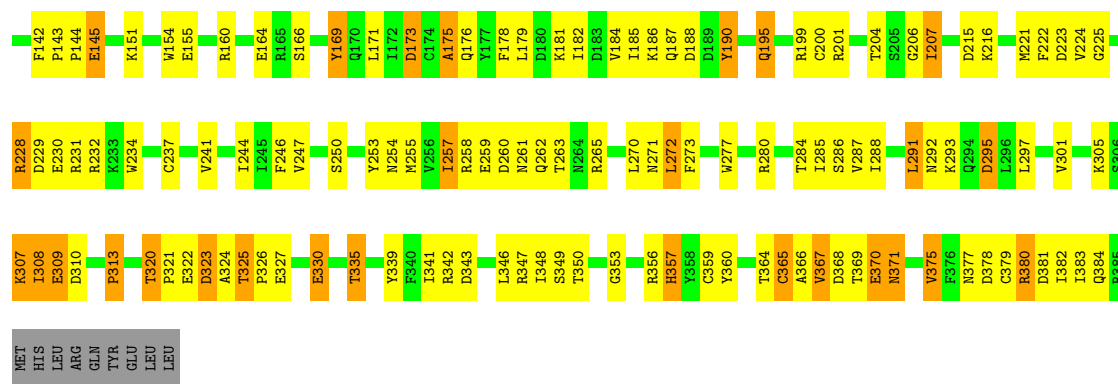


• Molecule 2: Adenylate cyclase type 2



• Molecule 3: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	1003 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.923	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 10.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5744	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, CA, FKP, TAT, CL, GSP

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:H201	4:A:101:FKP:H173	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:N	3:C:295:ASP:OD1	2.31	0.62
1:A:388:ASP:HB3	1:A:389:ASN:ND2	2.14	0.62
2:B:1067:LYS:HG3	2:B:1067:LYS:O	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:H	3:C:42:ARG:HD3	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
1:A:388:ASP:HB3	1:A:389:ASN:HD22	1.66	0.60
2:B:1030:MET:HE3	2:B:1042:THR:HG23	1.83	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:CD	2:B:1044:GLU:H	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:1000:ILE:CG2	2:B:1001:ASN:N	2.69	0.56
2:B:1040:GLN:HA	2:B:1073:TYR:O	2.05	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
1:A:479:VAL:HG13	1:A:481:VAL:HG22	1.88	0.55
3:C:253:TYR:CE1	3:C:308:ILE:HG12	2.41	0.55
3:C:330:GLU:OE2	3:C:335:THR:HG23	2.07	0.55
2:B:1030:MET:HE3	2:B:1042:THR:CG2	2.35	0.55
2:B:1045:THR:HG22	2:B:1049:LEU:HD12	1.82	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
1:A:467:ILE:HA	1:A:470:ILE:CG2	2.38	0.54
2:B:948:THR:HB	2:B:968:HIS:HB2	1.88	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:195:GLN:HA	3:C:195:GLN:NE2	2.24	0.53
3:C:201:ARG:HB2	8:C:395:GSP:O3'	2.09	0.53
3:C:326:PRO:HB3	3:C:335:THR:HG21	1.89	0.53
1:A:435:ILE:HG12	1:A:444:CYS:HA	1.91	0.52
3:C:368:ASP:O	3:C:370:GLU:N	2.42	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
1:A:427:ALA:HA	1:A:462:MET:CE	2.39	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
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
1:A:493:HIS:O	1:A:506:VAL:HA	2.11	0.50
2:B:884:CYS:O	2:B:968:HIS:NE2	2.36	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
1:A:512:THR:HG22	1:A:516:HIS:HD2	1.77	0.49
3:C:114:VAL:O	3:C:114:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:277:TRP:CE2	3:C:349:SER:HA	2.46	0.49
3:C:307:LYS:HB2	3:C:310:ASP:OD2	2.12	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
2:B:1047:LEU:O	2:B:1050:GLN:HB2	2.13	0.49
3:C:207:ILE:HG12	3:C:223:ASP:O	2.12	0.49
3:C:100:LYS:HE2	3:C:134:VAL:HG23	1.95	0.48
1:A:452:ARG:HE	1:A:454:ASP:HB2	1.77	0.48
1:A:517:MET:HE2	1:A:527:HIS:CD2	2.49	0.48
1:A:382:ILE:H	1:A:382:ILE:HG13	1.46	0.48
3:C:182:ILE:O	3:C:185:ILE:N	2.45	0.48
3:C:320:THR:HA	3:C:321:PRO:HD3	1.76	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
1:A:427:ALA:HA	1:A:462:MET:HE2	1.96	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
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:206:GLY:O	3:C:207:ILE:HG13	2.15	0.47
3:C:277:TRP:CD1	3:C:348:ILE:HG22	2.50	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:H201	4:A:101:FKP:C17	2.37	0.46
1:A:391:SER:OG	1:A:456:ALA:HA	2.16	0.46
2:B:1060:GLY:O	2:B:1071:LYS:HA	2.15	0.46
3:C:53:LYS:C	3:C:55:THR:H	2.18	0.46
1:A:417:ASN:HA	2:B:1010:ILE:HD12	1.98	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
3:C:137:VAL:CG1	3:C:138:PRO:HD2	2.46	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
1:A:415:THR:O	1:A:418:GLU:HB3	2.15	0.45
2:B:892:ILE:HG22	2:B:892:ILE:O	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
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:322:GLU:C	3:C:324:ALA:H	2.21	0.45
3:C:175:ALA:O	3:C:176:GLN:C	2.54	0.45
4:A:101:FKP:H163	4:A:101:FKP:H171	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:215:ASP:OD2	3:C:380:ARG:NH2	2.51	0.44
3:C:364:THR:HG22	3:C:375:VAL:HG21	1.99	0.44
2:B:891:SER:CB	2:B:943:THR:HG23	2.47	0.44
2:B:911:CYS:O	2:B:914:LEU:N	2.44	0.44
2:B:1000:ILE:HB	2:B:1041:VAL:HG12	1.98	0.44
2:B:1030:MET:CE	2:B:1042:THR:HG22	2.47	0.44
3:C:265:ARG:NH1	10:C:400:HOH:O	2.50	0.44
2:B:1022:ASN:HD22	2:B:1022:ASN:C	2.19	0.44
2:B:1062:ILE:O	2:B:1069:ASP:HA	2.18	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:121:ASN:HA	3:C:122:PRO:HD2	1.72	0.44
3:C:143:PRO:HA	3:C:144:PRO:HD3	1.89	0.44
3:C:244:ILE:CG2	3:C:287:VAL:HG13	2.48	0.44
3:C:292:ASN:HA	3:C:364:THR:O	2.18	0.44
3:C:87:GLU:C	3:C:89:ALA:H	2.21	0.43
3:C:109:ALA:HA	3:C:112:ASN:HB2	2.00	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
2:B:950:LEU:HD12	2:B:950:LEU:H	1.82	0.43
3:C:125:GLN:O	3:C:128:VAL:HB	2.18	0.43
3:C:260:ASP:OD1	3:C:261:ASN:N	2.52	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:228:ARG:HB2	3:C:259:GLU:HG2	2.00	0.43
3:C:257:ILE:HD12	3:C:263:THR:HB	2.01	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
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:99:LEU:O	3:C:100:LYS:C	2.57	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:349:SER:HB2	3:C:359:CYS:HB2	2.02	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
2:B:979:LEU:O	2:B:983:LEU:N	2.43	0.42
3:C:130:TYR:O	3:C:134:VAL:HG13	2.19	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
1:A:430:ASN:O	1:A:431:HIS:HB2	2.20	0.42
2:B:1075:VAL:CG1	2:B:1076:ASN:N	2.83	0.42
3:C:346:LEU:O	3:C:350:THR:HB	2.20	0.42
1:A:517:MET:CE	1:A:527:HIS:CD2	3.03	0.42
3:C:46:LEU:O	3:C:247:VAL:HG23	2.19	0.42
3:C:293:LYS:HA	8:C:395:GSP:O6	2.20	0.42
4:A:101:FKP:O7	4:A:101:FKP:H1	2.19	0.41
3:C:257:ILE:O	3:C:261:ASN:HA	2.19	0.41
3:C:368:ASP:O	3:C:371:ASN:N	2.50	0.41
1:A:485:VAL:HG21	1:A:526:ILE:HG12	2.02	0.41
2:B:1030:MET:HA	2:B:1040:GLN:HE21	1.83	0.41
1:A:457:HIS:HD2	1:A:540:TYR:HE1	1.67	0.41
3:C:188:ASP:OD1	3:C:188:ASP:N	2.50	0.41
3:C:231:ARG:HG2	3:C:234:TRP:CZ2	2.55	0.41
3:C:377:ASN:C	3:C:379:CYS:H	2.24	0.41
1:A:418:GLU:HB3	1:A:419:LEU:H	1.69	0.41
1:A:530:LYS:H	1:A:530:LYS:HG3	1.64	0.41
2:B:891:SER:O	2:B:996:LEU:HD12	2.21	0.41
3:C:160:ARG:HH11	3:C:160:ARG:HG2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:368:ASP:O	3:C:369:THR:C	2.57	0.41
2:B:923:ASP:OD1	2:B:944:TYR:OH	2.24	0.41
2:B:992:ASN:ND2	3:C:232:ARG:HB2	2.36	0.41
3:C:325:THR:O	3:C:325:THR:OG1	2.36	0.41
3:C:343:ASP:HA	3:C:346:LEU:HB2	2.03	0.41
1:A:549:GLU:HG2	1:A:549:GLU:H	1.76	0.41
1:A:453:ALA:C	1:A:455:HIS:H	2.23	0.41
1:A:507:TRP:O	1:A:508:SER:HB3	2.21	0.41
2:B:880:GLN:O	2:B:880:GLN:NE2	2.54	0.41
2:B:1059:ARG:HD3	2:B:1072:THR:OG1	2.20	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
3:C:277:TRP:CZ3	3:C:357:HIS:CE1	3.09	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
1:A:552:ALA:O	1:A:554:LEU:N	2.54	0.40
3:C:134:VAL:O	3:C:137:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	188/225 (84%)	156 (83%)	26 (14%)	6 (3%)	4	22
2	B	184/212 (87%)	153 (83%)	26 (14%)	5 (3%)	5	26
3	C	324/394 (82%)	264 (82%)	49 (15%)	11 (3%)	3	20
All	All	696/831 (84%)	573 (82%)	101 (14%)	22 (3%)	4	22

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	10
2	B	161/184 (88%)	134 (83%)	27 (17%)	2	11
3	C	295/351 (84%)	249 (84%)	46 (16%)	2	13
All	All	615/724 (85%)	514 (84%)	101 (16%)	2	11

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

Sometimes 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 monosaccharides 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	-	39,42,42	1.00	1 (2%)	49,68,68	1.33	7 (14%)
8	GSP	C	395	7	26,34,34	1.95	2 (7%)	28,54,54	1.88	6 (21%)
6	TAT	B	1	5	24,33,33	1.34	4 (16%)	29,52,52	1.47	4 (13%)

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	-	-	3/14/97/97	0/4/4/4
8	GSP	C	395	7	-	4/17/38/38	0/3/3/3
6	TAT	B	1	5	-	3/14/38/38	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	-8.68	1.71	1.90
4	A	101	FKP	O4-C21	3.85	1.45	1.34
6	B	1	TAT	O4'-C1'	3.42	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1	TAT	PA-O5'	3.32	1.63	1.57
8	C	395	GSP	C6-N1	2.33	1.37	1.33
6	B	1	TAT	PG-O1A	2.28	1.63	1.54
6	B	1	TAT	PG-O3G	2.10	1.62	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	395	GSP	C2-N3-C4	4.76	120.79	115.36
8	C	395	GSP	N3-C2-N1	-4.52	121.20	127.22
6	B	1	TAT	N3-C2-N1	-4.25	122.04	128.68
4	A	101	FKP	O4-C21-C22	4.16	120.46	111.50
8	C	395	GSP	PA-O3A-PB	-4.03	119.01	132.83
6	B	1	TAT	O4'-C1'-C2'	-3.82	101.34	106.93
4	A	101	FKP	C3-C4-C5	3.57	113.10	107.96
4	A	101	FKP	C13-O1-C8	3.03	124.65	119.84
6	B	1	TAT	C4-C5-N7	-2.76	106.53	109.40
8	C	395	GSP	C4-C5-N7	-2.75	106.53	109.40
8	C	395	GSP	C3'-C2'-C1'	2.60	104.89	100.98
8	C	395	GSP	C5-C6-N1	-2.54	119.96	123.43
4	A	101	FKP	C7-O4-C21	-2.48	112.97	118.00
4	A	101	FKP	C13-C14-C15	-2.40	117.24	128.88
6	B	1	TAT	PB-O3B-PG	-2.32	124.85	132.83
4	A	101	FKP	O4-C21-O5	-2.15	118.51	123.70
4	A	101	FKP	C10-C5-C4	-2.13	114.68	116.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

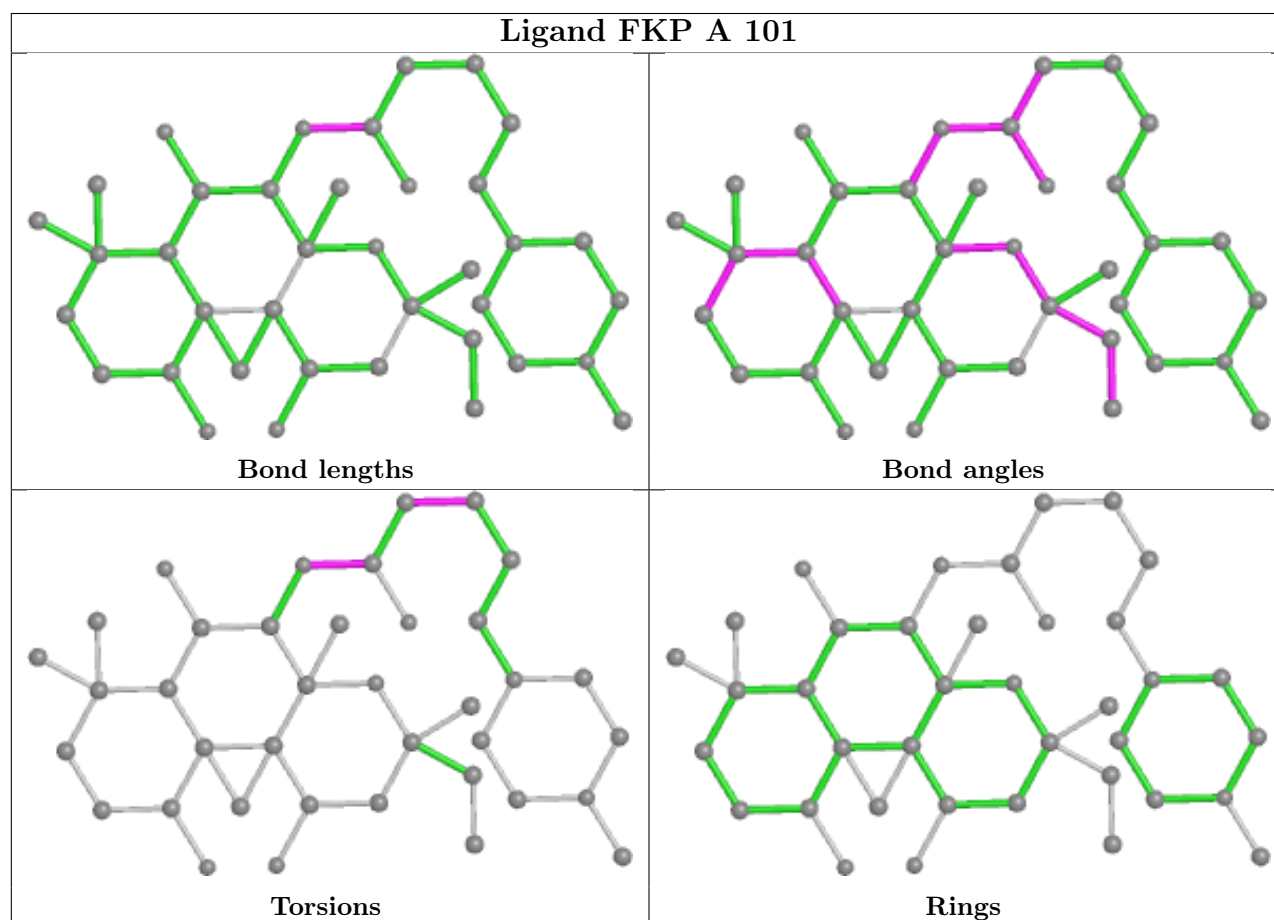
Mol	Chain	Res	Type	Atoms
8	C	395	GSP	C3'-C4'-C5'-O5'
8	C	395	GSP	O4'-C4'-C5'-O5'
4	A	101	FKP	C22-C21-O4-C7
4	A	101	FKP	O5-C21-O4-C7
4	A	101	FKP	C21-C22-C23-C24
8	C	395	GSP	PA-O3A-PB-O2B
6	B	1	TAT	O4'-C4'-C5'-O5'
8	C	395	GSP	C4'-C5'-O5'-PA
6	B	1	TAT	C3'-C4'-C5'-O5'
6	B	1	TAT	PA-O3A-PB-O2B

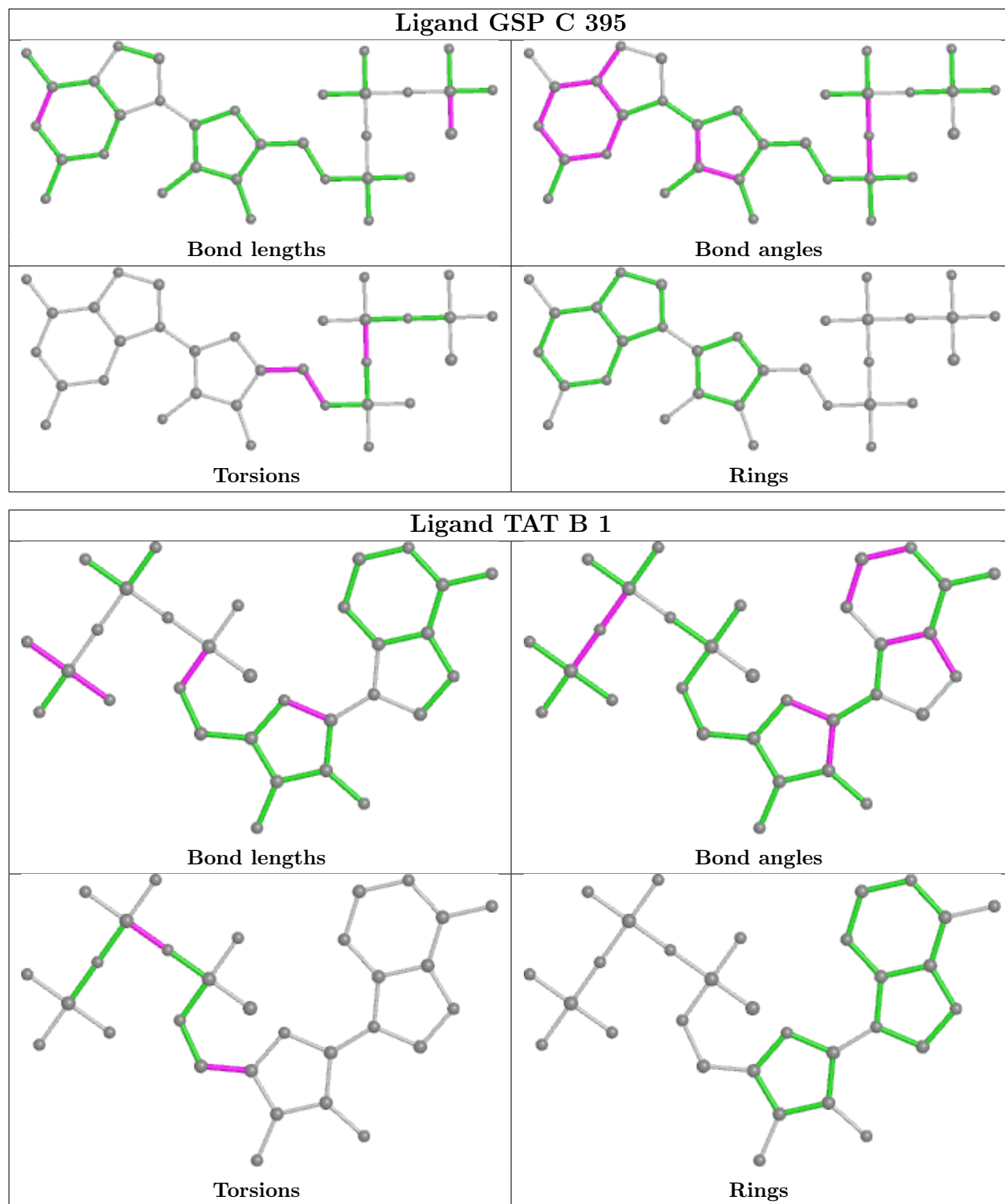
There are no ring outliers.

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	190/225 (84%)	-0.55	0 100 100	17, 39, 66, 75	0
2	B	188/212 (88%)	-0.63	0 100 100	17, 23, 54, 73	0
3	C	328/394 (83%)	-0.69	0 100 100	17, 26, 47, 78	0
All	All	706/831 (84%)	-0.63	0 100 100	17, 28, 58, 78	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

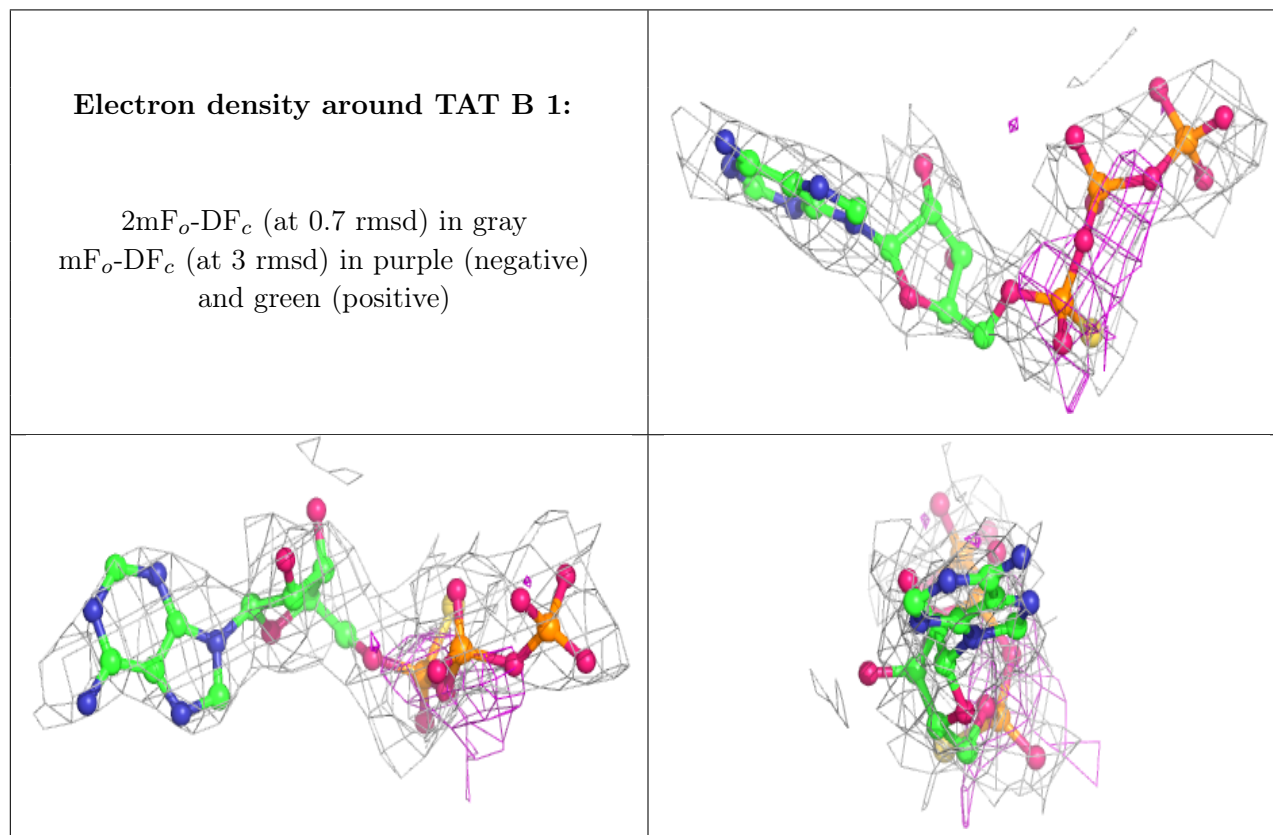
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

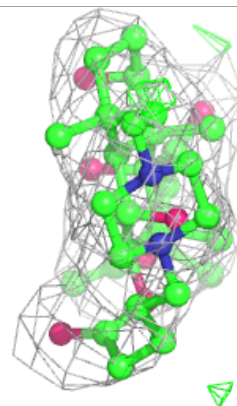
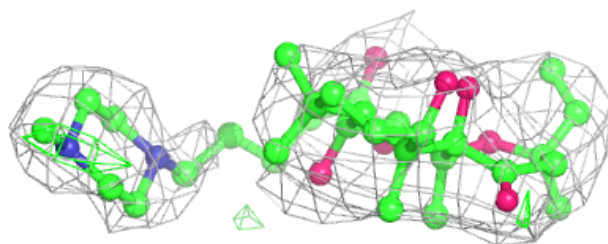
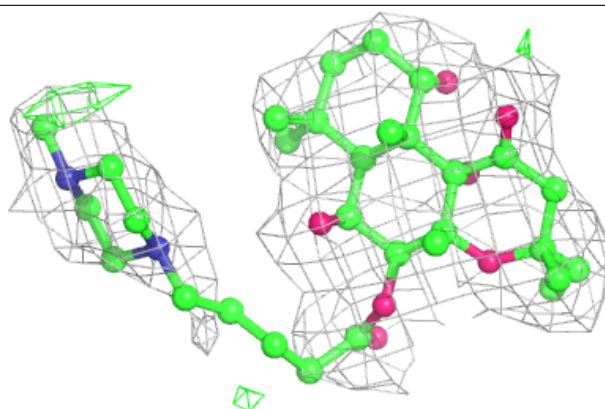
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	C	396	1/1	0.70	0.20	45,45,45,45	0
6	TAT	B	1	31/31	0.82	0.30	68,77,107,108	0
5	CA	A	581	1/1	0.84	0.15	66,66,66,66	0
4	FKP	A	101	39/39	0.94	0.23	36,50,93,95	0
8	GSP	C	395	32/32	0.95	0.15	17,22,66,73	0
9	CL	C	397	1/1	0.98	0.19	50,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

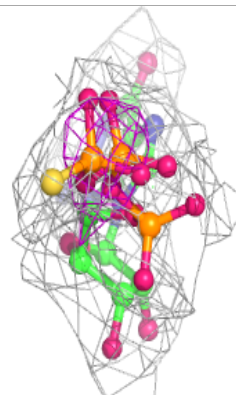
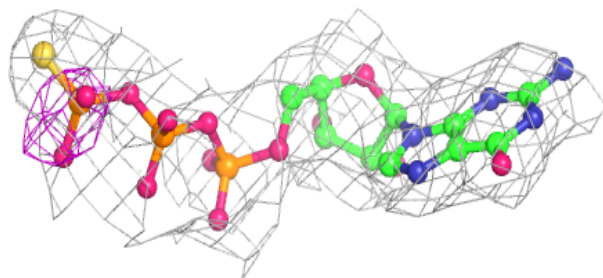
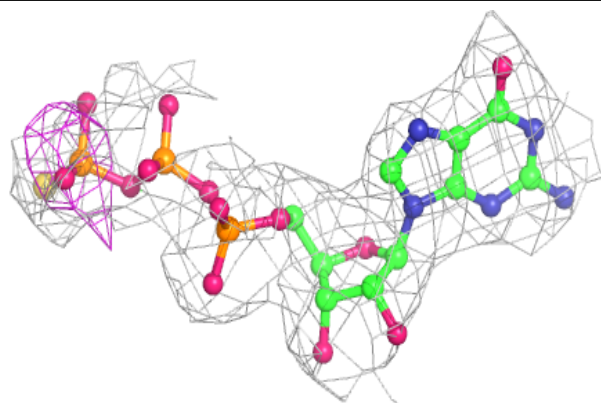


Electron density around FKP A 101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GSP C 395:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.