



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:56 AM EDT

PDB ID : 2GVD / pdb_00002gvd
Title : Complex Of Gs- With The Catalytic Domains Of Mammalian Adenylyl Cy-
clase: 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

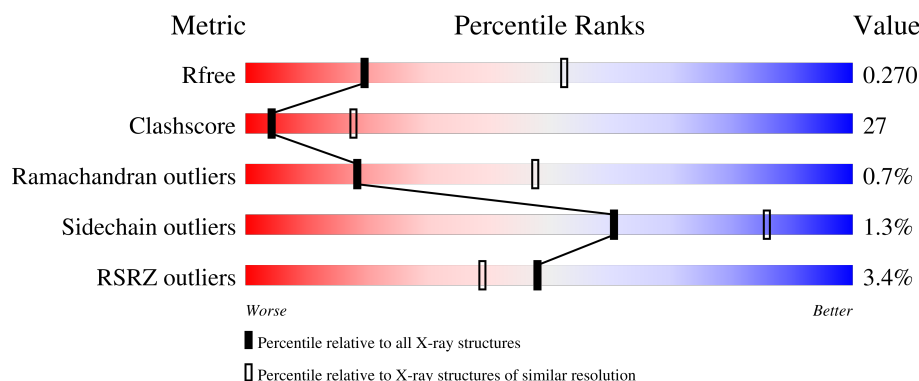
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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 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 mutation	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 (CCD ID: MN) (formula: Mn).

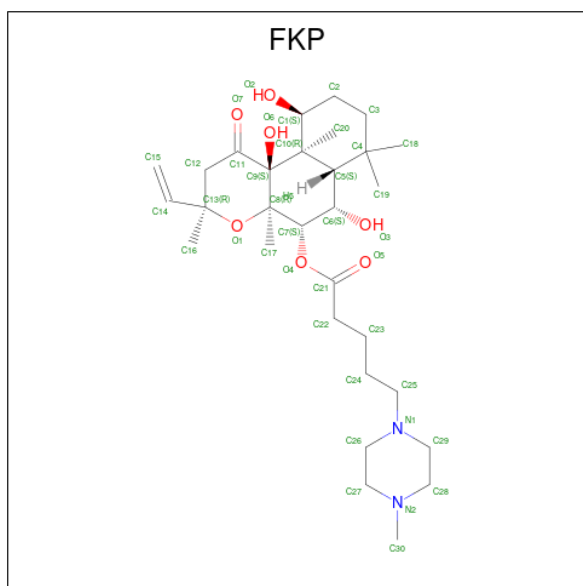
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

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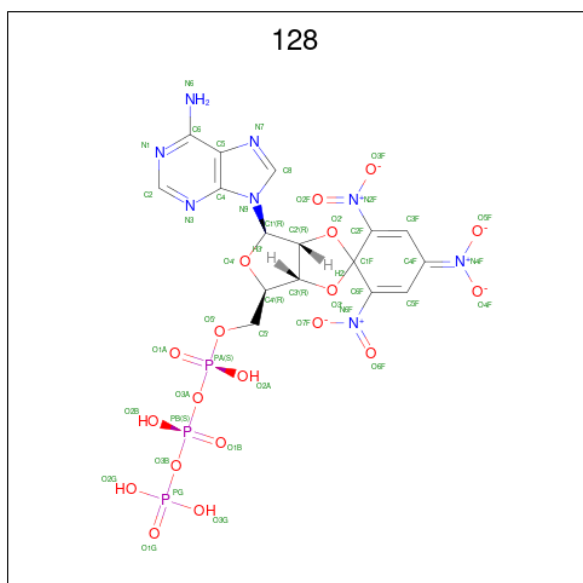
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	Mn		0	0
			1	1			

- Molecule 5 is METHYLPIPERAZINOFORSKOLIN (CCD ID: 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 (CCD ID: 128) (formula: $C_{16}H_{16}N_8O_{19}P_3$).

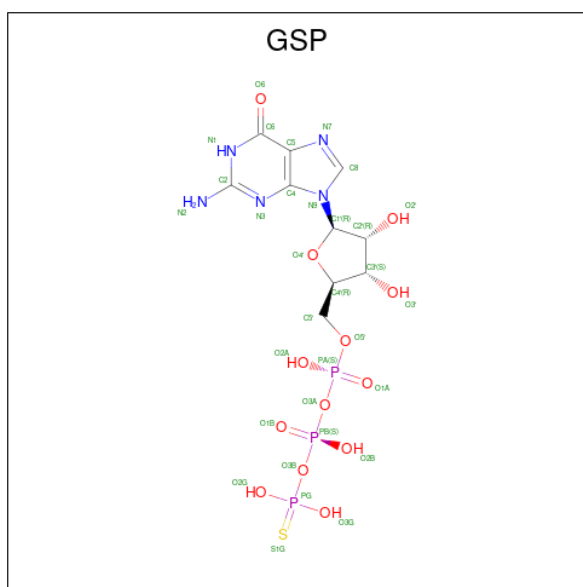


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	
			46	16	8	19	3	
							0	0

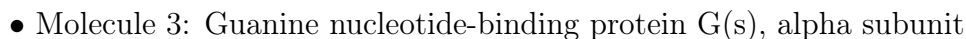
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

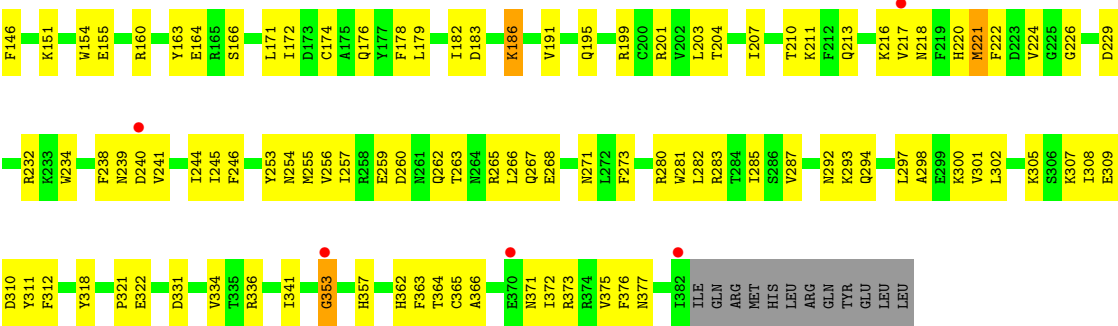
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



- 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, α , β , γ	118.20Å 133.40Å 70.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.96 – 2.90 14.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.5 (14.96-2.90) 74.0 (14.96-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.279 0.235 , 0.270	Depositor DCC
R_{free} test set	925 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.900	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5758	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: CL, 128, GSP, MN, 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	0.49	0/1512	0.79	1/2038 (0.0%)
2	B	0.58	0/1492	0.83	1/2014 (0.0%)
3	C	0.55	0/2691	0.79	0/3643
All	All	0.54	0/5695	0.80	2/7695 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	VAL	N-CA-C	5.98	117.20	108.53
1	A	467	ILE	N-CA-C	5.14	115.58	110.23

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	104	0
2	B	1467	0	1470	69	0
3	C	2635	0	2582	136	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	A	39	0	50	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
9	B	15	0	0	2	0
9	C	25	0	0	4	0
All	All	5758	0	5579	305	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 27.

All (305) 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:107:VAL:HA	3:C:110:MET:HE2	1.65	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:H201	5:A:583:FKP:H173	1.67	0.74
3:C:210:THR:HB	3:C:221:MET:HB3	1.67	0.73
1:A:528:ILE:H	1:A:528:ILE:HD13	1.52	0.73
3:C:257:ILE:HD12	3:C:268:GLU:HG2	1.70	0.72
1:A:452:ARG:HH11	1:A:452:ARG:HB2	1.53	0.72
1:A:403:LEU:H	1:A:403:LEU:HD23	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
1:A:395:ALA:HB1	1:A:483:MET:HE3	1.73	0.70
1:A:426:LEU:HB3	1:A:462:MET:HE1	1.74	0.70
2:B:890:ALA:HB1	2:B:996:LEU:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:VAL:HG12	1:A:480:ASN:H	1.58	0.69
1:A:452:ARG:HB2	1:A:452:ARG:NH1	2.07	0.69
2:B:905:ASN:HB2	2:B:910:GLU:HB2	1.73	0.69
3:C:45:LEU:HD11	3:C:221:MET:HE2	1.74	0.69
3:C:365:CYS:H	3:C:371:ASN:ND2	1.91	0.69
1:A:378:MET:HE1	3:C:283:ARG:H	1.58	0.68
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
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:H193	5:A:583:FKP:H202	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:462:MET:HA	1:A:462:MET:HE3	1.79	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:1044:GLU:CD	2:B:1044:GLU:H	2.04	0.64
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:N	1:A:526:ILE:HD12	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:H	3:C:119:LEU:HD12	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:393:LEU:C	1:A:393:LEU:HD23	2.25	0.60
1:A:426:LEU:CB	1:A:462:MET:HE1	2.31	0.60
3:C:61:ARG:O	3:C:65:VAL:HB	2.01	0.60
1:A:378:MET:CE	3:C:283:ARG:H	2.15	0.60
2:B:1026:VAL:HG21	2:B:1067:LYS:HZ2	1.67	0.60
1:A:378:MET:HE1	3:C:283:ARG:HG2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:888:MET:SD	2:B:972:MET:HE2	2.43	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
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:59:GLN:HG3	3:C:372:ILE:HG12	1.86	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
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:HH11	1:A:452:ARG:CB	2.17	0.57
1:A:408:THR:HB	9:A:11:HOH:O	2.03	0.57
1:A:423:PHE:HE2	1:A:483:MET:HE2	1.68	0.56
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:434:ARG:C	1:A:434:ARG:HD2	2.33	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
1:A:527:HIS:NE2	1:A:561:THR:HB	2.24	0.52
3:C:45:LEU:CD1	3:C:221:MET:HE2	2.38	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:221:MET:HE3	3:C:221:MET:HA	1.92	0.51
3:C:294:GLN:HG3	3:C:363:PHE:HB3	1.92	0.51
1:A:423:PHE:CE2	1:A:483:MET:HE2	2.44	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
1:A:470:ILE:HD13	1:A:482:ASN:C	2.36	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:54:SER:O	3:C:58:LYS:HG3	2.12	0.50
3:C:257:ILE:CG1	3:C:259:GLU:HG2	2.38	0.50
2:B:1033:THR:HG22	2:B:1059:ARG:NH2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:256:VAL:C	3:C:265:ARG:HG3	2.38	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
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:58:LYS:HA	3:C:61:ARG:NH1	2.29	0.47
3:C:124:ASN:O	3:C:128:VAL:HG23	2.14	0.47
1:A:470:ILE:HG12	1:A:470:ILE:O	2.14	0.47
3:C:103:ILE:HG23	3:C:104:GLU:N	2.28	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:59:GLN:CG	3:C:372:ILE:HG12	2.45	0.47
3:C:100:LYS:C	3:C:102:ALA:H	2.22	0.47
3:C:285:ILE:N	3:C:285:ILE:HD12	2.30	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:372:ILE:HD12	3:C:372:ILE:C	2.39	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:88:LYS:C	3:C:92:VAL:HG23	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:A:530:LYS:N	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
2:B:972:MET:HE3	2:B:975:PHE:HB3	1.99	0.45
2:B:1009:VAL:HG13	2:B:1016:GLN:C	2.42	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
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:H201	5:A:583:FKP:C17	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
2:B:1062:ILE:HD13	2:B:1063:ASN:H	1.77	0.44
3:C:100:LYS:C	3:C:102:ALA:N	2.76	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:HG23	1:A:481:VAL:O	2.17	0.44
3:C:104:GLU:HB2	3:C:135:MET:HE2	2.00	0.43
1:A:461:GLU:O	1:A:464:MET:HB2	2.18	0.43
1:A:525:ARG:C	1:A:526:ILE:HD12	2.43	0.43
2:B:995:LYS:HD2	2:B:1037:ASP:OD2	2.18	0.43
3:C:123:GLU:OE1	3:C:123:GLU:N	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:HG3	1:A:434:ARG:HH11	1.83	0.43
3:C:42:ARG:HA	3:C:220:HIS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:372:ILE:O	3:C:376:PHE:HB2	2.18	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
3:C:43:LEU:HB2	3:C:221:MET:HE3	2.01	0.43
3:C:203:LEU:HD23	3:C:203:LEU:C	2.44	0.43
3:C:292:ASN:CG	3:C:293:LYS:N	2.76	0.43
2:B:922:PHE:CG	2:B:979:LEU:HD22	2.54	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
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:107:VAL:CA	3:C:110:MET:HE2	2.45	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:952:ALA:O	2:B:953:ILE:C	2.62	0.42
2:B:1048:ILE:O	2:B:1052:LEU:HG	2.20	0.42
3:C:127:ARG:O	3:C:131:ILE:HG12	2.20	0.42
1:A:550:ARG:HG2	1:A:550:ARG:HH11	1.84	0.42
1:A:408:THR:HG23	1:A:411:GLU:OE2	2.19	0.42
1:A:526:ILE:N	1:A:526:ILE:CD1	2.82	0.42
3:C:245:ILE:HG23	9:C:404:HOH:O	2.19	0.42
1:A:462:MET:HE2	1:A:466:MET:HG3	2.02	0.42
3:C:98:ASN:O	3:C:102:ALA:HB2	2.19	0.42
3:C:213:GLN:HG3	3:C:217:VAL:C	2.45	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:201:ARG:HD3	3:C:201:ARG:C	2.45	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
2:B:1044:GLU:CD	2:B:1044:GLU:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LYS:HA	3:C:61:ARG:HH12	1.86	0.41
3:C:174:CYS:HB3	3:C:199:ARG:O	2.20	0.41
3:C:322:GLU:OE1	3:C:322:GLU:HA	2.20	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
1:A:377:MET:O	1:A:378:MET:C	2.63	0.41
3:C:99:LEU:HD21	3:C:182:ILE:HD12	2.01	0.41
3:C:372:ILE:HA	3:C:375:VAL:CG2	2.51	0.41
3:C:107:VAL:HG23	3:C:108:ALA:H	1.84	0.41
3:C:218:ASN:N	3:C:218:ASN:HD22	2.18	0.41
1:A:485:VAL:HB	1:A:526:ILE:HA	2.01	0.41
1:A:491:ARG:HH21	2:B:901:GLU:HB3	1.85	0.41
1:A:379:PHE:CD1	1:A:379:PHE:N	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:1030:MET:HE2	2:B:1042:THR:HG23	2.03	0.41
3:C:145:GLU:O	3:C:146:PHE:C	2.64	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:477:THR:O	1:A:478:GLY:C	2.63	0.40
1:A:401:THR:OG1	2:B:1065:LYS:HE3	2.21	0.40
3:C:377:ASN:OD1	3:C:377:ASN:C	2.64	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:1055:THR:C	2:B:1076:ASN:HD22	2.29	0.40
2:B:879:HIS:N	2:B:879:HIS:CD2	2.90	0.40
3:C:55:THR:CG2	3:C:366:ALA:HB1	2.51	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%)	170 (90%)	15 (8%)	3 (2%)	7	27
2	B	185/212 (87%)	174 (94%)	10 (5%)	1 (0%)	24	54
3	C	318/394 (81%)	285 (90%)	32 (10%)	1 (0%)	36	65
All	All	691/831 (83%)	629 (91%)	57 (8%)	5 (1%)	18	48

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 ⓘ

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%)	61	86
2	B	162/184 (88%)	158 (98%)	4 (2%)	42	74
3	C	290/351 (83%)	288 (99%)	2 (1%)	76	92
All	All	611/724 (84%)	603 (99%)	8 (1%)	61	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	ILE
1	A	528	ILE
2	B	879	HIS
2	B	921	ASP

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Mol	Chain	Res	Type
2	B	1044	GLU
2	B	1062	ILE
3	C	186	LYS
3	C	221	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	A	482	ASN
1	A	503	GLN
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	1022	ASN
2	B	1025	ASN
2	B	1050	GLN
2	B	1076	ASN
3	C	41	HIS
3	C	97	ASN
3	C	98	ASN
3	C	136	ASN
3	C	218	ASN
3	C	220	HIS
3	C	267	GLN
3	C	271	ASN
3	C	294	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	40,42,42	2.47	18 (45%)	52,68,68	2.09	12 (23%)
8	GSP	C	395	4	33,34,34	2.19	5 (15%)	47,54,54	1.54	8 (17%)
6	128	A	584	4	42,50,50	3.96	19 (45%)	55,80,80	2.91	22 (40%)

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	-	-	11/14/97/97	0/4/4/4
8	GSP	C	395	4	-	2/21/38/38	0/3/3/3
6	128	A	584	4	-	2/26/80/80	0/5/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	584	128	PB-O3A	11.54	1.72	1.59
6	A	584	128	PB-O2B	-11.07	1.04	1.55
6	A	584	128	O2'-C1F	9.20	1.54	1.41
6	A	584	128	PB-O1B	-8.77	1.20	1.50
6	A	584	128	O3'-C1F	8.20	1.53	1.41
8	C	395	GSP	PG-O2G	-8.12	1.28	1.54
8	C	395	GSP	PB-O3B	7.03	1.67	1.59
5	A	583	FKP	C10-C5	6.28	1.66	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	584	128	C5F-C6F	5.10	1.51	1.37
5	A	583	FKP	C12-C11	4.61	1.57	1.50
5	A	583	FKP	C9-C11	4.35	1.59	1.54
5	A	583	FKP	C4-C5	4.34	1.62	1.56
5	A	583	FKP	C6-C7	4.26	1.61	1.53
6	A	584	128	PA-O3A	3.77	1.63	1.59
6	A	584	128	C5'-C4'	3.60	1.62	1.51
5	A	583	FKP	C27-C26	-3.55	1.38	1.51
5	A	583	FKP	C2-C1	3.46	1.57	1.52
5	A	583	FKP	C17-C8	3.45	1.57	1.51
6	A	584	128	C4-N3	3.33	1.40	1.34
5	A	583	FKP	C5-C6	3.23	1.63	1.54
6	A	584	128	PG-O1G	3.18	1.60	1.50
5	A	583	FKP	C9-C10	3.09	1.65	1.57
6	A	584	128	C2'-C3'	3.02	1.59	1.53
5	A	583	FKP	C3-C2	2.96	1.59	1.53
6	A	584	128	C3'-C4'	-2.89	1.45	1.52
6	A	584	128	C6-N1	2.83	1.43	1.35
6	A	584	128	C5-N7	-2.78	1.34	1.39
5	A	583	FKP	C20-C10	2.73	1.58	1.53
5	A	583	FKP	C22-C21	2.55	1.58	1.50
6	A	584	128	O7F-N6F	-2.50	1.18	1.35
5	A	583	FKP	C25-N1	2.47	1.53	1.47
5	A	583	FKP	C29-N1	2.47	1.53	1.46
6	A	584	128	C2-N3	2.44	1.38	1.33
6	A	584	128	PG-O3G	-2.44	1.45	1.54
8	C	395	GSP	PB-O3A	2.42	1.62	1.59
6	A	584	128	C2-N1	2.39	1.38	1.33
6	A	584	128	PA-O1A	2.35	1.58	1.50
5	A	583	FKP	C23-C22	2.15	1.60	1.52
5	A	583	FKP	C26-N1	2.12	1.52	1.46
8	C	395	GSP	PB-O1B	-2.05	1.43	1.50
5	A	583	FKP	C8-C7	2.03	1.57	1.53
8	C	395	GSP	C4-N3	2.00	1.38	1.34

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	584	128	C5-C4-N3	-7.52	116.37	126.72
6	A	584	128	C4'-O4'-C1'	7.38	125.75	109.47
6	A	584	128	O3'-C1F-C6F	-6.74	101.25	110.47
5	A	583	FKP	O1-C8-C7	6.52	109.33	103.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	584	128	N3-C4-N9	5.96	137.30	127.17
5	A	583	FKP	C10-C5-C4	-5.73	111.39	116.32
5	A	583	FKP	C19-C4-C18	-5.21	100.28	107.87
6	A	584	128	O4'-C1'-C2'	-5.14	97.75	106.59
6	A	584	128	O2'-C1F-C2F	-5.04	103.57	110.47
6	A	584	128	C2-N3-C4	4.94	123.90	111.83
6	A	584	128	N3-C2-N1	-4.91	121.15	128.58
6	A	584	128	O2'-C2'-C3'	4.89	111.42	103.63
6	A	584	128	O3A-PB-O1B	-4.82	96.21	110.70
8	C	395	GSP	O2B-PB-O3B	4.56	119.59	107.27
8	C	395	GSP	O6-C6-N1	4.10	127.83	120.11
5	A	583	FKP	O1-C8-C17	-3.88	105.16	110.17
8	C	395	GSP	O3B-PB-O1B	-3.66	99.68	110.70
6	A	584	128	O2B-PB-O3B	3.65	117.14	107.27
5	A	583	FKP	C17-C8-C7	-3.58	104.04	111.56
5	A	583	FKP	C19-C4-C5	3.55	124.29	111.92
5	A	583	FKP	C17-C8-C9	3.16	118.68	115.19
5	A	583	FKP	C19-C4-C3	-3.10	102.56	109.01
5	A	583	FKP	C4-C5-C6	-2.98	111.28	115.09
6	A	584	128	O3'-C3'-C2'	2.89	108.23	103.63
6	A	584	128	O2G-PG-O3B	2.88	114.28	104.64
6	A	584	128	O4'-C4'-C3'	-2.84	98.92	104.92
6	A	584	128	C2'-C3'-C4'	2.73	110.11	103.78
6	A	584	128	C6-C5-C4	2.71	120.88	117.18
6	A	584	128	C1F-O2'-C2'	-2.67	101.75	107.85
6	A	584	128	C5'-C4'-C3'	2.39	122.33	114.38
8	C	395	GSP	C2'-C3'-C4'	2.35	107.15	102.61
6	A	584	128	C1'-N9-C8	2.34	132.29	127.09
8	C	395	GSP	O2A-PA-O1A	2.33	123.30	112.44
8	C	395	GSP	PB-O3B-PG	-2.33	124.64	133.17
6	A	584	128	C4-N9-C8	-2.18	103.45	105.74
5	A	583	FKP	O7-C11-C12	-2.17	117.61	121.97
5	A	583	FKP	O4-C7-C6	2.16	112.20	107.71
6	A	584	128	O2A-PA-O5'	2.09	117.03	107.57
8	C	395	GSP	O3G-PG-O3B	2.07	111.56	104.64
6	A	584	128	O2'-C1F-C6F	2.07	113.30	110.47
8	C	395	GSP	O3'-C3'-C4'	-2.05	105.18	111.08
5	A	583	FKP	O4-C21-C22	2.02	115.85	111.48

There are no chirality outliers.

All (15) torsion outliers are listed below:

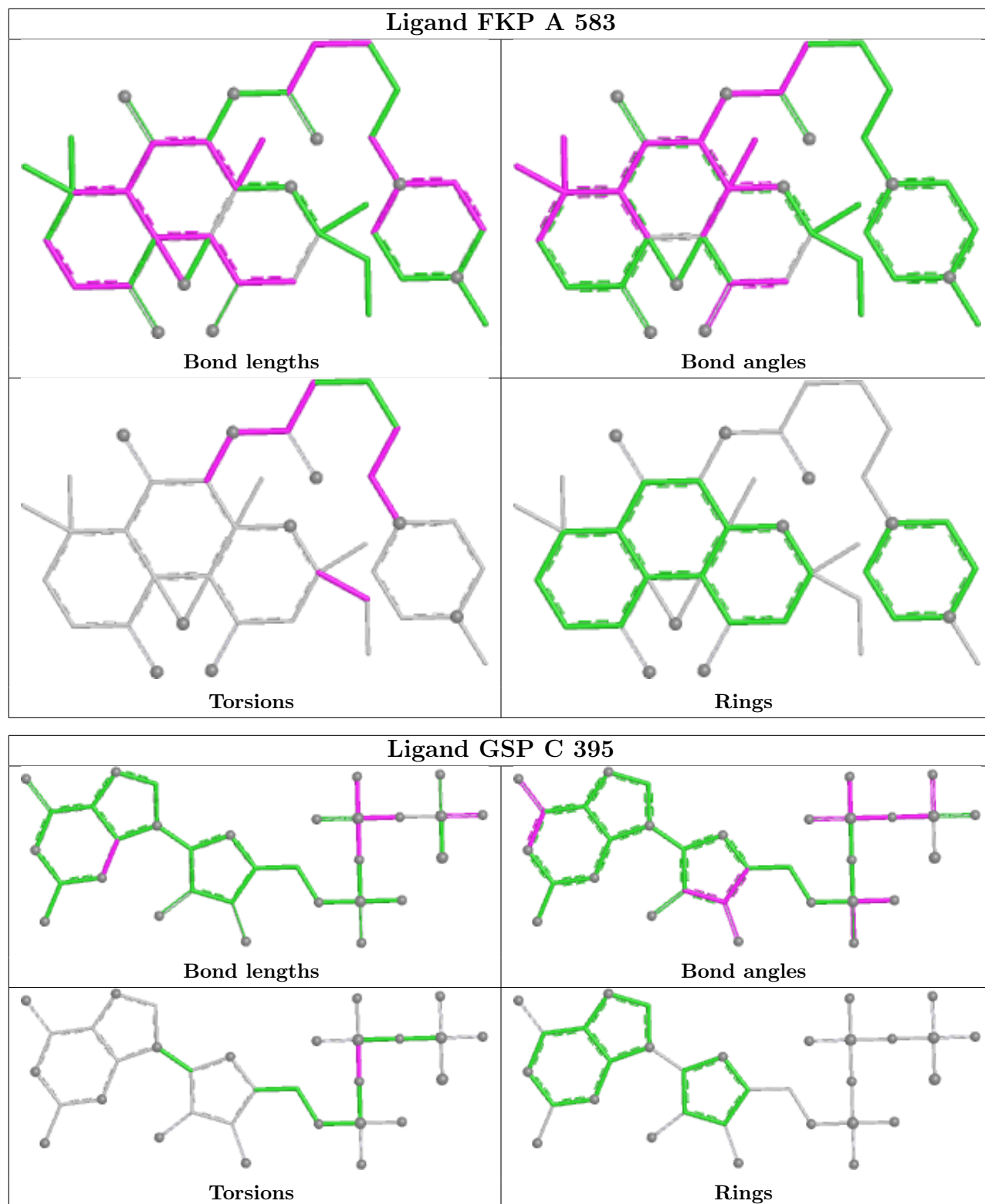
Mol	Chain	Res	Type	Atoms
5	A	583	FKP	C6-C7-O4-C21
5	A	583	FKP	C8-C7-O4-C21
5	A	583	FKP	O1-C13-C14-C15
5	A	583	FKP	C12-C13-C14-C15
5	A	583	FKP	C16-C13-C14-C15
6	A	584	128	C3'-C4'-C5'-O5'
5	A	583	FKP	C23-C24-C25-N1
6	A	584	128	O4'-C4'-C5'-O5'
5	A	583	FKP	C24-C25-N1-C26
5	A	583	FKP	C24-C25-N1-C29
5	A	583	FKP	C22-C21-O4-C7
5	A	583	FKP	O5-C21-O4-C7
8	C	395	GSP	PA-O3A-PB-O1B
8	C	395	GSP	PA-O3A-PB-O2B
5	A	583	FKP	O4-C21-C22-C23

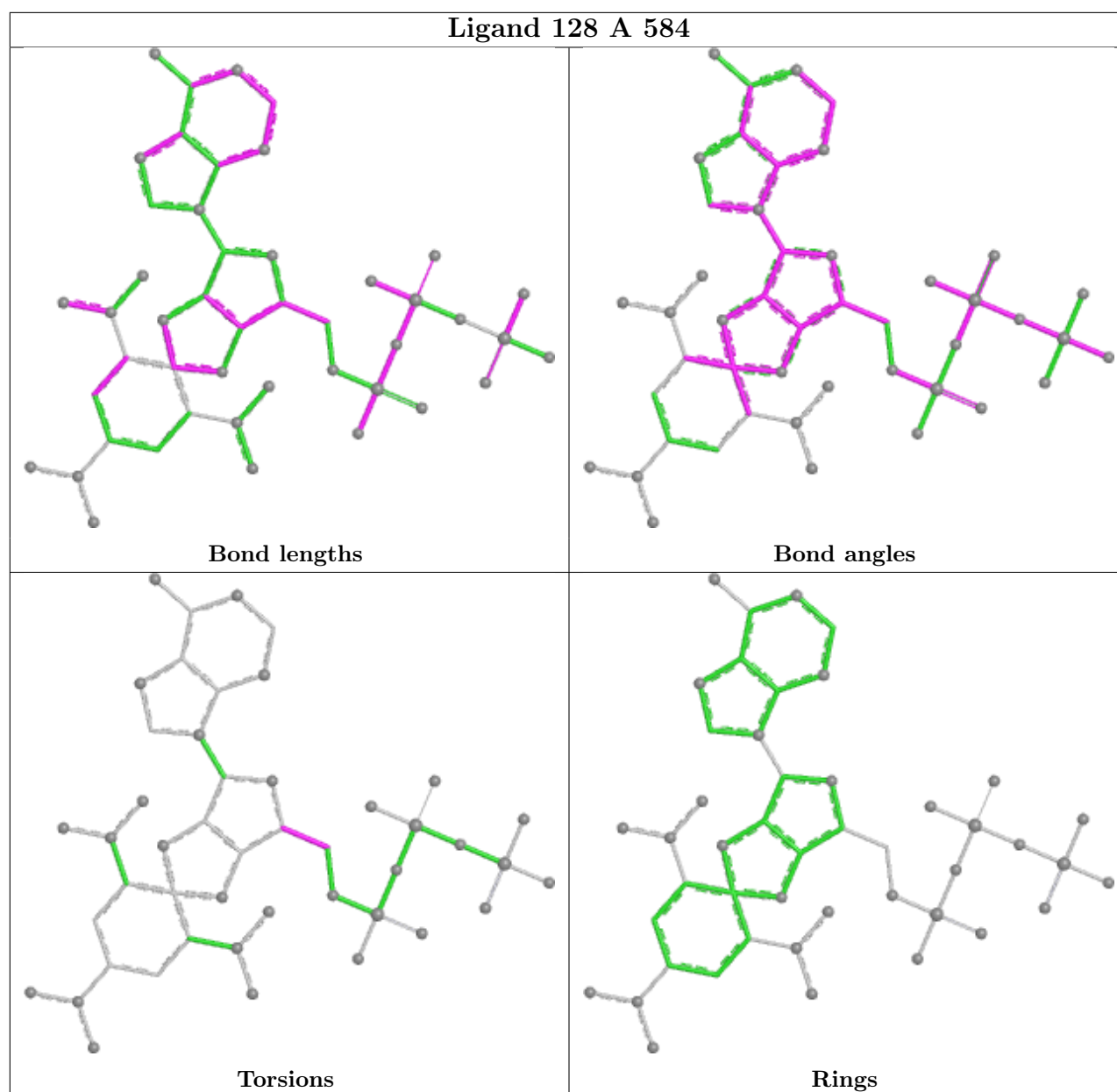
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	583	FKP	4	0
8	C	395	GSP	3	0
6	A	584	128	3	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	190/225 (84%)	0.63	15 (7%) 18 15	21, 56, 102, 127	0
2	B	189/212 (89%)	0.02	2 (1%) 78 71	13, 35, 68, 106	0
3	C	322/394 (81%)	0.12	7 (2%) 62 53	15, 38, 75, 95	0
All	All	701/831 (84%)	0.23	24 (3%) 48 39	13, 42, 81, 127	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	39	ALA	3.9
1	A	479	VAL	3.4
1	A	377	MET	3.3
3	C	353	GLY	3.3
3	C	217	VAL	3.1
1	A	467	ILE	2.9
3	C	382	ILE	2.9
2	B	1012	ALA	2.9
1	A	473	VAL	2.8
1	A	478	GLY	2.8
1	A	476	MET	2.6
1	A	472	LEU	2.4
1	A	458	CYS	2.4
3	C	370	GLU	2.4
2	B	952	ALA	2.3
1	A	481	VAL	2.3
1	A	469	ALA	2.3
1	A	565	LEU	2.3
1	A	450	GLU	2.2
3	C	240	ASP	2.2
1	A	379	PHE	2.1
3	C	40	THR	2.1
1	A	453	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	400	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

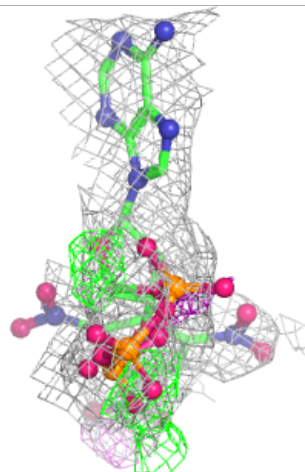
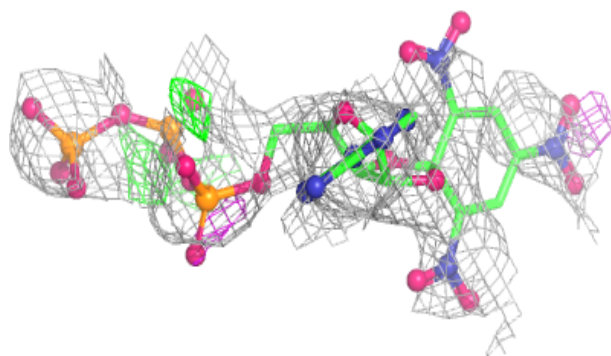
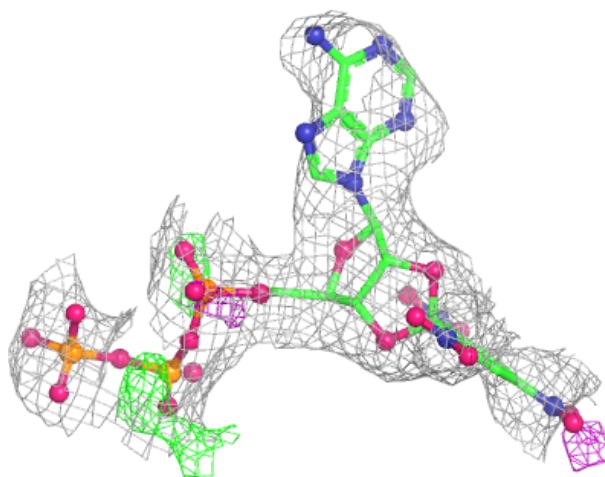
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	128	A	584	46/46	0.87	0.15	60,70,87,92	0
5	FKP	A	583	39/39	0.91	0.12	18,26,77,78	0
4	MN	C	396	1/1	0.94	0.05	40,40,40,40	0
4	MN	A	581	1/1	0.96	0.04	56,56,56,56	0
8	GSP	C	395	32/32	0.96	0.08	11,26,59,61	0
7	CL	C	397	1/1	0.97	0.06	25,25,25,25	0
4	MN	A	582	1/1	0.99	0.02	20,20,20,20	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.

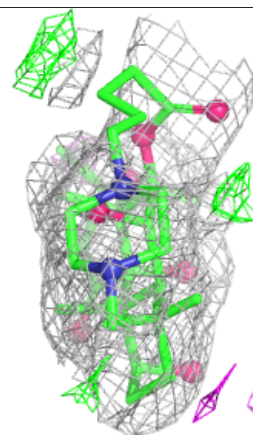
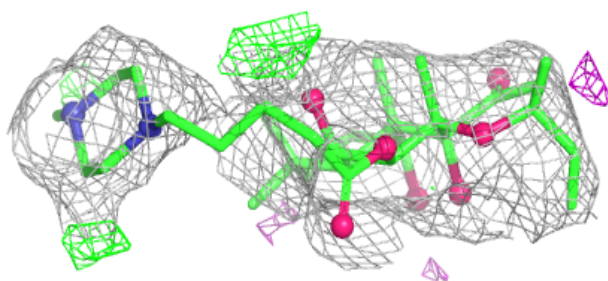
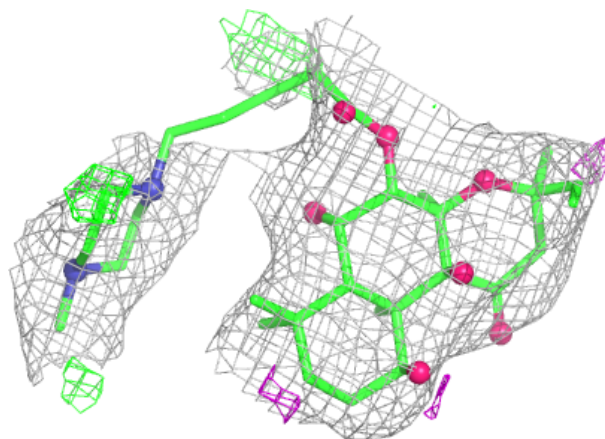
Electron density around 128 A 584:

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

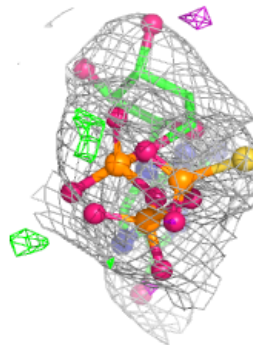
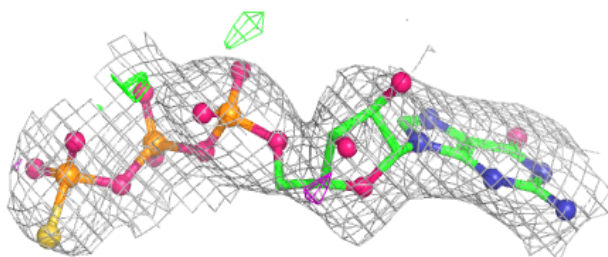
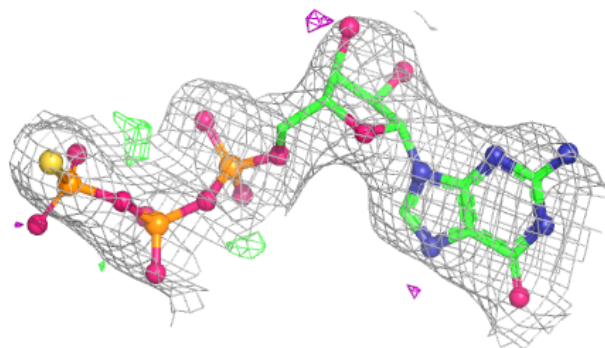


Electron density around FKP A 583:

$2mF_o-DF_c$ (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.