



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:11 PM UTC

PDB ID : 6QH5 / pdb_00006qh5
Title : AP2 clathrin adaptor mu2T156-phosphorylated core in closed conformation
Authors : Wrobel, A.G.; Owen, D.J.; McCoy, A.J.; Evans, P.R.
Deposited on : 2019-01-15
Resolution : 2.56 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

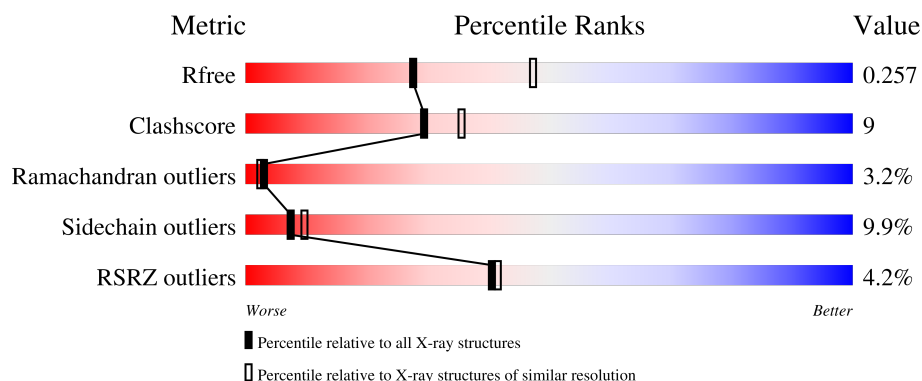
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	621	
2	B	592	
3	N	446	
4	M	446	
5	S	142	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13770 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 AP-2 complex subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	1	0
			4748	3023	819	885	21			

- Molecule 2 is a protein called AP-2 complex subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	579	Total	C	N	O	S	0	0	0
			4578	2919	762	872	25			

- Molecule 3 is a protein called AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	141	Total	C	N	O	S	0	0	0
			1138	731	198	204	5			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	237	MET	-	insertion	UNP P84092
N	238	GLU	-	insertion	UNP P84092
N	239	GLN	-	insertion	UNP P84092
N	240	LYS	-	insertion	UNP P84092
N	241	LEU	-	insertion	UNP P84092
N	242	ILE	-	insertion	UNP P84092
N	243	SER	-	insertion	UNP P84092
N	244	GLU	-	insertion	UNP P84092
N	245	GLU	-	insertion	UNP P84092
N	246	ASP	-	insertion	UNP P84092
N	247	LEU	-	insertion	UNP P84092

- Molecule 4 is a protein called AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	255	Total	C	N	O	S	0	2	0
			2070	1330	365	361	14			

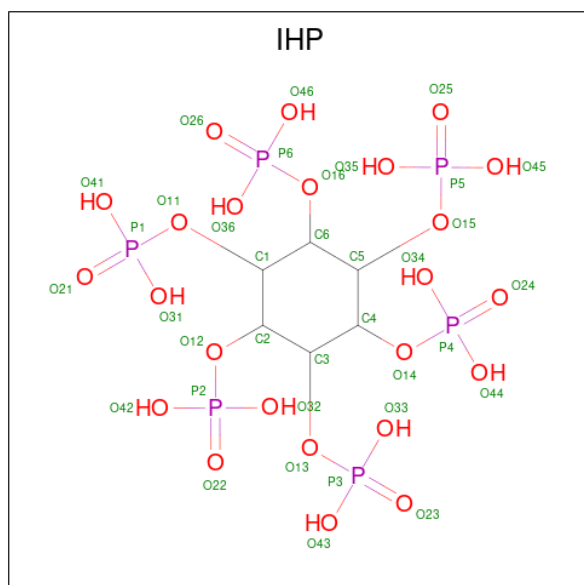
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	222O	MET	-	insertion	UNP P84092
M	222P	GLU	-	insertion	UNP P84092
M	222Q	GLN	-	insertion	UNP P84092
M	222R	LYS	-	insertion	UNP P84092
M	222S	LEU	-	insertion	UNP P84092
M	222T	ILE	-	insertion	UNP P84092
M	222U	SER	-	insertion	UNP P84092
M	222V	GLU	-	insertion	UNP P84092
M	222W	GLU	-	insertion	UNP P84092
M	222X	ASP	-	insertion	UNP P84092
M	222Y	LEU	-	insertion	UNP P84092

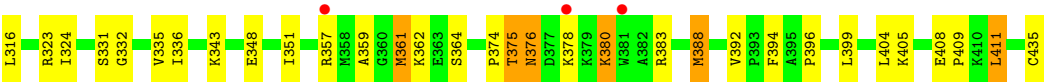
- Molecule 5 is a protein called AP-2 complex subunit sigma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S	142	Total	C	N	O	S	0	0	0
			1200	778	200	215	7			

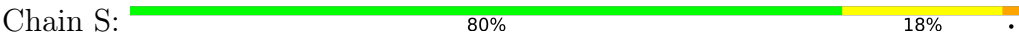
- Molecule 6 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			36	6	24	6		



● Molecule 5: AP-2 complex subunit sigma



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.04Å 121.04Å 257.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.52 – 2.56 60.52 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.7 (60.52-2.56) 99.7 (60.52-2.56)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.225 , 0.257 0.227 , 0.257	Depositor DCC
R_{free} test set	3551 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13770	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: IHP

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	1.02	3/4833 (0.1%)	1.16	5/6555 (0.1%)
2	B	1.01	4/4650 (0.1%)	1.18	12/6309 (0.2%)
3	N	0.92	0/1160	1.11	0/1565
4	M	1.07	1/2111 (0.0%)	1.09	3/2839 (0.1%)
5	S	1.15	3/1224 (0.2%)	1.14	4/1650 (0.2%)
All	All	1.03	11/13978 (0.1%)	1.15	24/18918 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	7
4	M	0	1
All	All	0	9

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	65	LEU	C-O	-6.38	1.16	1.24
5	S	53	ARG	CA-C	-6.28	1.46	1.52
2	B	286	PRO	CA-C	6.25	1.57	1.52
5	S	53	ARG	C-O	-5.79	1.19	1.24
2	B	533	ASP	CA-C	5.65	1.58	1.52
1	A	248	THR	C-O	-5.54	1.17	1.23
2	B	577	PRO	CA-C	5.51	1.57	1.52
1	A	471	ASN	N-CA	5.39	1.53	1.46
2	B	43	VAL	CA-C	5.16	1.59	1.53
4	M	332	GLY	N-CA	5.07	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ASP	C-O	-5.04	1.17	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	286	PRO	N-CA-C	8.39	120.94	110.70
4	M	392	VAL	N-CA-C	7.05	114.97	109.19
2	B	359	LYS	N-CA-C	-6.90	103.82	111.82
4	M	219	LYS	N-CA-C	6.54	118.41	111.28
1	A	493	HIS	N-CA-C	6.24	119.31	110.14
2	B	220	ILE	N-CA-C	5.89	116.63	110.62
1	A	122	SER	N-CA-C	-5.82	103.25	110.41
2	B	359	LYS	N-CA-CB	5.69	119.11	110.28
2	B	385	GLU	N-CA-C	5.58	118.13	111.71
1	A	323	GLU	CA-C-N	-5.39	113.47	119.19
1	A	323	GLU	C-N-CA	-5.39	113.47	119.19
4	M	343	LYS	N-CA-C	5.34	116.63	108.52
5	S	64	GLY	CA-C-N	5.30	130.32	123.00
5	S	64	GLY	C-N-CA	5.30	130.32	123.00
5	S	73	VAL	CB-CA-C	-5.27	105.14	112.04
2	B	114	ARG	N-CA-C	5.23	116.71	109.54
1	A	603	PRO	N-CA-C	5.18	117.03	110.70
2	B	441	GLU	CA-C-N	5.15	124.59	119.24
2	B	441	GLU	C-N-CA	5.15	124.59	119.24
2	B	184	LEU	N-CA-C	5.12	117.26	111.11
2	B	233	ASP	CA-C-N	5.05	130.79	121.70
2	B	233	ASP	C-N-CA	5.05	130.79	121.70
5	S	65	LEU	N-CA-C	5.05	117.20	109.07
2	B	321	ILE	N-CA-C	5.00	115.73	110.62

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	ARG	Peptide
2	B	159	GLN	Peptide
2	B	189	GLU	Peptide
2	B	190	SER	Peptide
2	B	191	HIS	Peptide
2	B	198	ASP	Peptide
2	B	452	VAL	Peptide
2	B	568	GLY	Peptide

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Mol	Chain	Res	Type	Group
4	M	374	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4748	0	4842	83	0
2	B	4578	0	4686	101	1
3	N	1138	0	1143	23	0
4	M	2070	0	2162	25	0
5	S	1200	0	1193	26	0
6	A	36	0	6	1	0
All	All	13770	0	14032	238	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (238) 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)
5:S:61:ARG:NH2	5:S:62:TYR:O	1.71	1.24
5:S:61:ARG:NH2	5:S:62:TYR:C	2.22	0.96
1:A:198:ASP:O	1:A:232:ARG:NH2	2.07	0.88
2:B:289:VAL:HG22	2:B:323:VAL:HG21	1.61	0.81
5:S:61:ARG:NH2	5:S:65:LEU:H	1.79	0.81
5:S:61:ARG:NH1	5:S:62:TYR:H	1.82	0.78
2:B:500:GLN:HA	2:B:503:VAL:HG12	1.67	0.76
4:M:316:LEU:HB3	4:M:357:ARG:HD2	1.67	0.76
2:B:219:GLN:O	2:B:222:ILE:HB	1.90	0.71
1:A:10:MET:HE3	1:A:56:LYS:HE3	1.71	0.71
1:A:585:ARG:CZ	2:B:543:SER:HB2	2.20	0.71
2:B:203:ASN:O	2:B:207:LEU:HG	1.93	0.69
2:B:312:LYS:O	2:B:314:PRO:HD3	1.93	0.68
4:M:361:MET:HE2	4:M:361:MET:HA	1.74	0.68
4:M:287:PHE:CD2	4:M:388:MET:HE1	2.28	0.68
5:S:61:ARG:HE	5:S:63:ALA:C	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:452:VAL:HG11	2:B:466:LEU:HD13	1.75	0.67
2:B:511:THR:HG23	2:B:524:TYR:CZ	2.30	0.67
1:A:360:GLU:H	1:A:360:GLU:CD	2.02	0.66
1:A:16:PHE:CZ	1:A:20:ILE:HD11	2.32	0.65
1:A:473:ASP:C	1:A:473:ASP:OD1	2.41	0.64
5:S:61:ARG:NH1	5:S:62:TYR:N	2.46	0.64
4:M:310[A]:ASN:CG	4:M:310[A]:ASN:O	2.37	0.64
1:A:535:VAL:HG12	1:A:538:ARG:HH21	1.64	0.63
1:A:32:ARG:NH1	1:A:36:GLU:HG2	2.12	0.62
5:S:61:ARG:CZ	5:S:62:TYR:N	2.62	0.62
3:N:21:ARG:NH1	3:N:118:PHE:O	2.33	0.62
5:S:15:ARG:NH1	5:S:100:GLU:OE2	2.29	0.62
2:B:75:ASN:OD1	3:N:18:ARG:NH2	2.32	0.62
1:A:473:ASP:OD1	1:A:474:ASP:N	2.34	0.61
5:S:15:ARG:HH12	5:S:100:GLU:CD	2.09	0.61
5:S:61:ARG:NH1	5:S:61:ARG:HA	2.16	0.61
2:B:276:TYR:O	2:B:279:MET:N	2.33	0.60
1:A:32:ARG:HH12	1:A:36:GLU:HG2	1.68	0.59
1:A:401:ASN:O	1:A:402:ALA:C	2.46	0.58
1:A:10:MET:CE	1:A:56:LYS:HG2	2.33	0.58
2:B:299:GLN:O	2:B:300:TYR:C	2.47	0.58
2:B:297:GLU:HB3	3:N:79:PHE:CE1	2.39	0.58
1:A:473:ASP:C	1:A:475:VAL:H	2.11	0.57
2:B:237:ALA:HA	2:B:240:ILE:HD12	1.85	0.57
2:B:564:ILE:O	2:B:567:ILE:HG23	2.05	0.56
4:M:162:ARG:NH2	4:M:206:LEU:O	2.38	0.56
2:B:324:PHE:O	2:B:338:LYS:HG3	2.06	0.56
4:M:376:ASN:ND2	4:M:378:LYS:O	2.39	0.56
2:B:249:SER:OG	2:B:255:VAL:HG11	2.05	0.56
2:B:208:LEU:HB3	2:B:243:ARG:HG2	1.87	0.56
3:N:18:ARG:NH1	3:N:113:ASP:OD1	2.39	0.56
1:A:473:ASP:O	1:A:475:VAL:N	2.39	0.56
3:N:111:LEU:HD23	3:N:133:ILE:CD1	2.35	0.55
2:B:474:HIS:C	2:B:476:GLU:H	2.14	0.55
1:A:467:GLN:O	1:A:470:ILE:HG12	2.06	0.55
2:B:453:GLY:HA3	2:B:454:GLU:HB3	1.89	0.55
1:A:174:ARG:HH11	1:A:174:ARG:CG	2.19	0.55
2:B:271:PRO:HB3	2:B:277:TYR:CD1	2.42	0.54
2:B:297:GLU:HB3	3:N:79:PHE:CD1	2.41	0.54
2:B:143:VAL:HG11	3:N:117:ASP:HB3	1.89	0.54
2:B:453:GLY:HA3	2:B:454:GLU:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:PRO:O	2:B:178:ALA:HB3	2.08	0.54
2:B:287:PRO:O	2:B:291:LEU:HD13	2.07	0.53
2:B:529:LEU:HD23	2:B:537:ALA:HA	1.91	0.53
3:N:111:LEU:HD23	3:N:133:ILE:HD13	1.91	0.53
4:M:287:PHE:CG	4:M:388:MET:HE1	2.43	0.53
3:N:115:ILE:HG13	3:N:124:SER:CB	2.39	0.53
1:A:492:CYS:SG	1:A:529:LYS:HE3	2.49	0.52
1:A:374:ILE:HD13	1:A:408:GLU:HG3	1.91	0.52
1:A:217:LYS:C	1:A:219:PRO:HD3	2.35	0.52
1:A:421:ARG:NH1	1:A:453:ALA:HB2	2.25	0.52
1:A:585:ARG:CZ	2:B:543:SER:CB	2.88	0.52
3:N:74:ASN:HB3	3:N:77:MET:HE2	1.92	0.52
5:S:49:PHE:CE2	5:S:77:ASN:HB3	2.45	0.52
1:A:585:ARG:CZ	1:A:585:ARG:CB	2.88	0.51
5:S:61:ARG:CZ	5:S:65:LEU:N	2.74	0.51
2:B:492:PHE:HD1	2:B:499:THR:HG1	1.57	0.51
5:S:36:HIS:CE1	5:S:40:THR:HG21	2.46	0.51
1:A:174:ARG:HH11	1:A:174:ARG:HG2	1.75	0.51
1:A:487:LEU:HD11	1:A:500:GLY:HA3	1.93	0.51
2:B:451:ILE:O	2:B:454:GLU:O	2.28	0.51
2:B:502:LEU:HD12	2:B:503:VAL:N	2.25	0.51
1:A:459:GLU:HG2	1:A:463:TYR:CZ	2.45	0.51
2:B:492:PHE:HD1	2:B:499:THR:OG1	1.94	0.51
4:M:173:LEU:HD12	4:M:173:LEU:C	2.36	0.51
5:S:61:ARG:CZ	5:S:62:TYR:C	2.84	0.51
1:A:357:ALA:HB2	1:A:366:VAL:HG11	1.93	0.51
2:B:82:ASP:HA	2:B:85:ILE:HD12	1.92	0.51
1:A:79:ALA:HA	1:A:82:LEU:HD12	1.93	0.50
2:B:295:GLU:O	2:B:299:GLN:HG3	2.10	0.50
1:A:365:ALA:O	1:A:368:THR:HB	2.11	0.50
1:A:346:ARG:NH1	1:A:380:GLU:OE2	2.44	0.50
3:N:8:TYR:HB2	3:N:64:TRP:HB2	1.92	0.50
2:B:285:ALA:HB3	2:B:286:PRO:CD	2.42	0.49
2:B:165:LEU:HD23	2:B:184:LEU:HD13	1.95	0.49
5:S:61:ARG:CZ	5:S:65:LEU:H	2.24	0.49
2:B:305:ASN:OD1	2:B:572:SER:HB2	2.12	0.49
1:A:213:THR:HA	1:A:216:GLN:OE1	2.12	0.49
5:S:3:ARG:HD2	5:S:21:MET:HE2	1.94	0.49
2:B:299:GLN:O	2:B:302:ALA:N	2.46	0.49
4:M:202:MET:HE2	4:M:204:SER:HB3	1.95	0.48
4:M:252:VAL:HG13	4:M:263:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:SER:O	2:B:294:GLY:O	2.31	0.48
1:A:585:ARG:NH2	2:B:543:SER:HB2	2.28	0.48
2:B:249:SER:OG	2:B:250:HIS:N	2.45	0.48
1:A:263:ARG:NH2	5:S:74:ASN:O	2.47	0.48
2:B:85:ILE:HD13	2:B:117:LYS:HD2	1.94	0.48
4:M:408:GLU:CG	4:M:411:LEU:HB2	2.44	0.48
3:N:73:VAL:HG12	3:N:74:ASN:N	2.29	0.48
2:B:251:ALA:HB3	2:B:255:VAL:HG23	1.95	0.48
1:A:488:GLN:HA	1:A:525:LEU:HD11	1.96	0.48
3:N:84:LYS:HA	3:N:87:ASP:HB2	1.95	0.48
2:B:130:LEU:HB3	2:B:168:LEU:HD11	1.96	0.48
2:B:216:GLU:CG	2:B:251:ALA:HB2	2.44	0.48
3:N:12:GLY:HA2	3:N:37:ILE:HD13	1.95	0.48
2:B:350:ASN:C	2:B:352:ALA:N	2.72	0.47
1:A:10:MET:HE1	1:A:93:ILE:CD1	2.43	0.47
1:A:118:ASN:O	1:A:122:SER:N	2.47	0.47
1:A:585:ARG:NH2	2:B:543:SER:CB	2.77	0.47
1:A:124:ASN:O	1:A:128:MET:HG3	2.14	0.47
1:A:185:MET:HE3	1:A:185:MET:HA	1.96	0.47
2:B:511:THR:HG23	2:B:524:TYR:CE1	2.48	0.47
1:A:231:SER:HB3	1:A:235:ARG:HH21	1.79	0.47
2:B:292:LEU:HD12	2:B:292:LEU:N	2.30	0.47
3:N:108:ILE:O	3:N:112:LEU:HG	2.14	0.47
5:S:61:ARG:NH2	5:S:65:LEU:N	2.57	0.47
1:A:469:VAL:O	1:A:470:ILE:HG23	2.15	0.47
1:A:585:ARG:NH1	2:B:539:GLU:O	2.47	0.46
1:A:589:VAL:HG12	1:A:590:ALA:N	2.29	0.46
3:N:115:ILE:HG13	3:N:124:SER:HB2	1.97	0.46
1:A:370:ILE:HG23	1:A:371:GLU:N	2.30	0.46
4:M:394:PHE:O	4:M:396:PRO:HD3	2.15	0.46
2:B:354:VAL:O	2:B:358:LEU:HG	2.15	0.46
2:B:574:TYR:CZ	3:N:49:ASN:HB2	2.50	0.46
2:B:474:HIS:C	2:B:476:GLU:N	2.72	0.46
5:S:92:ASN:OD1	5:S:97:ASN:HA	2.15	0.46
1:A:188:TRP:O	1:A:189:THR:C	2.59	0.46
2:B:166:ARG:HD3	2:B:197:LEU:HB2	1.96	0.46
4:M:216:MET:SD	4:M:399:LEU:HD11	2.55	0.46
2:B:9:THR:HG21	5:S:99:CYS:HB3	1.97	0.46
2:B:90:SER:HA	2:B:93:LYS:HG2	1.98	0.46
1:A:590:ALA:HB1	1:A:594:ILE:HG21	1.98	0.46
2:B:267:LEU:HD21	2:B:281:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ASP:HA	2:B:166:ARG:HD2	1.98	0.46
2:B:297:GLU:HB2	3:N:83:TYR:OH	2.15	0.46
2:B:357:GLU:HA	2:B:357:GLU:OE1	2.16	0.45
1:A:590:ALA:HB2	2:B:536:THR:CG2	2.46	0.45
1:A:201:LEU:HD11	1:A:244:LEU:HD22	1.97	0.45
2:B:245:THR:HB	2:B:246:PRO:HD3	1.99	0.45
4:M:168:TYR:OH	4:M:269:ASP:OD1	2.33	0.45
1:A:10:MET:CE	1:A:56:LYS:HE3	2.43	0.45
5:S:99:CYS:O	5:S:100:GLU:C	2.60	0.45
1:A:397:CYS:SG	1:A:431:LEU:HD22	2.57	0.45
1:A:468:ILE:O	1:A:470:ILE:N	2.44	0.45
2:B:71:LEU:HD22	3:N:109:TYR:HB3	1.99	0.45
3:N:1:MET:O	3:N:69:THR:HG23	2.17	0.45
1:A:446:ILE:HG21	1:A:465:VAL:HB	1.99	0.45
2:B:353:GLN:O	2:B:356:ALA:N	2.50	0.45
4:M:359:ALA:HB3	4:M:362:LYS:HD3	1.99	0.45
1:A:470:ILE:HD13	1:A:605:PHE:N	2.32	0.45
2:B:180:ALA:O	2:B:184:LEU:HD22	2.17	0.45
1:A:454:GLY:HA2	1:A:457:VAL:HG23	1.98	0.44
2:B:239:SER:O	2:B:240:ILE:C	2.61	0.44
2:B:243:ARG:O	2:B:246:PRO:HD2	2.17	0.44
4:M:383:ARG:HG2	4:M:435:CYS:SG	2.57	0.44
5:S:62:TYR:O	5:S:63:ALA:HB3	2.16	0.44
2:B:286:PRO:O	2:B:290:THR:HG23	2.17	0.44
2:B:364:GLU:OE1	2:B:364:GLU:HA	2.17	0.44
1:A:483:VAL:CG1	1:A:500:GLY:HA2	2.48	0.44
1:A:197:ASN:HD21	1:A:228:LEU:HD22	1.83	0.44
1:A:506:GLU:OE2	1:A:602:MET:HB2	2.18	0.44
1:A:527:HIS:HA	1:A:545:TYR:OH	2.18	0.44
1:A:16:PHE:CE1	1:A:20:ILE:HD11	2.53	0.44
2:B:259:ALA:O	2:B:262:VAL:N	2.50	0.44
1:A:273:ASP:OD1	1:A:273:ASP:C	2.61	0.43
1:A:470:ILE:HD13	1:A:605:PHE:H	1.83	0.43
2:B:8:THR:O	2:B:9:THR:C	2.61	0.43
5:S:3:ARG:HB3	5:S:21:MET:CE	2.47	0.43
1:A:309:VAL:O	1:A:310:LEU:C	2.61	0.43
2:B:129:CYS:HA	2:B:132:ASP:HB2	2.00	0.43
2:B:214:CYS:SG	2:B:218:GLY:HA3	2.58	0.43
4:M:310[B]:ASN:HA	4:M:361:MET:HE3	2.00	0.43
2:B:328:TYR:CE1	2:B:329:ASN:HB3	2.53	0.43
4:M:376:ASN:ND2	4:M:376:ASN:C	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ASN:HB3	1:A:405:ILE:HG13	2.01	0.43
3:N:112:LEU:HA	3:N:115:ILE:HG22	2.00	0.43
1:A:105:ASN:OD1	1:A:107:GLU:HB3	2.18	0.43
2:B:216:GLU:HG3	2:B:251:ALA:HB2	1.99	0.43
4:M:241:ILE:HB	5:S:27:GLU:HG2	2.00	0.43
1:A:382:ASP:OD1	1:A:384:SER:OG	2.27	0.43
1:A:563:LEU:O	1:A:569:LEU:HG	2.19	0.43
2:B:303:LEU:N	2:B:303:LEU:HD12	2.34	0.43
2:B:463:ASP:OD1	2:B:463:ASP:N	2.51	0.43
1:A:535:VAL:HG12	1:A:538:ARG:NH2	2.31	0.43
5:S:69:ILE:HG22	5:S:71:VAL:HG13	2.00	0.43
2:B:177:VAL:O	2:B:181:VAL:HG23	2.19	0.43
2:B:222:ILE:O	2:B:223:LEU:C	2.61	0.43
1:A:470:ILE:HG13	1:A:471:ASN:N	2.32	0.43
2:B:476:GLU:CG	2:B:480:VAL:HG11	2.49	0.42
4:M:324:ILE:HB	4:M:351:ILE:HB	2.02	0.42
2:B:326:VAL:HB	2:B:361:TYR:CZ	2.55	0.42
2:B:198:ASP:C	2:B:200:ASN:N	2.78	0.42
2:B:259:ALA:O	2:B:260:VAL:C	2.63	0.42
3:N:56:PHE:CG	3:N:78:VAL:HG11	2.54	0.42
2:B:217:TRP:O	2:B:221:PHE:CE2	2.73	0.42
1:A:59:VAL:HG21	1:A:82:LEU:CD1	2.50	0.42
1:A:59:VAL:HG21	1:A:82:LEU:HD11	2.02	0.42
1:A:386:ARG:O	1:A:387:GLN:C	2.61	0.42
2:B:555:ILE:HG23	2:B:560:LEU:HB2	2.02	0.42
2:B:211:LEU:HD11	2:B:223:LEU:HD21	2.00	0.41
2:B:233:ASP:HA	2:B:234:ASP:HB2	2.02	0.41
4:M:298:ARG:NH1	4:M:376:ASN:O	2.53	0.41
1:A:245:GLN:HE21	1:A:245:GLN:HA	1.85	0.41
1:A:539:ALA:HB1	1:A:579:ARG:CZ	2.50	0.41
4:M:298:ARG:NH1	4:M:375:THR:O	2.53	0.41
1:A:486:ALA:HB1	1:A:496:LEU:HD21	2.02	0.41
1:A:605:PHE:CZ	2:B:520:ARG:HD3	2.55	0.41
2:B:345:LEU:O	2:B:347:SER:N	2.53	0.41
4:M:163:ARG:O	4:M:209:MET:HE1	2.20	0.41
1:A:40:ILE:HG23	1:A:58:TYR:HB3	2.03	0.41
1:A:58:TYR:OH	6:A:701:IHP:O44	2.30	0.41
1:A:330:ALA:O	1:A:331:CYS:C	2.61	0.41
1:A:360:GLU:CD	1:A:360:GLU:N	2.75	0.41
2:B:41:MET:HG2	2:B:47:VAL:HG21	2.03	0.41
2:B:480:VAL:O	2:B:481:GLN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ASP:OD2	5:S:46:HIS:HA	2.21	0.41
2:B:40:ALA:HB3	2:B:47:VAL:HG11	2.03	0.41
2:B:285:ALA:HB3	2:B:286:PRO:HD3	2.02	0.41
2:B:473:PHE:O	2:B:476:GLU:HB3	2.21	0.41
1:A:506:GLU:OE2	1:A:601:GLU:O	2.38	0.41
1:A:585:ARG:HH12	2:B:539:GLU:C	2.28	0.41
1:A:603:PRO:HG2	2:B:524:TYR:CE2	2.56	0.41
2:B:227:SER:OG	2:B:262:VAL:HG22	2.20	0.41
2:B:262:VAL:C	2:B:264:MET:H	2.29	0.41
3:N:115:ILE:HG13	3:N:124:SER:HB3	2.02	0.41
2:B:292:LEU:N	2:B:292:LEU:CD1	2.84	0.41
4:M:216:MET:HE1	4:M:275:MET:HE1	2.03	0.41
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.91	0.40
2:B:570:LEU:HG	2:B:574:TYR:CE2	2.56	0.40
4:M:376:ASN:C	4:M:376:ASN:HD22	2.30	0.40
2:B:315:GLU:O	2:B:316:ILE:C	2.64	0.40
2:B:326:VAL:HG13	2:B:335:LYS:HG2	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLU:O	2:B:213:GLU:O[4_557]	2.01	0.19

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	599/621 (96%)	542 (90%)	39 (6%)	18 (3%)	3	3
2	B	577/592 (98%)	461 (80%)	86 (15%)	30 (5%)	1	0
3	N	139/446 (31%)	116 (84%)	20 (14%)	3 (2%)	5	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	M	251/446 (56%)	231 (92%)	17 (7%)	3 (1%)	10	14
5	S	140/142 (99%)	133 (95%)	6 (4%)	1 (1%)	18	25
All	All	1706/2247 (76%)	1483 (87%)	168 (10%)	55 (3%)	3	2

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	TYR
1	A	470	ILE
1	A	471	ASN
1	A	474	ASP
1	A	491	ALA
1	A	601	GLU
2	B	179	ASN
2	B	234	ASP
2	B	238	GLN
2	B	250	HIS
2	B	294	GLY
2	B	352	ALA
2	B	462	ALA
3	N	2	ILE
1	A	417	ASP
1	A	590	ALA
2	B	152	ASN
2	B	199	LEU
2	B	222	ILE
2	B	260	VAL
2	B	271	PRO
2	B	312	LYS
2	B	316	ILE
2	B	500	GLN
2	B	552	THR
3	N	27	ASN
1	A	189	THR
1	A	554	GLU
2	B	263	LEU
2	B	277	TYR
2	B	346	ALA
2	B	501	GLU
2	B	550	GLU
4	M	375	THR

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Mol	Chain	Res	Type
4	M	380	LYS
4	M	409	PRO
1	A	419	SER
1	A	602	MET
2	B	9	THR
2	B	99	ASN
2	B	193	ASN
2	B	227	SER
2	B	247	ARG
5	S	63	ALA
1	A	186	GLY
1	A	492	CYS
2	B	454	GLU
2	B	532	THR
1	A	469	VAL
1	A	555	VAL
2	B	256	VAL
1	A	606	PRO
1	A	370	ILE
2	B	289	VAL
3	N	14	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	527/543 (97%)	485 (92%)	42 (8%)	11	16
2	B	516/533 (97%)	447 (87%)	69 (13%)	4	4
3	N	122/398 (31%)	109 (89%)	13 (11%)	6	7
4	M	233/397 (59%)	212 (91%)	21 (9%)	9	12
5	S	131/131 (100%)	125 (95%)	6 (5%)	24	35
All	All	1529/2002 (76%)	1378 (90%)	151 (10%)	7	10

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	47	ASP
1	A	50	LEU
1	A	87	ARG
1	A	103	ASN
1	A	109	ILE
1	A	117	LYS
1	A	161	MET
1	A	165	LYS
1	A	174	ARG
1	A	224	THR
1	A	241	SER
1	A	244	LEU
1	A	245	GLN
1	A	283	CYS
1	A	320	HIS
1	A	339	GLN
1	A	352	SER
1	A	354	CYS
1	A	360	GLU
1	A	388	ARG
1	A	423	GLU
1	A	458	SER
1	A	468	ILE
1	A	469	VAL
1	A	473	ASP
1	A	483	VAL
1	A	493	HIS
1	A	511	ILE
1	A	520	LEU
1	A	528	SER
1	A	535	VAL
1	A	540	LEU
1	A	554	GLU
1	A	555	VAL
1	A	570	LYS
1	A	577	GLN
1	A	584	LEU
1	A	585	ARG
1	A	586	LEU
1	A	591	SER
1	A	608	ARG
2	B	4	SER

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Mol	Chain	Res	Type
2	B	25	GLU
2	B	27	LYS
2	B	61	ASP
2	B	63	LEU
2	B	95	CYS
2	B	124	GLU
2	B	133	GLU
2	B	140	THR
2	B	151	ILE
2	B	155	MET
2	B	158	ASP
2	B	159	GLN
2	B	161	PHE
2	B	163	ASP
2	B	177	VAL
2	B	184	LEU
2	B	199	LEU
2	B	215	THR
2	B	226	LEU
2	B	228	ASN
2	B	238	GLN
2	B	249	SER
2	B	252	ASN
2	B	253	SER
2	B	267	LEU
2	B	269	LEU
2	B	273	ASP
2	B	284	LEU
2	B	286	PRO
2	B	291	LEU
2	B	295	GLU
2	B	298	VAL
2	B	317	LEU
2	B	338	LYS
2	B	339	LEU
2	B	340	ASP
2	B	343	ILE
2	B	347	SER
2	B	348	GLN
2	B	351	ILE
2	B	354	VAL
2	B	359	LYS

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Mol	Chain	Res	Type
2	B	374	VAL
2	B	379	ARG
2	B	383	LYS
2	B	386	GLN
2	B	387	SER
2	B	389	GLU
2	B	406	VAL
2	B	432	LEU
2	B	436	LEU
2	B	457	GLU
2	B	458	ARG
2	B	459	ILE
2	B	463	ASP
2	B	464	GLU
2	B	468	SER
2	B	478	THR
2	B	482	LEU
2	B	494	LYS
2	B	501	GLU
2	B	513	ASP
2	B	529	LEU
2	B	535	VAL
2	B	539	GLU
2	B	567	ILE
2	B	570	LEU
2	B	579	ASN
3	N	6	PHE
3	N	24	ILE
3	N	30	ASP
3	N	43	VAL
3	N	50	ILE
3	N	58	VAL
3	N	59	LYS
3	N	61	SER
3	N	62	ASN
3	N	69	THR
3	N	87	ASP
3	N	116	LEU
3	N	117	ASP
4	M	199	ARG
4	M	221	VAL
4	M	255	SER

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Mol	Chain	Res	Type
4	M	261	ARG
4	M	263	ILE
4	M	281	LYS
4	M	299	THR
4	M	300	LYS
4	M	323	ARG
4	M	331	SER
4	M	335	VAL
4	M	336	ILE
4	M	348	GLU
4	M	361	MET
4	M	364	SER
4	M	376	ASN
4	M	380	LYS
4	M	388	MET
4	M	404	LEU
4	M	405	LYS
4	M	411	LEU
5	S	41	VAL
5	S	54	ASN
5	S	57	ILE
5	S	61	ARG
5	S	116	GLU
5	S	129	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	245	GLN
1	A	495	ASN
1	A	509	ASN
2	B	159	GLN
2	B	202	GLN
2	B	278	ASN
4	M	365	GLN
4	M	376	ASN
5	S	8	GLN
5	S	106	ASN
5	S	139	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	IHP	A	701	-	36,36,36	1.36	4 (11%)	60,60,60	2.62	26 (43%)

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
6	IHP	A	701	-	-	6/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	IHP	P1-O11	3.66	1.65	1.59
6	A	701	IHP	P3-O13	3.18	1.65	1.59
6	A	701	IHP	C2-C1	2.47	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	IHP	P6-O16	2.22	1.63	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	IHP	P3-O13-C3	7.06	142.28	123.43
6	A	701	IHP	O13-C3-C2	7.05	123.75	108.76
6	A	701	IHP	P2-O12-C2	-5.39	109.04	123.43
6	A	701	IHP	C5-C4-C3	4.86	121.08	110.43
6	A	701	IHP	O13-C3-C4	4.85	119.08	108.76
6	A	701	IHP	O15-C5-C4	4.46	118.26	108.76
6	A	701	IHP	P4-O14-C4	-3.96	112.85	123.43
6	A	701	IHP	O44-P4-O34	3.89	122.37	107.80
6	A	701	IHP	O11-C1-C2	3.48	116.16	108.76
6	A	701	IHP	O12-C2-C1	3.46	116.12	108.76
6	A	701	IHP	C6-C1-C2	3.41	117.91	110.43
6	A	701	IHP	C3-C2-C1	3.39	117.88	110.43
6	A	701	IHP	P1-O11-C1	3.10	131.72	123.43
6	A	701	IHP	P5-O15-C5	-3.08	115.20	123.43
6	A	701	IHP	C5-C6-C1	2.83	116.64	110.43
6	A	701	IHP	O16-C6-C1	2.67	114.44	108.76
6	A	701	IHP	O12-C2-C3	2.60	114.28	108.76
6	A	701	IHP	O46-P6-O36	2.51	117.20	107.80
6	A	701	IHP	O11-C1-C6	2.46	114.00	108.76
6	A	701	IHP	O14-C4-C5	2.44	113.96	108.76
6	A	701	IHP	O41-P1-O31	2.37	116.70	107.80
6	A	701	IHP	O41-P1-O11	2.33	114.95	105.85
6	A	701	IHP	O33-P3-O23	2.31	119.84	110.83
6	A	701	IHP	O14-C4-C3	2.16	113.36	108.76
6	A	701	IHP	O33-P3-O13	2.07	113.90	105.85
6	A	701	IHP	O11-P1-O21	-2.02	102.12	109.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

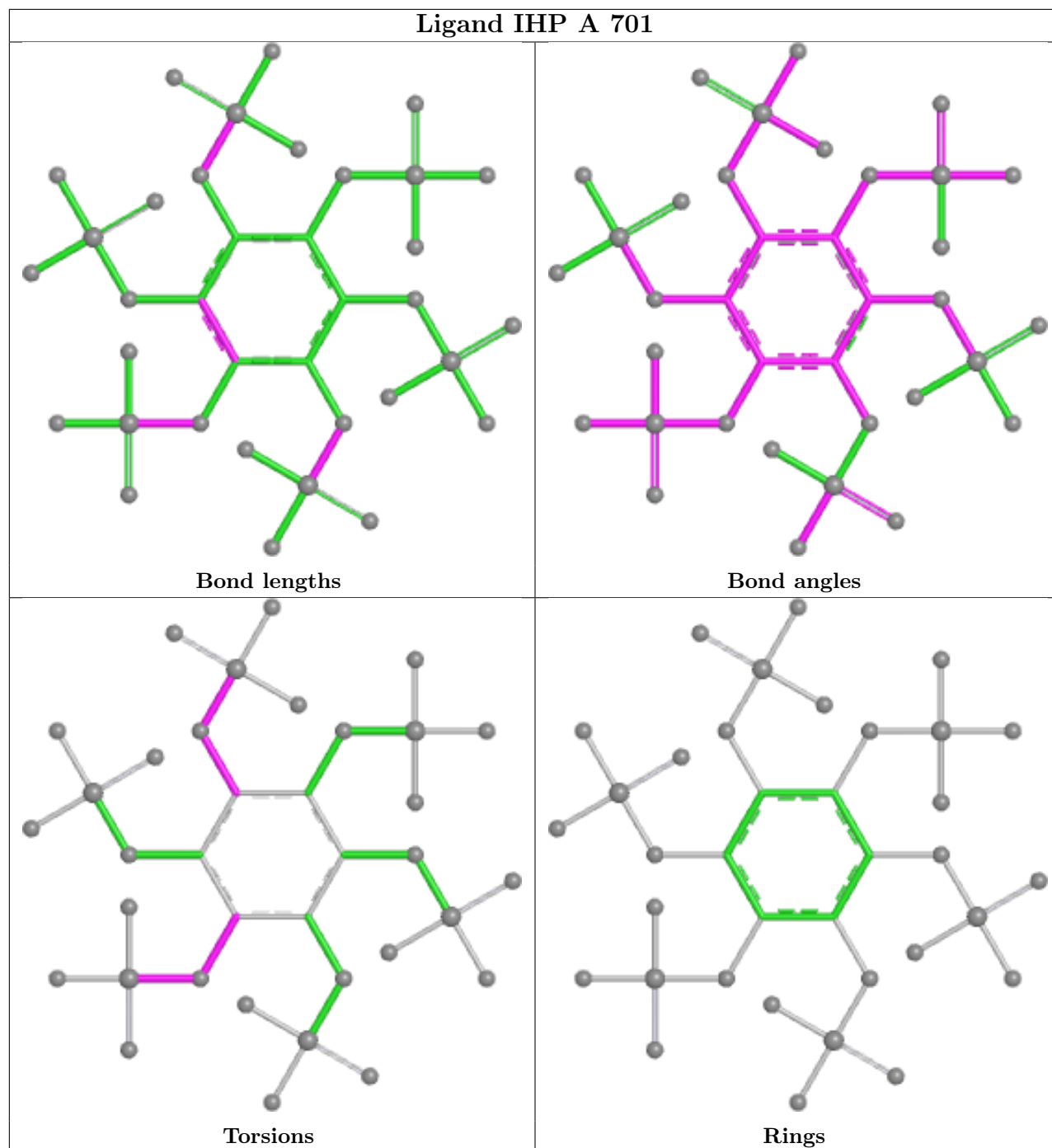
Mol	Chain	Res	Type	Atoms
6	A	701	IHP	C6-C1-O11-P1
6	A	701	IHP	C1-O11-P1-O21
6	A	701	IHP	C2-C1-O11-P1
6	A	701	IHP	C2-C3-O13-P3
6	A	701	IHP	C4-C3-O13-P3
6	A	701	IHP	C3-O13-P3-O23

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	701	IHP	1	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	600/621 (96%)	-0.23	4 (0%) 84 86	29, 53, 85, 123	1 (0%)
2	B	579/592 (97%)	0.74	54 (9%) 14 14	35, 92, 144, 178	0
3	N	141/446 (31%)	0.89	9 (6%) 25 25	60, 91, 122, 146	0
4	M	255/446 (57%)	-0.17	5 (1%) 65 65	22, 49, 89, 169	2 (0%)
5	S	142/142 (100%)	-0.55	0 100 100	28, 40, 65, 92	0
All	All	1717/2247 (76%)	0.17	72 (4%) 40 41	22, 64, 129, 178	3 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	253	SER	8.2
2	B	582	VAL	5.6
2	B	257	LEU	5.4
2	B	270	LEU	4.4
2	B	248	LEU	4.1
3	N	43	VAL	4.1
2	B	85	ILE	3.8
2	B	262	VAL	3.7
2	B	276	TYR	3.4
2	B	256	VAL	3.3
2	B	115	VAL	3.3
2	B	199	LEU	3.2
2	B	263	LEU	3.1
2	B	39	ALA	3.1
2	B	266	PHE	3.0
2	B	84	ALA	3.0
2	B	197	LEU	2.9
4	M	378	LYS	2.9
2	B	98	PRO	2.8
4	M	222	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
3	N	132	PHE	2.7
4	M	159	ILE	2.7
2	B	252	ASN	2.6
2	B	241	CYS	2.6
1	A	608	ARG	2.5
2	B	27	LYS	2.5
3	N	24	ILE	2.5
2	B	226	LEU	2.5
2	B	280	LEU	2.5
2	B	43	VAL	2.5
3	N	44	ARG	2.5
3	N	138	ILE	2.5
2	B	122	LEU	2.5
2	B	215	THR	2.5
2	B	273	ASP	2.4
2	B	222	ILE	2.4
2	B	581	PHE	2.4
1	A	590	ALA	2.4
2	B	285	ALA	2.4
2	B	168	LEU	2.4
2	B	267	LEU	2.4
2	B	227	SER	2.4
2	B	112	CYS	2.3
2	B	290	THR	2.3
3	N	19	VAL	2.3
2	B	250	HIS	2.2
1	A	470	ILE	2.2
2	B	567	ILE	2.2
3	N	126	THR	2.2
2	B	239	SER	2.2
2	B	192	PRO	2.2
2	B	255	VAL	2.2
2	B	436	LEU	2.2
2	B	178	ALA	2.2
2	B	254	ALA	2.2
2	B	259	ALA	2.2
2	B	187	ILE	2.2
2	B	220	ILE	2.2
2	B	174	PRO	2.2
4	M	381	TRP	2.2
1	A	469	VAL	2.1
2	B	169	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	165	LEU	2.1
3	N	111	LEU	2.1
2	B	105	LEU	2.1
2	B	306	ILE	2.1
3	N	115	ILE	2.1
2	B	283	LYS	2.1
2	B	210	ALA	2.0
2	B	302	ALA	2.0
4	M	357	ARG	2.0
2	B	233	ASP	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](#)

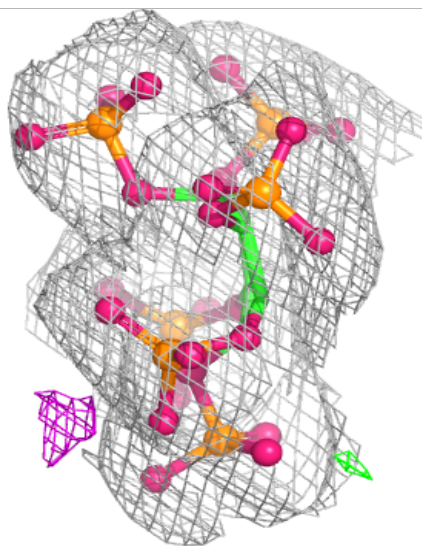
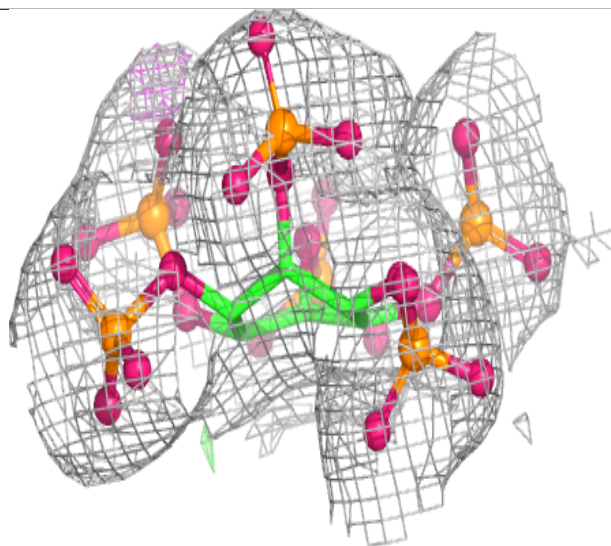
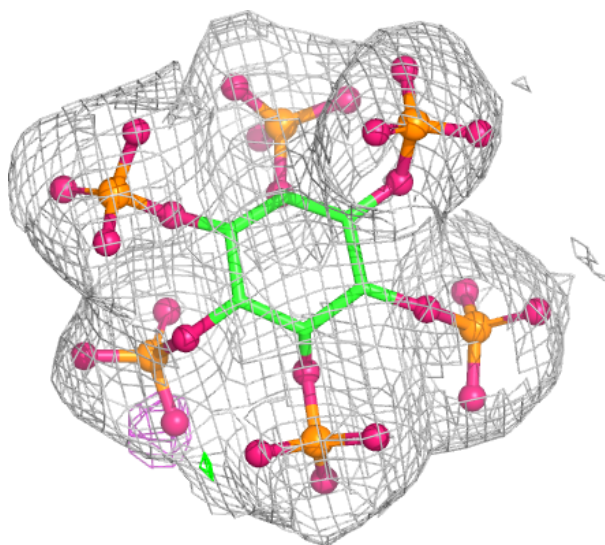
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IHP	A	701	36/36	0.93	0.06	44,71,85,87	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 IHP A 701:

$2mF_o-DF_c$ (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.