Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2020 – 12:05 PM BST

PDB ID	:	6QH5
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 (i) symbol.

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

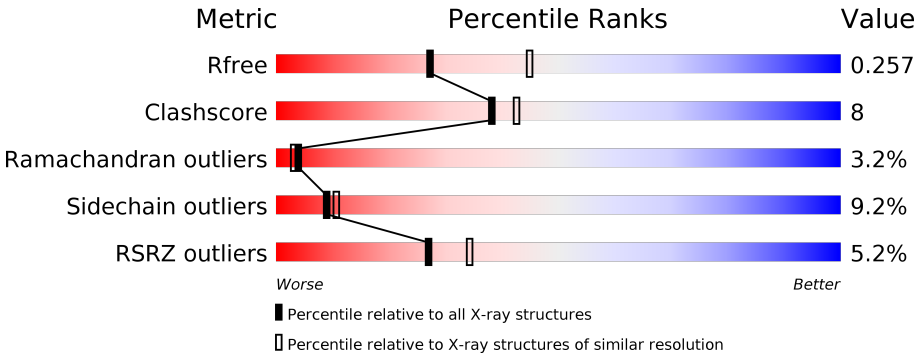
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 on 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 <=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	% 76% 17%
2	B	592	13% 66% 26% 6%
3	N	446	23% 8% 68%
4	M	446	% 46% 10% 43%
5	S	142	80% 17%

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			

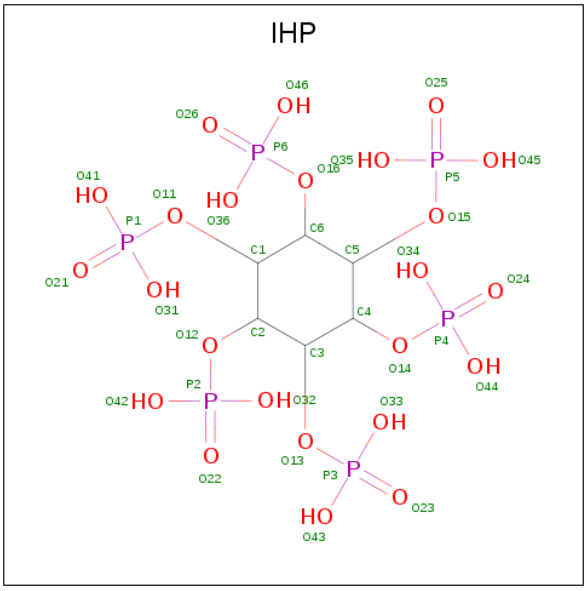
There are 11 discrepancies between the modelled and reference sequences:

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 (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).

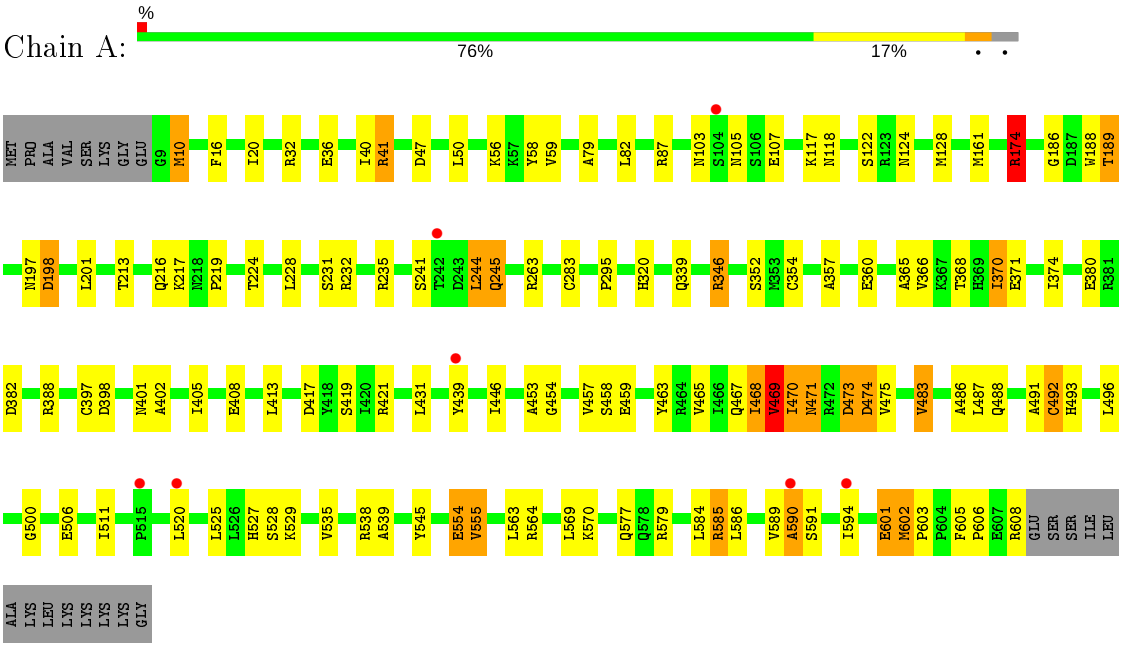


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			36	6	24	6		

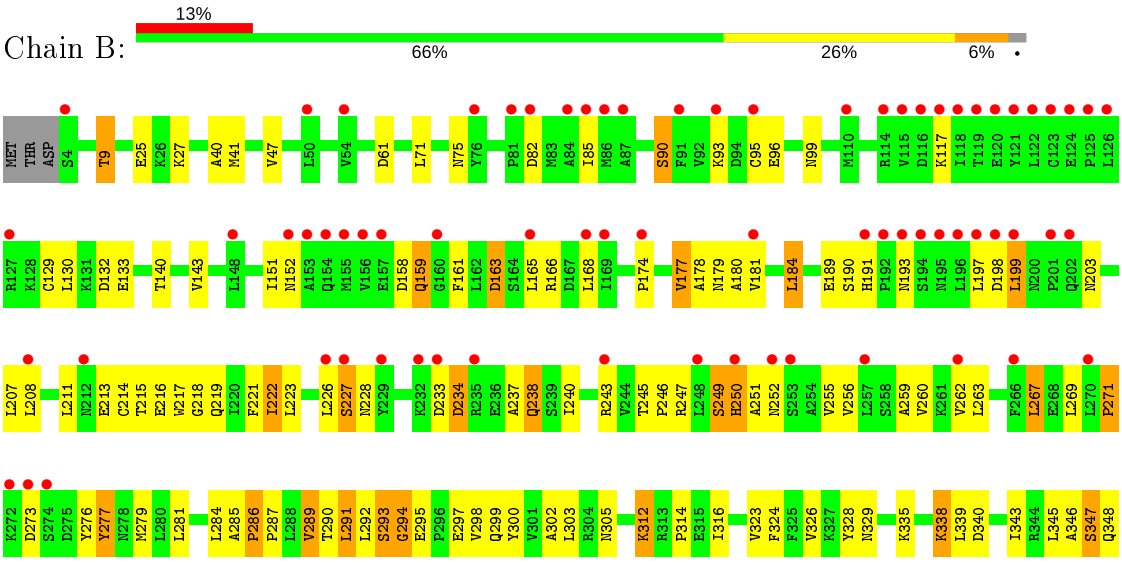
3 Residue-property plots (i)

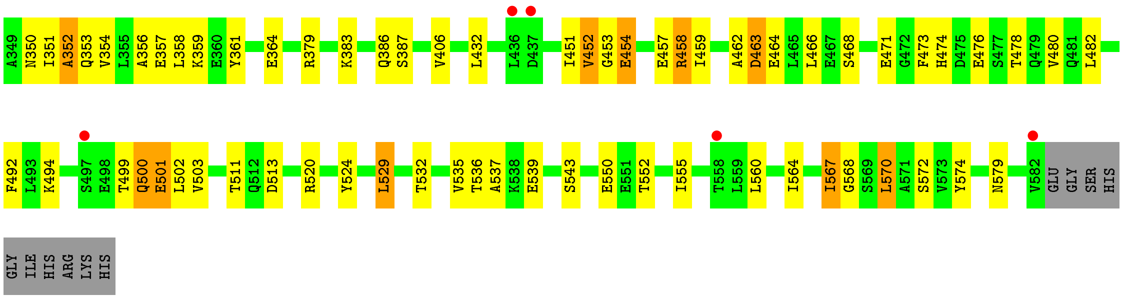
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: AP-2 complex subunit alpha



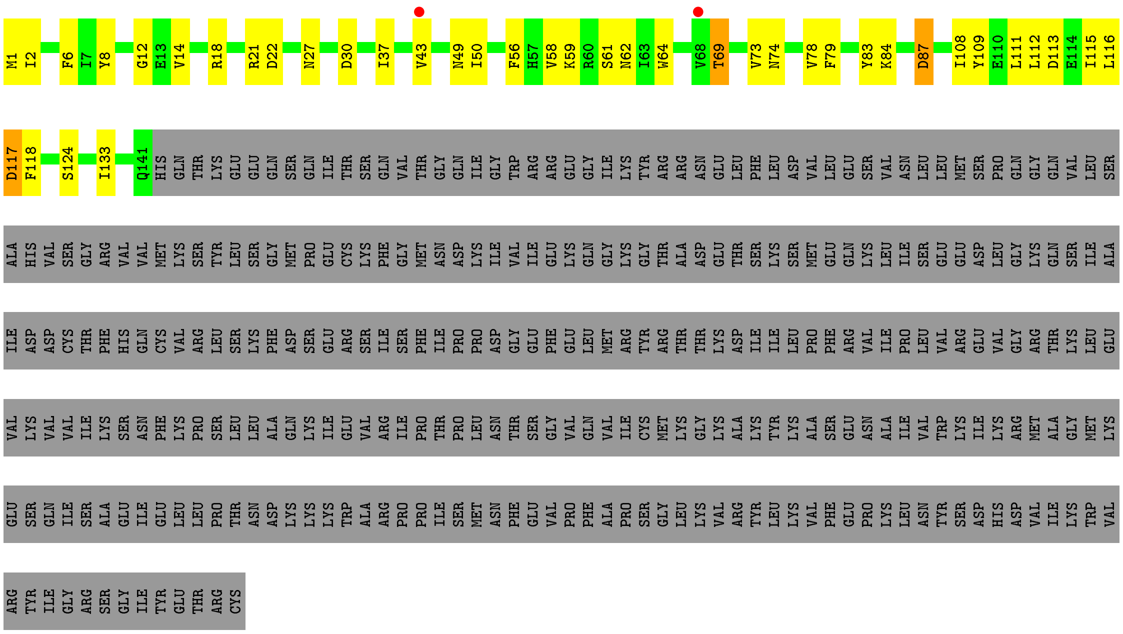
- Molecule 2: AP-2 complex subunit beta





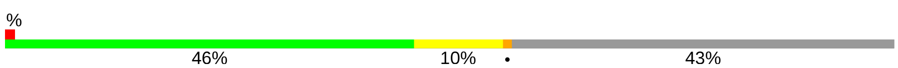
• Molecule 3: AP-2 complex subunit mu

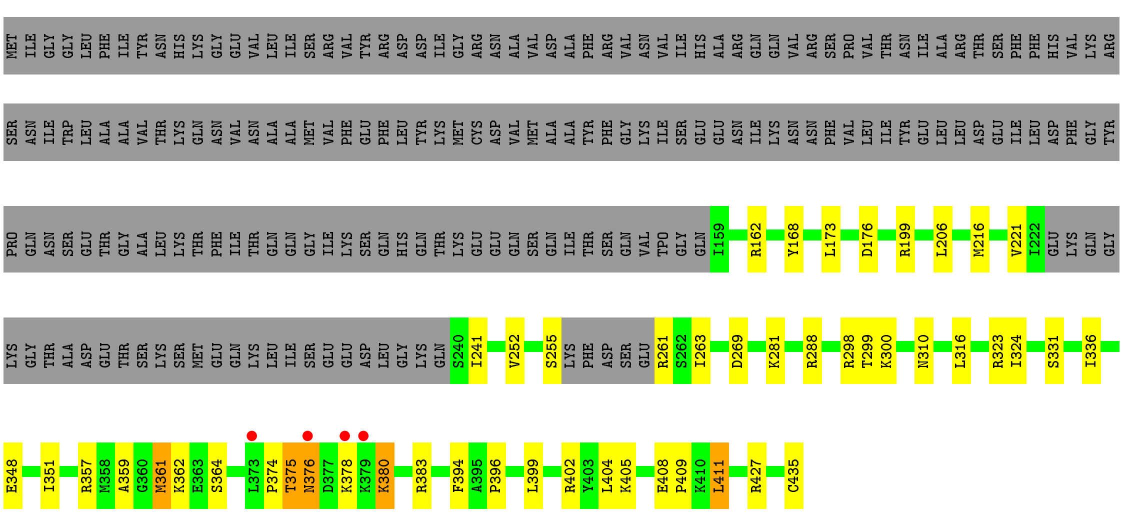
Chain N:



• Molecule 4: AP-2 complex subunit mu

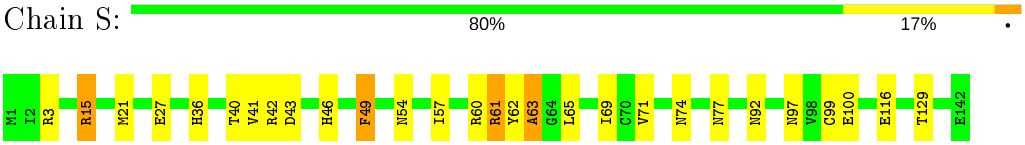
Chain M:





• Molecule 5: AP-2 complex subunit sigma

Chain S:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (4.99%)	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)	0.32 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.74	0/4833	0.88	5/6555 (0.1%)
2	B	0.70	0/4650	0.86	1/6309 (0.0%)
3	N	0.66	0/1160	0.82	0/1565
4	M	0.78	0/2111	0.95	4/2839 (0.1%)
5	S	0.82	0/1224	0.96	2/1650 (0.1%)
All	All	0.73	0/13978	0.89	12/18918 (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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	174	ARG	NE-CZ-NH1	8.18	124.39	120.30
4	M	288	ARG	NE-CZ-NH1	7.94	124.27	120.30
4	M	288	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	174	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	346	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	198	ASP	CB-CG-OD2	-5.91	112.98	118.30
5	S	43	ASP	CB-CG-OD1	5.72	123.44	118.30
2	B	458	ARG	NE-CZ-NH1	5.69	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	398	ASP	CB-CG-OD2	-5.57	113.28	118.30
5	S	42	ARG	NE-CZ-NH1	5.52	123.06	120.30
4	M	427	ARG	NE-CZ-NH1	5.49	123.05	120.30
4	M	402	ARG	NE-CZ-NH1	5.04	122.82	120.30

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
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	74	0
2	B	4578	0	4686	92	1
3	N	1138	0	1143	22	0
4	M	2070	0	2162	17	0
5	S	1200	0	1193	26	0
6	A	36	0	6	1	0
All	All	13770	0	14032	212	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 8.

All (212) 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	0.91
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: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
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:16:PHE:CZ	1:A:20:ILE:HD11	2.32	0.65
5:S:61:ARG:NH1	5:S:62:TYR:N	2.46	0.64
5:S:61:ARG:HE	5:S:63:ALA:C	2.02	0.63
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
1:A:360:GLU:CD	1:A:360:GLU:H	2.02	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:61:ARG:HA	5:S:61:ARG:NH1	2.16	0.61
2:B:276:TYR:O	2:B:279:MET:N	2.33	0.60
1:A:473:ASP:OD1	1:A:473:ASP:C	2.41	0.59
4:M:310[A]:ASN:CG	4:M:310[A]:ASN:O	2.37	0.59
1:A:32:ARG:HH12	1:A:36:GLU:HG2	1.68	0.59
1:A:10:MET:CE	1:A:56:LYS:HG2	2.33	0.58
2:B:297:GLU:HB3	3:N:79:PHE:CE1	2.39	0.58
2:B:237:ALA:HA	2:B:240:ILE:HD12	1.85	0.57
5:S:15:ARG:HH12	5:S:100:GLU:CD	2.09	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:111:LEU:HD23	3:N:133:ILE:CD1	2.35	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
1:A:401:ASN:O	1:A:402:ALA:C	2.46	0.54
2:B:453:GLY:HA3	2:B:454:GLU:CB	2.38	0.54
2:B:174:PRO:O	2:B:178:ALA:HB3	2.08	0.54
2:B:299:GLN:O	2:B:300:TYR:C	2.47	0.54
2:B:287:PRO:O	2:B:291:LEU:HD13	2.07	0.53
1:A:473:ASP:C	1:A:475:VAL:H	2.11	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
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: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
5:S:49:PHE:CE2	5:S:77:ASN:HB3	2.45	0.52
1:A:585:ARG:CB	1:A:585:ARG:CZ	2.88	0.51
5:S:61:ARG:CZ	5:S:65:LEU:N	2.74	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
1:A:357:ALA:HB2	1:A:366:VAL:HG11	1.93	0.51
2:B:474:HIS:C	2:B:476:GLU:H	2.14	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
2:B:492:PHE:HD1	2:B:499:THR:HG1	1.58	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
1:A:10:MET:HE2	1:A:56:LYS:HE3	1.94	0.50
2:B:285:ALA:HB3	2:B:286:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:299:GLN:O	2:B:302:ALA:N	2.46	0.49
4:M:252:VAL:HG13	4:M:263:ILE:HG23	1.95	0.48
1:A:10:MET:CE	1:A:56:LYS:HE3	2.43	0.48
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
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
1:A:263:ARG:NH2	5:S:74:ASN:O	2.47	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
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:217:LYS:C	1:A:219:PRO:HD3	2.35	0.47
2:B:511:THR:HG23	2:B:524:TYR:CE1	2.48	0.47
5:S:61:ARG:NH2	5:S:65:LEU:N	2.57	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
1:A:469:VAL:O	1:A:470:ILE:HG23	2.15	0.47
4:M:173:LEU:C	4:M:173:LEU:HD12	2.36	0.47
1:A:589:VAL:HG12	1:A:590:ALA:N	2.29	0.46
1:A:585:ARG:NH1	2:B:539:GLU:O	2.47	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
5:S:92:ASN:OD1	5:S:97:ASN:HA	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:THR:HG21	5:S:99:CYS:HB3	1.97	0.46
5:S:61:ARG:CZ	5:S:62:TYR:C	2.84	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
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:364:GLU:OE1	2:B:364:GLU:HA	2.17	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: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: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
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:527:HIS:HA	1:A:545:TYR:OH	2.18	0.44
1:A:506:GLU:OE2	1:A:602:MET:HB2	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:470:ILE:HD13	1:A:605:PHE:H	1.83	0.43
1:A:470:ILE:HG13	1:A:471:ASN:N	2.32	0.43
5:S:3:ARG:HB3	5:S:21:MET:CE	2.47	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
2:B:328:TYR:CE1	2:B:329:ASN:HB3	2.53	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:563:LEU:O	1:A:569:LEU:HG	2.19	0.43
2:B:303:LEU:HD12	2:B:303:LEU:N	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:350:ASN:C	2:B:352:ALA:N	2.72	0.42
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
4:M:361:MET:CE	4:M:361:MET:HA	2.50	0.42
3:N:56:PHE:CG	3:N:78:VAL:HG11	2.54	0.42
2:B:474:HIS:C	2:B:476:GLU:N	2.72	0.42
5:S:3:ARG:HB3	5:S:21:MET:HE2	2.02	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
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:188:TRP:O	1:A:189:THR:C	2.59	0.41
1:A:245:GLN:HA	1:A:245:GLN:HE21	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
2:B:345:LEU:O	2:B:347:SER:N	2.53	0.41
1:A:605:PHE:CZ	2:B:520:ARG:HD3	2.55	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
2:B:41:MET:HG2	2:B:47:VAL:HG21	2.03	0.41
1:A:382:ASP:OD2	5:S:46:HIS:HA	2.21	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
2:B:40:ALA:HB3	2:B:47:VAL:HG11	2.03	0.41
1:A:506:GLU:OE2	1:A:601:GLU:O	2.38	0.41
2:B:227:SER:OG	2:B:262:VAL:HG22	2.20	0.41
1:A:603:PRO:HG2	2:B:524:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:S:99:CYS:O	5:S:100:GLU:C	2.60	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%)	4 4
2	B	577/592 (98%)	461 (80%)	86 (15%)	30 (5%)	2 1
3	N	139/446 (31%)	116 (84%)	20 (14%)	3 (2%)	6 7
4	M	251/446 (56%)	231 (92%)	17 (7%)	3 (1%)	13 17
5	S	140/142 (99%)	133 (95%)	6 (4%)	1 (1%)	22 29
All	All	1706/2247 (76%)	1483 (87%)	168 (10%)	55 (3%)	4 3

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	TYR
1	A	470	ILE
1	A	471	ASN

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	527/543 (97%)	488 (93%)	39 (7%)	13 18
2	B	516/533 (97%)	455 (88%)	61 (12%)	5 5
3	N	122/398 (31%)	109 (89%)	13 (11%)	6 7
4	M	233/397 (59%)	214 (92%)	19 (8%)	11 14
5	S	131/131 (100%)	122 (93%)	9 (7%)	15 19
All	All	1529/2002 (76%)	1388 (91%)	141 (9%)	9 11

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	41	ARG
1	A	47	ASP
1	A	50	LEU
1	A	87	ARG
1	A	103	ASN
1	A	117	LYS
1	A	161	MET
1	A	174	ARG

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Mol	Chain	Res	Type
1	A	224	THR
1	A	241	SER
1	A	244	LEU
1	A	245	GLN
1	A	283	CYS
1	A	295	PRO
1	A	320	HIS
1	A	339	GLN
1	A	352	SER
1	A	354	CYS
1	A	388	ARG
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	554	GLU
1	A	555	VAL
1	A	564	ARG
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	25	GLU
2	B	27	LYS
2	B	61	ASP
2	B	90	SER
2	B	95	CYS
2	B	96	GLU
2	B	133	GLU
2	B	140	THR
2	B	151	ILE
2	B	158	ASP
2	B	159	GLN
2	B	161	PHE

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Mol	Chain	Res	Type
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	267	LEU
2	B	269	LEU
2	B	273	ASP
2	B	284	LEU
2	B	286	PRO
2	B	291	LEU
2	B	293	SER
2	B	298	VAL
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	359	LYS
2	B	379	ARG
2	B	383	LYS
2	B	386	GLN
2	B	387	SER
2	B	406	VAL
2	B	432	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	471	GLU
2	B	478	THR
2	B	482	LEU
2	B	494	LYS

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Mol	Chain	Res	Type
2	B	501	GLU
2	B	513	ASP
2	B	529	LEU
2	B	535	VAL
2	B	567	ILE
2	B	570	LEU
2	B	579	ASN
3	N	6	PHE
3	N	22	ASP
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	176	ASP
4	M	199	ARG
4	M	221	VAL
4	M	255	SER
4	M	261	ARG
4	M	281	LYS
4	M	299	THR
4	M	300	LYS
4	M	323	ARG
4	M	331	SER
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	404	LEU
4	M	405	LYS
4	M	411	LEU
5	S	15	ARG
5	S	41	VAL
5	S	49	PHE

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Mol	Chain	Res	Type
5	S	54	ASN
5	S	57	ILE
5	S	60	ARG
5	S	61	ARG
5	S	116	GLU
5	S	129	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	245	GLN
1	A	550	ASN
1	A	568	GLN
2	B	24	ASN
2	B	200	ASN
2	B	307	ASN
2	B	579	ASN
4	M	376	ASN
5	S	8	GLN

5.3.3 RNA (i)

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)

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	1.33	4 (11%)	54,60,60	2.21	17 (31%)

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	-	-	7/30/54/54	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	3.51	1.65	1.59
6	A	701	IHP	P3-O13	3.07	1.65	1.59
6	A	701	IHP	C2-C1	2.45	1.57	1.52
6	A	701	IHP	P6-O16	2.17	1.63	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	701	IHP	O13-C3-C2	6.39	123.75	108.69
6	A	701	IHP	C5-C4-C3	4.87	121.08	110.41
6	A	701	IHP	O13-C3-C4	4.41	119.08	108.69
6	A	701	IHP	O15-C5-C4	4.06	118.26	108.69
6	A	701	IHP	O44-P4-O34	3.85	122.37	107.64
6	A	701	IHP	C6-C1-C2	3.42	117.91	110.41
6	A	701	IHP	C3-C2-C1	3.41	117.88	110.41
6	A	701	IHP	O11-C1-C2	3.17	116.16	108.69
6	A	701	IHP	O12-C2-C1	3.15	116.12	108.69
6	A	701	IHP	C5-C6-C1	2.84	116.64	110.41
6	A	701	IHP	O46-P6-O36	2.50	117.20	107.64
6	A	701	IHP	O16-C6-C1	2.44	114.44	108.69
6	A	701	IHP	O12-C2-C3	2.37	114.28	108.69
6	A	701	IHP	O41-P1-O31	2.37	116.70	107.64
6	A	701	IHP	O33-P3-O23	2.34	119.84	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	701	IHP	O11-C1-C6	2.25	114.00	108.69
6	A	701	IHP	O14-C4-C5	2.24	113.96	108.69

There are no chirality outliers.

All (7) 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	C3-O13-P3-O23
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-O43

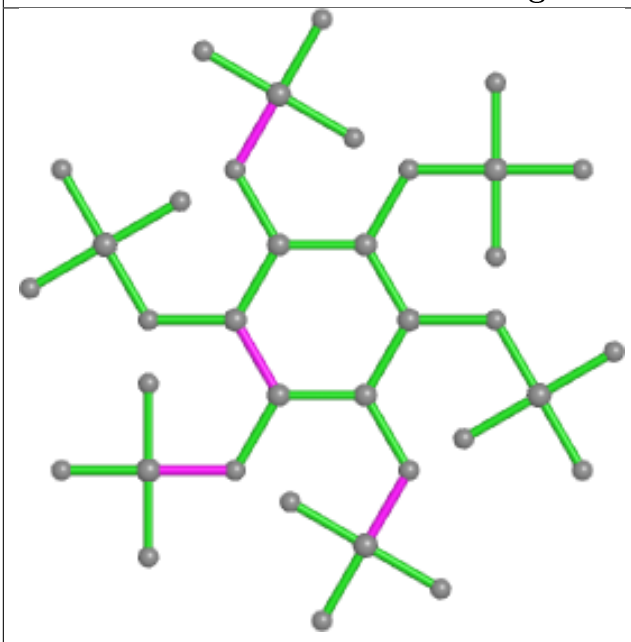
There are no ring outliers.

1 monomer is involved in 1 short contact:

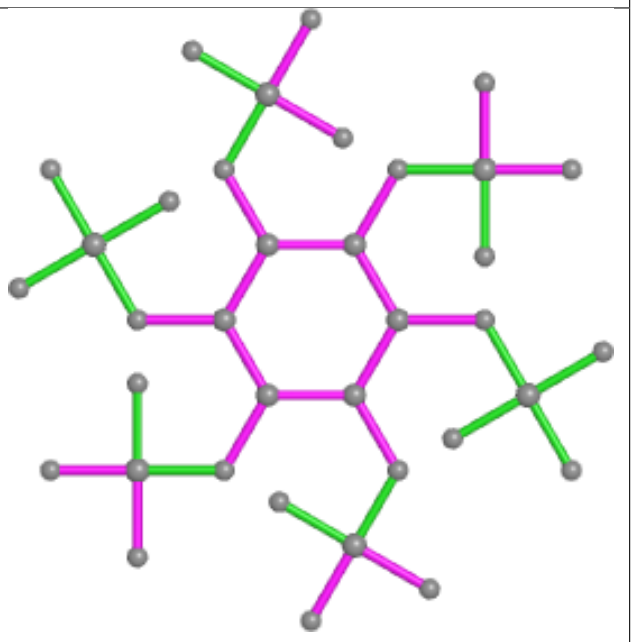
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	701	IHP	1	0

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 then 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.

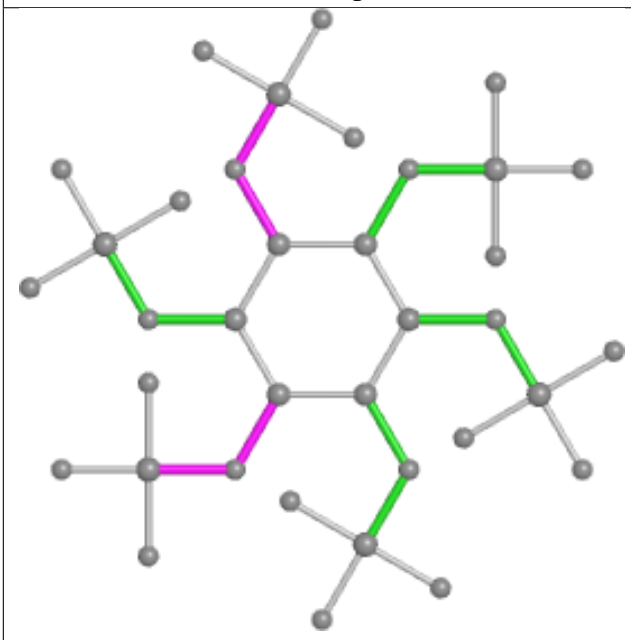
Ligand IHP A 701



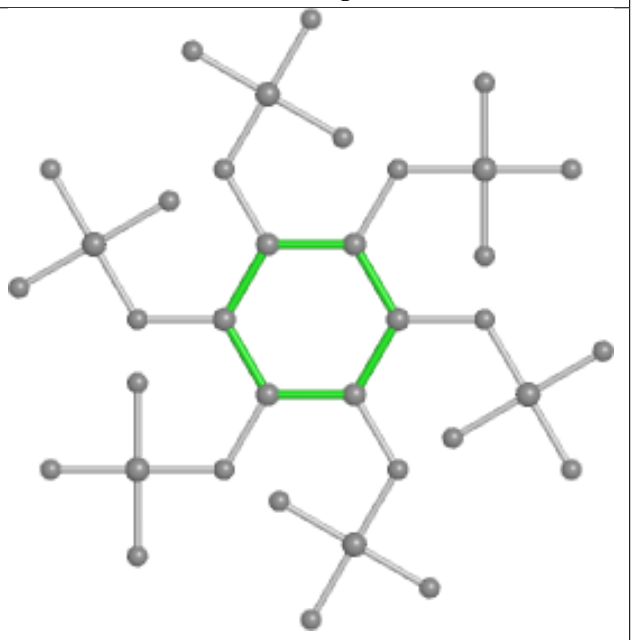
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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%)	-0.19	7 (1%) 79 84	29, 53, 85, 123	0
2	B	579/592 (97%)	0.71	77 (13%) 3 4	35, 92, 144, 178	0
3	N	141/446 (31%)	0.38	2 (1%) 75 81	60, 91, 122, 146	0
4	M	255/446 (57%)	-0.02	4 (1%) 72 78	29, 50, 89, 169	0
5	S	142/142 (100%)	-0.28	0 100 100	28, 40, 65, 92	0
All	All	1717/2247 (76%)	0.18	90 (5%) 27 34	28, 64, 129, 178	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	273	ASP	15.7
2	B	233	ASP	8.1
2	B	253	SER	7.5
2	B	115	VAL	7.2
2	B	153	ALA	7.1
1	A	590	ALA	6.8
2	B	155	MET	6.6
2	B	121	TYR	6.6
2	B	229	TYR	6.0
2	B	148	LEU	5.7
2	B	274	SER	5.7
2	B	119	THR	5.5
2	B	156	VAL	5.5
2	B	257	LEU	5.2
2	B	4	SER	4.9
2	B	122	LEU	4.9
2	B	582	VAL	4.9
2	B	194	SER	4.9
2	B	227	SER	4.9
2	B	85	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	154	GLN	4.4
2	B	262	VAL	4.3
2	B	232	LYS	4.2
2	B	212	ASN	4.1
2	B	86	MET	4.1
2	B	197	LEU	4.0
2	B	127	ARG	4.0
2	B	196	LEU	3.9
2	B	169	ILE	3.8
2	B	117	LYS	3.7
2	B	84	ALA	3.7
2	B	168	LEU	3.7
2	B	436	LEU	3.7
2	B	116	ASP	3.7
2	B	252	ASN	3.6
2	B	152	ASN	3.6
2	B	192	PRO	3.4
2	B	235	ARG	3.3
2	B	76	TYR	3.3
2	B	195	ASN	3.2
2	B	87	ALA	3.1
3	N	43	VAL	3.1
2	B	125	PRO	3.1
2	B	81	PRO	3.0
4	M	378	LYS	3.0
2	B	202	GLN	3.0
2	B	118	ILE	3.0
2	B	208	LEU	3.0
2	B	193	ASN	3.0
1	A	520	LEU	2.9
2	B	126	LEU	2.9
4	M	376	ASN	2.9
1	A	439	TYR	2.9
2	B	201	PRO	2.9
2	B	272	LYS	2.9
2	B	120	GLU	2.8
2	B	124	GLU	2.8
2	B	110	MET	2.8
2	B	181	VAL	2.8
2	B	191	HIS	2.8
3	N	68	VAL	2.7
2	B	95	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	123	CYS	2.7
2	B	248	LEU	2.7
2	B	174	PRO	2.7
2	B	160	GLY	2.6
2	B	437	ASP	2.6
2	B	250	HIS	2.6
4	M	373	LEU	2.5
2	B	82	ASP	2.5
2	B	91	PHE	2.5
2	B	165	LEU	2.5
2	B	199	LEU	2.5
4	M	379	LYS	2.5
1	A	594	ILE	2.4
2	B	114	ARG	2.4
2	B	270	LEU	2.4
2	B	54	VAL	2.3
2	B	558	THR	2.3
1	A	515	PRO	2.3
1	A	242	THR	2.2
2	B	157	GLU	2.2
2	B	226	LEU	2.2
1	A	104	SER	2.2
2	B	497	SER	2.2
2	B	243	ARG	2.1
2	B	198	ASP	2.1
2	B	93	LYS	2.1
2	B	266	PHE	2.1
2	B	50	LEU	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 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,

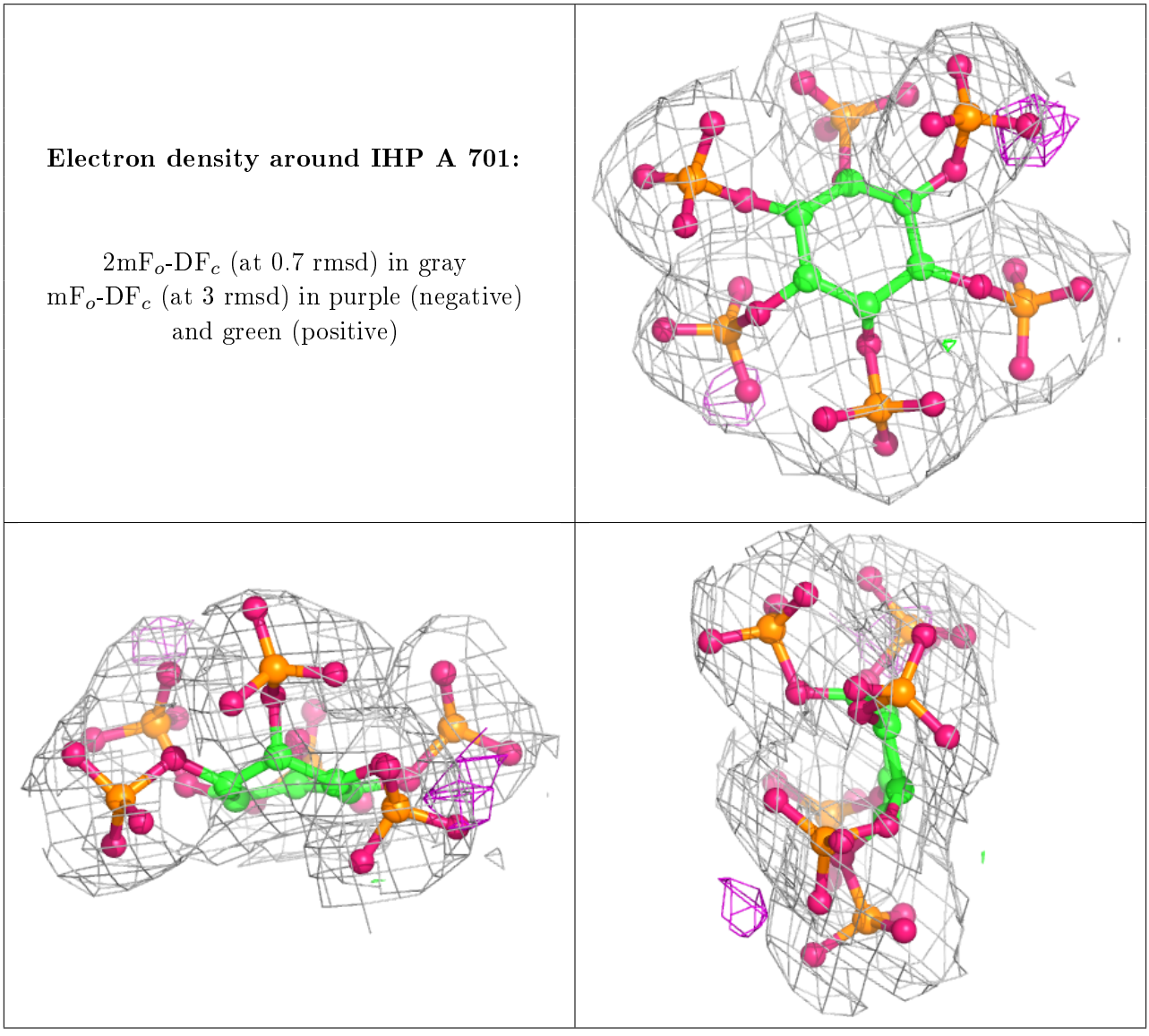
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	IHP	A	701	36/36	0.96	0.09	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

There are no such residues in this entry.