



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:58 PM UTC

PDB ID : 7W5O / pdb_00007w5o
Title : Crystal structure of ERK2 with an allosteric inhibitor
Authors : Yoshida, M.; Kinoshita, T.
Deposited on : 2021-11-30
Resolution : 2.35 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

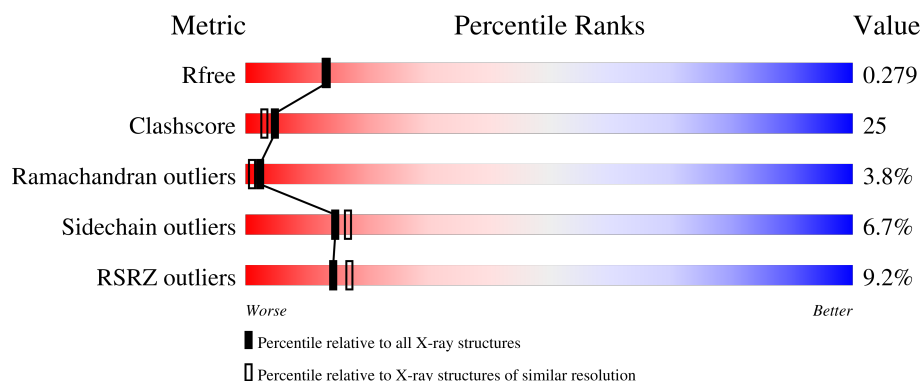
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	368	
1	B	368	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MLA	A	406	-	X	-	-
3	MLA	B	603	-	X	-	-
3	MLA	B	604	-	X	-	-
7	TAR	B	602	-	X	-	-
8	6GI	B	606	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6067 atoms, of which 94 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.

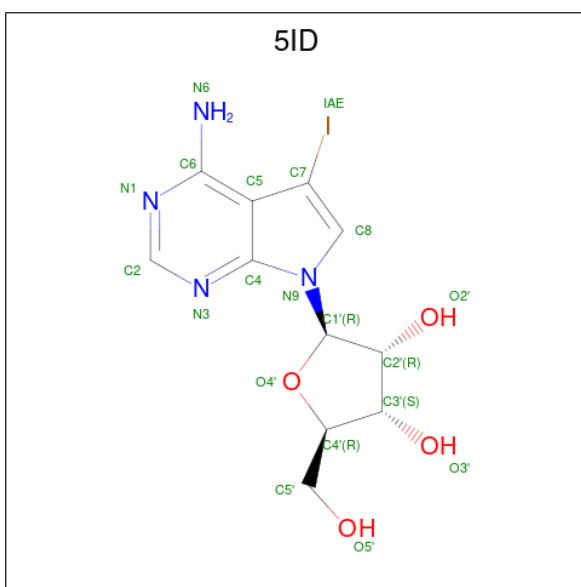
- Molecule 1 is a protein called Mitogen-activated protein kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	P	S	0	0	0
			2868	1838	490	524	1	15			
1	B	346	Total	C	N	O	P	S	0	0	0
			2831	1815	483	517	1	15			

There are 16 discrepancies between the modelled and reference sequences:

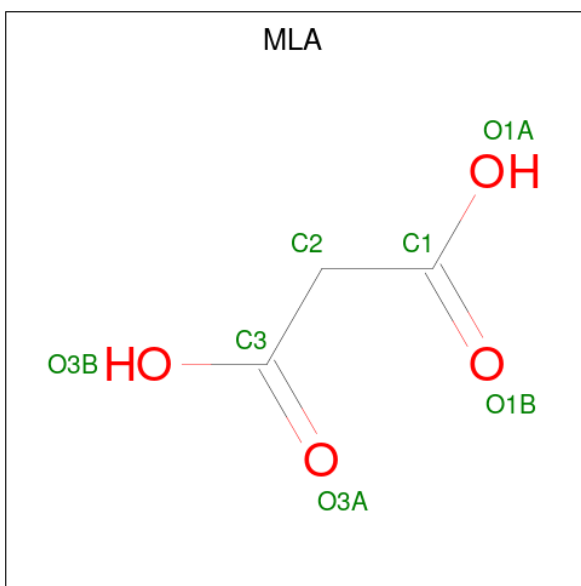
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P28482
A	-6	ASP	-	expression tag	UNP P28482
A	-5	LEU	-	expression tag	UNP P28482
A	-4	GLY	-	expression tag	UNP P28482
A	-3	SER	-	expression tag	UNP P28482
A	-2	ASP	-	expression tag	UNP P28482
A	-1	GLU	-	expression tag	UNP P28482
A	0	LEU	-	expression tag	UNP P28482
B	-7	GLY	-	expression tag	UNP P28482
B	-6	ASP	-	expression tag	UNP P28482
B	-5	LEU	-	expression tag	UNP P28482
B	-4	GLY	-	expression tag	UNP P28482
B	-3	SER	-	expression tag	UNP P28482
B	-2	ASP	-	expression tag	UNP P28482
B	-1	GLU	-	expression tag	UNP P28482
B	0	LEU	-	expression tag	UNP P28482

- Molecule 2 is (2R,3R,4S,5R)-2-(4-AMINO-5-iodo-7H-PYRROLO[2,3-D]PYRIMIDIN-7-YL)-5-(HYDROXYMETHYL)TETRAHYDROFURAN-3,4-DIOL (CCD ID: 5ID) (formula: C₁₁H₁₃IN₄O₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	I	N	O	0	0
			33	11	13	1	4	4		

- Molecule 3 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



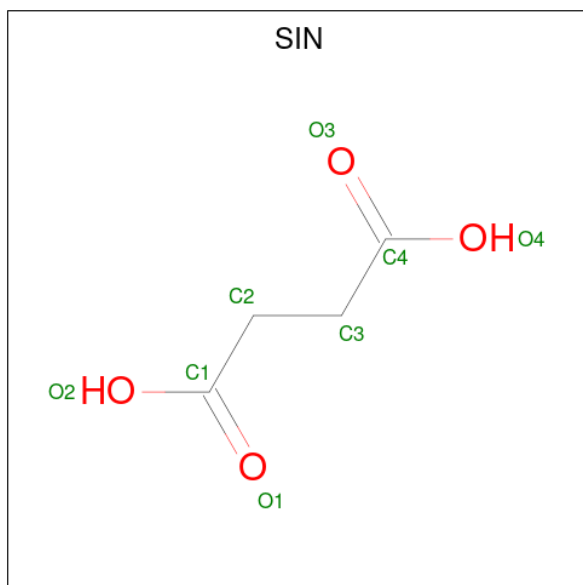
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			9	3	2	4		
3	A	1	Total	C	H	O	0	0
			9	3	2	4		
3	A	1	Total	C	H	O	0	0
			9	3	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			9	3	2	4		
3	B	1	Total	C	H	O	0	0
			9	3	2	4		
3	B	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 4 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).

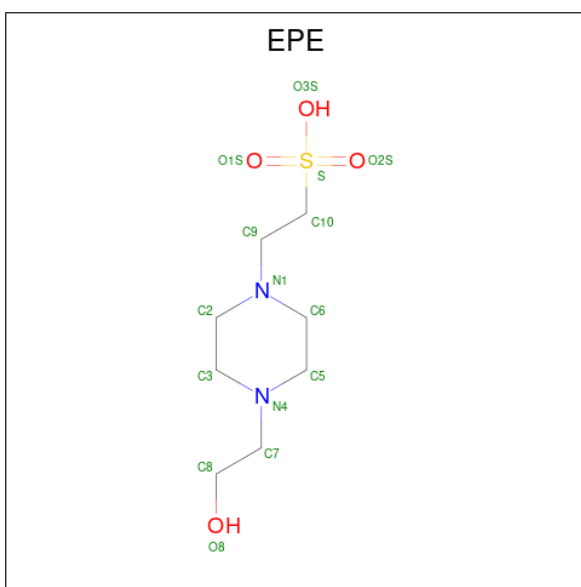


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			12	4	4	4		
4	A	1	Total	C	H	O	0	0
			12	4	4	4		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

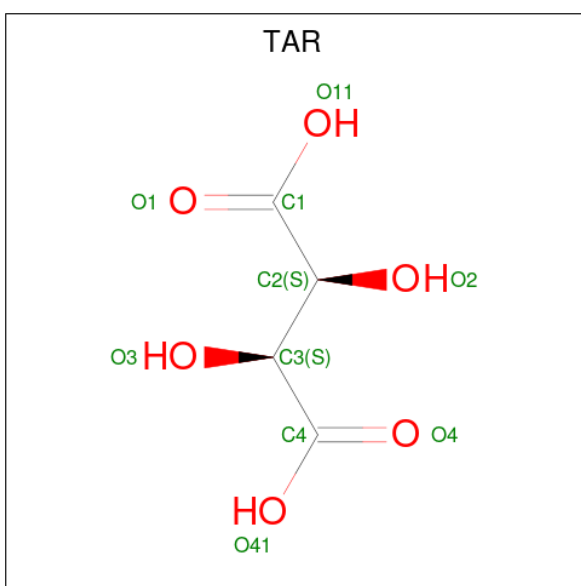
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
6	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

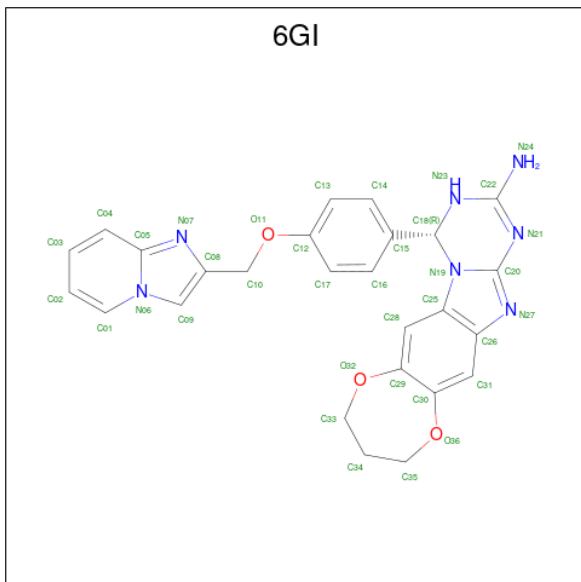
- Molecule 7 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			14	4	4	6		

- Molecule 8 is 13-[4-(Imidazo[1,2-a]pyridin-2-yl)methoxy]phenyl]-4,8-dioxa-12,14,16,18-tet

raazatetracyclo[9.7.0.0[^]{3,9}.0[^]{12,17}]octadeca-1(11),2,9,15,17-pentaen-15-amine (CCD ID: 6GI) (formula: C₂₆H₂₃N₇O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	0	0
			59	26	23	7	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	71	Total	O	0	0
			71	71		
9	B	48	Total	O	0	0
			48	48		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.81Å 82.81Å 274.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 2.35 49.32 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.32-2.35) 100.0 (49.32-2.35)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.225 , 0.279 0.226 , 0.279	Depositor DCC
R_{free} test set	2000 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6067	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, EPE, SIN, 6GI, TAR, 5ID, MLA, NEP

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	0.36	0/2922	0.53	0/3956
1	B	0.37	0/2883	0.58	0/3905
All	All	0.37	0/5805	0.56	0/7861

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	ARG	Sidechain
1	B	332	ASP	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	2868	0	2861	134	0
1	B	2831	0	2826	160	0
2	A	20	13	12	3	0
3	A	21	6	6	2	0
3	B	21	6	6	3	0
4	A	16	8	8	0	0
5	A	1	0	0	0	0
6	A	15	17	17	0	0
6	B	15	17	17	4	0
7	B	10	4	4	3	0
8	B	36	23	0	7	0
9	A	71	0	0	5	0
9	B	48	0	0	2	0
All	All	5973	94	5757	295	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (295) 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)
8:B:606:6GI:N23	8:B:606:6GI:C18	1.71	1.53
2:A:401:5ID:O4'	2:A:401:5ID:C1'	1.65	1.23
1:B:315:GLN:HG3	9:B:718:HOH:O	1.57	1.03
1:B:91:ARG:HH11	1:B:351:THR:HG23	1.21	1.02
1:B:78:PHE:O	1:B:79:ARG:HD3	1.64	0.96
1:B:297:ASN:HB3	1:B:300:LYS:HE3	1.52	0.91
1:A:137:LEU:HA	1:A:140:ILE:HD12	1.55	0.89
1:B:297:ASN:CB	1:B:300:LYS:HE3	2.03	0.89
1:A:335:LEU:HA	1:A:338:LEU:HD13	1.56	0.87
1:A:215:GLY:HA2	1:A:293:MET:HE3	1.55	0.86
1:B:91:ARG:NH1	1:B:351:THR:HG23	1.91	0.84
1:B:347:ILE:O	1:B:351:THR:HG22	1.78	0.83
1:A:331:PHE:CE1	1:A:334:GLU:HG2	2.15	0.82
1:B:24:ARG:NH1	1:B:44:ASP:OD2	2.14	0.81
1:B:148:ARG:HD3	1:B:170:LEU:O	1.80	0.81
1:A:297:ASN:HB3	1:A:300:LYS:HG2	1.63	0.80
1:A:262:ASN:OD1	1:A:263:TYR:N	2.14	0.79
1:B:30:TYR:HA	1:B:40:CYS:SG	2.23	0.79
1:A:89:ILE:HG21	1:A:351:THR:HG22	1.64	0.78
1:B:274:PRO:HD2	1:B:277:ARG:HG3	1.64	0.78
1:B:297:ASN:HB3	1:B:300:LYS:HG2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASP:OD1	1:A:178:HIS:HB2	1.84	0.77
1:A:62:GLN:HB2	1:A:340:LYS:HB3	1.67	0.76
1:A:229:PRO:HD2	1:A:239:HIS:CD2	2.21	0.76
1:A:30:TYR:HD2	1:A:38:MET:HE3	1.50	0.75
1:A:267:LEU:HD13	1:A:267:LEU:O	1.86	0.75
1:B:333:MET:HE1	1:B:346:LEU:HD21	1.67	0.75
1:A:257:ASN:OD1	1:A:260:ALA:N	2.20	0.75
1:B:179:ASP:HB3	1:B:203:LYS:HD3	1.69	0.75
1:B:94:THR:HG22	1:B:97:GLN:HE22	1.52	0.75
1:B:94:THR:HA	1:B:348:PHE:CZ	2.22	0.74
1:B:42:ALA:O	1:B:50:ARG:HG2	1.87	0.74
1:B:183:PHE:HZ	1:B:257:ASN:HB2	1.51	0.74
1:B:179:ASP:O	1:B:203:LYS:NZ	2.17	0.74
1:A:81:GLU:HG2	1:A:135:ARG:HH12	1.53	0.72
1:A:111:ASP:OD2	2:A:401:5ID:O3'	2.08	0.72
1:B:88:ASP:HA	1:B:354:PHE:CE1	2.25	0.72
1:A:178:HIS:O	1:A:178:HIS:ND1	2.22	0.72
1:A:175:ASP:HB3	1:A:178:HIS:HB3	1.72	0.71
1:B:88:ASP:HB3	1:B:104:VAL:HG22	1.72	0.71
1:A:350:GLU:OE2	9:A:501:HOH:O	2.07	0.71
1:B:199:MET:O	1:B:200:LEU:HB2	1.89	0.71
1:A:264:LEU:O	1:A:267:LEU:HD12	1.91	0.71
1:B:355:GLN:O	1:B:357:GLY:N	2.23	0.70
1:B:241:LEU:HD13	1:B:247:PRO:HD3	1.73	0.70
1:B:330:LYS:O	1:B:331:PHE:HB2	1.93	0.69
1:B:44:ASP:OD1	1:B:46:VAL:HG12	1.92	0.69
1:A:13:MET:O	1:A:14:VAL:HG12	1.93	0.69
1:A:256:ILE:O	1:A:258:LEU:N	2.26	0.68
1:A:259:LYS:HE2	1:A:262:ASN:HD21	1.58	0.68
1:B:28:LEU:HA	1:B:42:ALA:HA	1.75	0.68
1:B:182:GLY:O	1:B:183:PHE:HB2	1.92	0.68
1:B:94:THR:HG22	1:B:97:GLN:NE2	2.07	0.68
1:A:259:LYS:HD3	1:A:259:LYS:O	1.94	0.68
1:A:175:ASP:CG	1:A:178:HIS:HB2	2.19	0.67
1:B:200:LEU:O	1:B:202:SER:N	2.28	0.67
1:A:13:MET:O	1:A:18:VAL:HA	1.93	0.67
1:A:125:NEP:O1P	1:B:191:ARG:HD3	1.95	0.67
1:A:12:GLU:HB2	1:A:19:PHE:O	1.94	0.66
1:B:333:MET:SD	1:B:342:LYS:HE2	2.36	0.66
1:A:261:ARG:O	9:A:502:HOH:O	2.12	0.66
7:B:602:TAR:O41	7:B:602:TAR:O2	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ASP:OD1	3:B:603:MLA:HC21	1.97	0.65
1:A:257:ASN:O	1:A:260:ALA:N	2.22	0.65
1:B:95:ILE:HG22	1:B:344:LYS:HE2	1.78	0.65
1:A:265:LEU:HD12	1:A:265:LEU:H	1.62	0.64
1:B:183:PHE:CZ	1:B:257:ASN:HB2	2.33	0.64
1:A:262:ASN:CG	1:A:263:TYR:H	2.05	0.64
1:A:89:ILE:HG21	1:A:351:THR:CG2	2.28	0.64
1:B:201:ASN:O	1:B:203:LYS:HG2	1.97	0.64
1:B:59:PHE:CZ	1:B:98:MET:HE3	2.34	0.63
1:B:69:LEU:HD23	1:B:335:LEU:CD2	2.29	0.63
1:A:30:TYR:CD2	1:A:38:MET:HE3	2.31	0.63
1:A:30:TYR:OH	1:A:33:GLU:HG2	1.99	0.63
1:B:43:TYR:OH	1:B:48:LYS:HD3	1.99	0.62
1:B:198:ILE:O	1:B:202:SER:HA	2.00	0.62
1:B:252:LEU:HD12	1:B:252:LEU:O	1.99	0.62
1:B:333:MET:HE1	1:B:346:LEU:HD11	1.80	0.62
1:B:336:ASP:OD1	8:B:606:6GI:C04	2.47	0.62
1:A:248:SER:O	1:A:252:LEU:HD12	2.00	0.62
1:A:69:LEU:HD23	1:A:335:LEU:HD22	1.81	0.62
1:A:177:ASP:N	1:A:177:ASP:OD2	2.30	0.62
1:A:281:ASN:HB2	3:A:402:MLA:O1B	2.00	0.61
1:B:53:ILE:HG12	1:B:104:VAL:HG12	1.81	0.61
1:B:88:ASP:HB3	1:B:104:VAL:CG2	2.30	0.61
1:A:241:LEU:HD13	1:A:247:PRO:HD3	1.81	0.61
1:B:182:GLY:HA2	1:B:185:THR:HB	1.83	0.61
1:A:81:GLU:CG	1:A:135:ARG:HH12	2.13	0.61
1:B:12:GLU:O	1:B:13:MET:HB2	2.01	0.61
1:B:24:ARG:NE	1:B:46:VAL:HG11	2.15	0.61
1:B:297:ASN:H	1:B:300:LYS:HE3	1.65	0.61
1:B:333:MET:CE	1:B:346:LEU:HD11	2.32	0.60
1:A:179:ASP:OD1	1:A:203:LYS:HA	2.02	0.60
1:A:265:LEU:HD12	1:A:265:LEU:N	2.16	0.60
1:A:297:ASN:H	1:A:300:LYS:HZ3	1.49	0.60
1:A:188:VAL:N	3:A:406:MLA:O3A	2.26	0.60
1:B:179:ASP:OD2	1:B:206:THR:HG23	2.02	0.60
1:A:159:THR:OG1	1:B:259:LYS:NZ	2.34	0.60
1:A:60:GLU:O	1:A:340:LYS:NZ	2.25	0.60
1:B:297:ASN:HB3	1:B:300:LYS:CE	2.29	0.59
1:B:37:GLY:HA2	1:B:55:LYS:O	2.03	0.59
1:B:17:GLN:HA	1:B:17:GLN:OE1	2.02	0.59
1:B:88:ASP:HA	1:B:354:PHE:CD1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:SER:HB2	1:B:41:SER:OG	2.03	0.58
1:A:335:LEU:HD12	1:A:335:LEU:H	1.68	0.58
1:B:94:THR:HA	1:B:348:PHE:HZ	1.68	0.58
1:B:176:PRO:HB3	1:B:206:THR:HG22	1.84	0.57
1:A:111:ASP:OD2	1:A:114:LYS:HD3	2.04	0.57
1:A:149:ASP:HB2	1:A:170:LEU:HD12	1.86	0.57
1:A:37:GLY:HA3	1:A:55:LYS:O	2.04	0.57
1:A:264:LEU:O	1:A:267:LEU:HB3	2.04	0.57
1:B:39:VAL:HG22	1:B:54:LYS:HG3	1.85	0.57
1:B:178:HIS:HB3	1:B:180:HIS:NE2	2.19	0.57
1:B:72:ILE:HD11	1:B:103:ILE:HD11	1.87	0.57
1:A:54:LYS:HE3	1:A:56:ILE:HD11	1.87	0.57
1:B:128:TYR:HE2	1:B:161:CYS:HA	1.70	0.57
1:A:332:ASP:C	1:A:333:MET:HG2	2.30	0.56
1:B:67:ARG:HH12	6:B:605:EPE:H51	1.70	0.56
1:B:333:MET:O	1:B:333:MET:HG2	2.05	0.56
1:A:85:GLY:O	1:A:105:GLN:HG2	2.06	0.56
1:B:17:GLN:HE21	1:B:55:LYS:HZ3	1.53	0.56
1:B:179:ASP:HB3	1:B:203:LYS:CD	2.35	0.56
1:A:329:PHE:O	1:A:330:LYS:HE2	2.05	0.56
1:A:261:ARG:C	1:A:265:LEU:HD13	2.31	0.55
1:B:67:ARG:HH12	6:B:605:EPE:C5	2.18	0.55
1:A:66:GLN:O	1:A:70:ARG:HG3	2.06	0.55
1:B:88:ASP:CB	1:B:104:VAL:HG22	2.37	0.55
1:B:333:MET:HE1	1:B:346:LEU:CD2	2.37	0.55
1:B:59:PHE:HA	1:B:65:CYS:SG	2.47	0.54
1:B:172:ARG:HH22	8:B:606:6GI:C33	2.20	0.54
1:B:196:PRO:O	1:B:199:MET:O	2.24	0.54
1:B:203:LYS:O	1:B:209:ILE:HD11	2.07	0.54
1:A:261:ARG:O	1:A:262:ASN:HB3	2.07	0.54
1:A:72:ILE:O	1:A:76:LEU:HB2	2.08	0.54
1:A:253:ASN:HA	1:A:261:ARG:HH11	1.73	0.54
1:A:335:LEU:HD12	1:A:335:LEU:N	2.22	0.54
1:B:241:LEU:CD1	1:B:247:PRO:HD3	2.38	0.54
1:A:334:GLU:OE2	1:A:334:GLU:HA	2.08	0.53
1:A:60:GLU:HA	1:A:340:LYS:HZ2	1.73	0.53
1:B:274:PRO:HD2	1:B:277:ARG:CG	2.38	0.53
1:A:259:LYS:O	1:A:262:ASN:ND2	2.42	0.53
1:A:331:PHE:CD1	1:A:334:GLU:HG2	2.44	0.53
1:B:91:ARG:NH1	1:B:348:PHE:O	2.41	0.53
1:A:246:SER:OG	1:A:267:LEU:HD21	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLU:OE2	1:A:335:LEU:HD12	2.08	0.53
1:B:256:ILE:O	1:B:258:LEU:HG	2.09	0.52
1:A:218:LEU:HD23	1:A:293:MET:HE2	1.90	0.52
1:B:200:LEU:O	1:B:201:ASN:C	2.53	0.52
1:A:156:LEU:O	1:A:157:LEU:HD23	2.09	0.52
1:B:250:GLU:H	1:B:252:LEU:H	1.58	0.52
1:A:274:PRO:HG2	1:A:277:ARG:HH21	1.74	0.52
1:B:249:GLN:HA	1:B:252:LEU:HB3	1.92	0.51
1:A:19:PHE:CZ	1:A:55:LYS:HB2	2.45	0.51
1:B:67:ARG:HH11	8:B:606:6GI:C35	2.24	0.51
1:B:89:ILE:HG12	1:B:103:ILE:HG12	1.92	0.51
1:B:92:ALA:HB1	1:B:97:GLN:HG2	1.93	0.51
1:A:134:LEU:HD21	1:A:214:VAL:HG11	1.93	0.51
1:A:262:ASN:N	1:A:265:LEU:HD13	2.26	0.51
1:B:28:LEU:HD12	1:B:28:LEU:N	2.26	0.51
1:A:62:GLN:CB	1:A:340:LYS:HB3	2.40	0.51
1:A:28:LEU:N	1:A:28:LEU:HD12	2.26	0.51
1:B:79:ARG:HH12	1:B:86:ILE:H	1.58	0.51
1:A:182:GLY:O	1:A:185:THR:OG1	2.29	0.51
1:A:297:ASN:HB3	1:A:300:LYS:CG	2.35	0.51
1:B:62:GLN:O	1:B:63:THR:HB	2.12	0.50
1:B:181:THR:HG21	8:B:606:6GI:C13	2.40	0.50
1:A:259:LYS:HD3	1:A:259:LYS:C	2.37	0.50
1:A:343:LEU:HD23	1:A:346:LEU:HD12	1.94	0.50
1:B:146:LEU:HD11	1:B:174:ALA:HA	1.94	0.50
1:A:330:LYS:HE2	1:A:330:LYS:HA	1.94	0.49
1:A:175:ASP:HB3	1:A:178:HIS:CB	2.42	0.49
1:A:59:PHE:HA	1:A:65:CYS:SG	2.52	0.49
1:A:252:LEU:HD23	1:A:255:ILE:HD12	1.95	0.49
1:B:17:GLN:HE21	1:B:55:LYS:NZ	2.09	0.49
1:B:62:GLN:O	1:B:63:THR:CB	2.59	0.49
1:A:122:SER:HB3	6:B:605:EPE:H31	1.95	0.49
1:B:91:ARG:NH2	1:B:355:GLN:HG3	2.26	0.49
1:B:353:ARG:HG3	1:B:354:PHE:CD2	2.48	0.49
1:A:128:TYR:O	1:A:132:GLN:HG3	2.12	0.49
1:A:246:SER:OG	1:A:269:HIS:HA	2.11	0.49
1:B:94:THR:HA	1:B:348:PHE:CE1	2.48	0.49
1:B:311:PRO:O	1:B:314:GLU:HG2	2.13	0.49
1:A:305:GLU:HB2	9:A:503:HOH:O	2.13	0.48
1:B:76:LEU:HD23	1:B:86:ILE:HB	1.94	0.48
1:A:77:ARG:HG2	1:A:77:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:SER:N	1:B:41:SER:O	2.46	0.48
1:A:69:LEU:HD23	1:A:335:LEU:CD2	2.43	0.48
1:A:359:ARG:O	1:A:360:SER:HB2	2.12	0.48
1:A:276:ASN:N	1:A:276:ASN:OD1	2.47	0.48
1:B:95:ILE:CG2	1:B:344:LYS:HE2	2.42	0.47
1:B:275:TRP:NE1	1:B:291:ASP:OD1	2.41	0.47
1:A:13:MET:HA	1:A:18:VAL:HB	1.96	0.47
1:A:330:LYS:HA	1:A:330:LYS:CE	2.44	0.47
1:B:147:HIS:O	1:B:148:ARG:HB2	2.14	0.47
1:B:14:VAL:HG23	1:B:15:ARG:N	2.29	0.47
1:B:94:THR:HG22	1:B:97:GLN:CD	2.39	0.47
1:B:148:ARG:CD	1:B:170:LEU:O	2.57	0.47
1:B:67:ARG:HB3	3:B:603:MLA:O3B	2.15	0.47
1:B:297:ASN:N	1:B:300:LYS:HE3	2.30	0.47
1:A:182:GLY:HA3	1:A:185:THR:CG2	2.44	0.47
1:A:334:GLU:HG3	9:A:504:HOH:O	2.14	0.47
1:B:75:LEU:HB2	1:B:86:ILE:CD1	2.45	0.47
1:B:121:LEU:HB3	1:B:126:ILE:HG13	1.96	0.47
1:A:255:ILE:CG2	1:A:261:ARG:HG3	2.45	0.46
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.80	0.46
1:B:112:LEU:O	1:B:112:LEU:HG	2.15	0.46
1:A:226:PRO:HA	9:A:528:HOH:O	2.14	0.46
1:A:55:LYS:HG3	1:A:102:TYR:CE2	2.51	0.46
1:A:262:ASN:CG	1:A:263:TYR:N	2.68	0.46
1:B:75:LEU:HB2	1:B:86:ILE:HD12	1.96	0.46
1:B:228:PHE:HE1	1:B:243:ILE:HD12	1.80	0.46
1:B:97:GLN:OE1	1:B:97:GLN:N	2.45	0.46
1:B:333:MET:O	1:B:334:GLU:HB3	2.15	0.46
1:A:13:MET:CG	1:A:14:VAL:H	2.29	0.46
1:B:297:ASN:HB3	1:B:300:LYS:CG	2.40	0.46
1:B:15:ARG:HG3	1:B:30:TYR:CD1	2.51	0.45
1:A:162:ASP:HB2	1:B:259:LYS:CD	2.47	0.45
1:A:183:PHE:HZ	1:A:200:LEU:O	1.99	0.45
1:B:179:ASP:CB	1:B:203:LYS:HD3	2.43	0.45
1:A:265:LEU:H	1:A:265:LEU:CD1	2.26	0.45
1:B:270:LYS:NZ	9:B:705:HOH:O	2.49	0.45
1:B:156:LEU:HD13	7:B:602:TAR:H3	1.99	0.45
1:B:333:MET:HE1	1:B:346:LEU:CD1	2.47	0.45
1:A:227:ILE:HG23	1:A:228:PHE:CD2	2.52	0.44
1:B:107:LEU:HD12	1:B:108:MET:N	2.32	0.44
1:B:274:PRO:HB2	1:B:277:ARG:HG2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HD13	1:A:86:ILE:HD12	1.99	0.44
1:A:60:GLU:HA	1:A:340:LYS:NZ	2.32	0.44
1:A:332:ASP:OD1	1:A:332:ASP:N	2.48	0.44
1:B:12:GLU:O	1:B:13:MET:CB	2.64	0.44
1:B:183:PHE:HD1	1:B:183:PHE:HA	1.65	0.44
1:A:91:ARG:HD2	1:A:98:MET:SD	2.57	0.44
1:A:173:VAL:HG21	1:A:331:PHE:HD2	1.82	0.44
1:B:69:LEU:HD23	1:B:335:LEU:HD23	1.99	0.44
1:A:12:GLU:CB	1:A:19:PHE:O	2.65	0.44
1:A:26:THR:C	1:A:28:LEU:HD12	2.43	0.44
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.75	0.43
1:A:84:ILE:HD12	1:A:84:ILE:HA	1.84	0.43
1:B:105:GLN:OE1	7:B:602:TAR:O1	2.37	0.43
1:A:228:PHE:CE1	1:A:240:ILE:HA	2.54	0.43
1:B:54:LYS:O	1:B:102:TYR:HA	2.19	0.43
1:A:19:PHE:C	1:A:21:VAL:H	2.27	0.43
1:A:30:TYR:HD2	1:A:38:MET:CE	2.26	0.43
1:A:61:HIS:ND1	1:A:63:THR:HB	2.33	0.43
1:B:75:LEU:O	1:B:79:ARG:NH1	2.52	0.43
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.87	0.42
1:B:43:TYR:HA	1:B:50:ARG:HG2	2.00	0.42
1:B:333:MET:O	1:B:334:GLU:CB	2.66	0.42
1:B:21:VAL:HG21	1:B:28:LEU:HD11	2.00	0.42
1:B:69:LEU:HD23	1:B:335:LEU:HD22	2.00	0.42
1:B:275:TRP:CD1	1:B:291:ASP:HB2	2.53	0.42
1:A:255:ILE:CG2	1:A:260:ALA:HB3	2.49	0.42
1:B:63:THR:HG22	1:B:64:TYR:N	2.33	0.42
1:B:338:LEU:N	1:B:338:LEU:HD23	2.34	0.42
1:A:188:VAL:O	1:A:189:ALA:HB3	2.20	0.42
1:A:268:PRO:O	1:A:269:HIS:C	2.61	0.42
1:B:218:LEU:HD23	1:B:290:LEU:HD13	2.01	0.42
1:B:244:LEU:HD23	1:B:296:PHE:HB2	2.02	0.42
1:A:211:ILE:HG21	1:A:302:ILE:O	2.19	0.42
1:B:335:LEU:H	8:B:606:6GI:C03	2.32	0.42
1:A:108:MET:O	2:A:401:5ID:H2	2.20	0.42
1:A:261:ARG:HB3	1:A:265:LEU:HD11	2.01	0.42
1:B:182:GLY:HA2	1:B:185:THR:CB	2.49	0.42
1:B:297:ASN:HB2	1:B:300:LYS:HE3	1.97	0.42
1:B:339:PRO:HB2	1:B:341:GLU:OE1	2.20	0.42
1:A:259:LYS:O	1:A:262:ASN:CG	2.63	0.41
1:A:13:MET:HA	1:A:18:VAL:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD22	1:A:268:PRO:C	2.45	0.41
1:B:43:TYR:CD1	1:B:50:ARG:HG3	2.55	0.41
1:B:200:LEU:HA	1:B:257:ASN:HB3	2.01	0.41
1:B:255:ILE:HD12	1:B:261:ARG:HG3	2.02	0.41
1:B:297:ASN:H	1:B:300:LYS:CE	2.30	0.41
1:B:24:ARG:HH11	1:B:44:ASP:CG	2.20	0.41
1:A:22:GLY:HA2	1:A:23:PRO:C	2.45	0.41
1:A:261:ARG:HG3	1:A:261:ARG:H	1.71	0.41
1:A:310:HIS:CG	1:A:311:PRO:HD2	2.55	0.41
1:B:91:ARG:HB2	1:B:98:MET:HG3	2.01	0.41
1:A:178:HIS:O	1:A:178:HIS:CG	2.73	0.41
1:A:255:ILE:HG21	1:A:261:ARG:HG3	2.03	0.41
1:B:39:VAL:CG2	1:B:54:LYS:HG3	2.51	0.41
1:B:79:ARG:NH1	1:B:86:ILE:H	2.19	0.41
1:B:148:ARG:CZ	1:B:172:ARG:HG3	2.51	0.41
8:B:606:6GI:N23	8:B:606:6GI:C15	2.72	0.41
1:B:43:TYR:HD1	1:B:50:ARG:NH2	2.18	0.41
1:B:67:ARG:HH22	6:B:605:EPE:H51	1.86	0.41
1:B:81:GLU:HG3	1:B:135:ARG:HH12	1.85	0.41
1:B:195:ALA:HA	1:B:212:TRP:CD1	2.56	0.40
1:A:338:LEU:HD23	1:A:342:LYS:HG3	2.03	0.40
1:B:14:VAL:HG23	1:B:15:ARG:H	1.85	0.40
1:B:29:SER:O	1:B:30:TYR:O	2.39	0.40
1:B:46:VAL:O	1:B:46:VAL:HG22	2.19	0.40
1:B:167:ASP:OD1	3:B:603:MLA:C2	2.68	0.40
1:B:275:TRP:NE1	1:B:291:ASP:HB2	2.36	0.40
1:A:183:PHE:HE1	1:A:199:MET:O	2.04	0.40
1:B:73:LYS:HE3	1:B:73:LYS:HB3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	347/368 (94%)	313 (90%)	26 (8%)	8 (2%)	5	3
1	B	343/368 (93%)	287 (84%)	38 (11%)	18 (5%)	1	0
All	All	690/736 (94%)	600 (87%)	64 (9%)	26 (4%)	2	1

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	B	183	PHE
1	B	201	ASN
1	A	14	VAL
1	A	262	ASN
1	B	30	TYR
1	B	48	LYS
1	B	63	THR
1	B	181	THR
1	B	202	SER
1	B	249	GLN
1	B	250	GLU
1	A	261	ARG
1	B	13	MET
1	B	14	VAL
1	B	23	PRO
1	B	189	ALA
1	B	200	LEU
1	B	356	PRO
1	B	20	ASP
1	B	334	GLU
1	A	328	PRO
1	A	58	PRO
1	A	229	PRO
1	A	21	VAL
1	B	21	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	316/323 (98%)	294 (93%)	22 (7%)	14	15
1	B	312/323 (97%)	292 (94%)	20 (6%)	16	18
All	All	628/646 (97%)	586 (93%)	42 (7%)	15	17

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	14	VAL
1	A	36	TYR
1	A	57	SER
1	A	60	GLU
1	A	63	THR
1	A	76	LEU
1	A	79	ARG
1	A	90	ILE
1	A	94	THR
1	A	119	GLN
1	A	177	ASP
1	A	179	ASP
1	A	233	TYR
1	A	267	LEU
1	A	278	LEU
1	A	313	LEU
1	A	330	LYS
1	A	332	ASP
1	A	333	MET
1	A	334	GLU
1	A	335	LEU
1	B	26	THR
1	B	31	ILE
1	B	56	ILE
1	B	57	SER
1	B	63	THR
1	B	71	GLU
1	B	79	ARG
1	B	91	ARG
1	B	104	VAL
1	B	116	LEU
1	B	178	HIS
1	B	180	HIS
1	B	181	THR

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Mol	Chain	Res	Type
1	B	183	PHE
1	B	201	ASN
1	B	227	ILE
1	B	233	TYR
1	B	259	LYS
1	B	270	LYS
1	B	303	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	132	GLN
1	A	239	HIS
1	A	269	HIS
1	A	299	HIS
1	B	17	GLN
1	B	119	GLN
1	B	238	ASN
1	B	281	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are 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
1	NEP	A	125	1	11,14,15	3.12	3 (27%)	8,20,22	2.98	2 (25%)
1	NEP	B	125	1	11,14,15	3.42	3 (27%)	8,20,22	2.64	2 (25%)

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
1	NEP	A	125	1	-	2/5/12/14	0/1/1/1
1	NEP	B	125	1	-	2/5/12/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	125	NEP	P-O3P	9.53	1.60	1.46
1	A	125	NEP	P-O3P	8.57	1.59	1.46
1	B	125	NEP	P-O2P	-4.67	1.44	1.56
1	A	125	NEP	P-O2P	-4.65	1.44	1.56
1	B	125	NEP	CD2-CG	3.16	1.41	1.36
1	A	125	NEP	CD2-CG	2.49	1.40	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	NEP	O1P-P-O3P	-7.55	94.37	112.95
1	B	125	NEP	O1P-P-O3P	-6.88	96.02	112.95
1	A	125	NEP	O2P-P-O3P	3.56	121.71	112.95
1	B	125	NEP	O2P-P-O3P	2.39	118.83	112.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	125	NEP	CA-CB-CG-CD2
1	A	125	NEP	CA-CB-CG-ND1
1	B	125	NEP	CA-CB-CG-ND1
1	A	125	NEP	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	125	NEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SIN	A	403	-	7,7,7	1.10	0	8,8,8	1.54	2 (25%)
6	EPE	B	605	-	15,15,15	0.95	1 (6%)	19,20,20	1.56	4 (21%)
4	SIN	A	405	-	7,7,7	1.22	0	8,8,8	1.49	2 (25%)
6	EPE	A	408	-	15,15,15	0.72	1 (6%)	19,20,20	1.62	4 (21%)
3	MLA	B	604	-	6,6,6	3.65	5 (83%)	7,7,7	0.66	0
3	MLA	A	407	-	6,6,6	2.26	1 (16%)	7,7,7	1.21	1 (14%)
3	MLA	A	402	-	6,6,6	2.38	3 (50%)	7,7,7	1.47	2 (28%)
3	MLA	B	603	-	6,6,6	3.42	5 (83%)	7,7,7	1.70	3 (42%)
3	MLA	A	406	-	6,6,6	2.94	5 (83%)	7,7,7	1.79	2 (28%)
3	MLA	B	601	-	6,6,6	2.32	2 (33%)	7,7,7	1.01	0
8	6GI	B	606	-	41,42,42	5.01	32 (78%)	53,61,61	2.59	24 (45%)
2	5ID	A	401	-	21,22,22	3.57	8 (38%)	28,33,33	2.53	8 (28%)
7	TAR	B	602	-	9,9,9	1.91	4 (44%)	12,12,12	1.54	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SIN	A	403	-	-	5/5/5/5	-
6	EPE	B	605	-	-	5/9/19/19	0/1/1/1
4	SIN	A	405	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EPE	A	408	-	-	4/9/19/19	0/1/1/1
3	MLA	B	604	-	-	3/4/4/4	-
3	MLA	A	407	-	-	4/4/4/4	-
3	MLA	A	402	-	-	0/4/4/4	-
3	MLA	B	603	-	-	1/4/4/4	-
3	MLA	A	406	-	-	2/4/4/4	-
3	MLA	B	601	-	-	2/4/4/4	-
8	6GI	B	606	-	-	5/9/29/29	0/7/7/7
2	5ID	A	401	-	-	2/6/22/22	0/3/3/3
7	TAR	B	602	-	-	10/12/12/12	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	606	6GI	C20-N19	15.43	1.48	1.37
8	B	606	6GI	C18-N23	11.60	1.71	1.45
2	A	401	5ID	O4'-C1'	10.09	1.65	1.42
8	B	606	6GI	C10-C08	10.00	1.67	1.49
8	B	606	6GI	C34-C35	-7.48	1.32	1.51
2	A	401	5ID	C2'-C1'	-7.33	1.30	1.53
8	B	606	6GI	C18-N19	6.50	1.58	1.46
8	B	606	6GI	C20-N21	6.43	1.47	1.34
2	A	401	5ID	O4'-C4'	-6.39	1.30	1.45
8	B	606	6GI	C20-N27	6.03	1.39	1.32
8	B	606	6GI	C09-C08	5.63	1.45	1.36
3	B	604	MLA	C2-C1	5.60	1.59	1.51
8	B	606	6GI	C25-N19	5.59	1.51	1.40
3	B	603	MLA	C2-C1	5.50	1.59	1.51
3	A	407	MLA	C2-C3	5.30	1.59	1.51
8	B	606	6GI	O11-C10	5.15	1.54	1.42
8	B	606	6GI	C22-N24	5.05	1.46	1.34
3	B	604	MLA	C2-C3	4.99	1.58	1.51
8	B	606	6GI	C09-N06	4.97	1.45	1.37
3	B	601	MLA	C2-C1	4.77	1.58	1.51
3	A	402	MLA	C2-C1	4.59	1.58	1.51
8	B	606	6GI	C15-C18	4.58	1.59	1.52
2	A	401	5ID	C6-N6	4.49	1.45	1.34
8	B	606	6GI	O32-C29	4.44	1.46	1.38
8	B	606	6GI	C28-C29	4.44	1.46	1.38
3	A	406	MLA	C2-C3	4.42	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	606	6GI	C28-C25	4.36	1.46	1.39
8	B	606	6GI	C08-N07	4.22	1.46	1.38
3	B	603	MLA	C2-C3	4.21	1.57	1.51
8	B	606	6GI	C05-N07	3.93	1.40	1.33
2	A	401	5ID	O2'-C2'	3.90	1.52	1.43
8	B	606	6GI	C04-C05	3.84	1.49	1.41
8	B	606	6GI	C16-C15	3.63	1.44	1.39
8	B	606	6GI	O11-C12	3.57	1.45	1.37
3	A	406	MLA	C2-C1	3.50	1.56	1.51
7	B	602	TAR	C3-C2	3.44	1.64	1.53
8	B	606	6GI	C14-C13	3.43	1.44	1.38
8	B	606	6GI	C31-C26	3.36	1.45	1.40
8	B	606	6GI	C26-N27	3.16	1.46	1.39
2	A	401	5ID	O3'-C3'	-3.08	1.35	1.43
3	B	601	MLA	C2-C3	2.97	1.55	1.51
6	B	605	EPE	C10-S	2.92	1.81	1.77
3	B	604	MLA	O3A-C3	2.79	1.31	1.22
3	B	604	MLA	O1B-C1	2.78	1.31	1.22
8	B	606	6GI	C17-C16	2.65	1.43	1.38
3	B	603	MLA	O3A-C3	2.63	1.30	1.22
8	B	606	6GI	C13-C12	2.59	1.43	1.38
8	B	606	6GI	C30-C29	-2.55	1.35	1.40
2	A	401	5ID	C8-N9	-2.48	1.33	1.38
3	A	406	MLA	O1B-C1	2.46	1.30	1.22
3	A	402	MLA	O1B-C1	2.46	1.30	1.22
3	A	406	MLA	O3A-C3	2.44	1.30	1.22
3	B	603	MLA	O1B-C1	2.44	1.30	1.22
8	B	606	6GI	C05-N06	-2.34	1.34	1.39
7	B	602	TAR	C3-C4	2.31	1.56	1.52
3	B	603	MLA	O3B-C3	-2.29	1.23	1.30
8	B	606	6GI	O32-C33	-2.23	1.39	1.44
7	B	602	TAR	O4-C4	2.14	1.28	1.22
3	A	402	MLA	O1A-C1	-2.09	1.23	1.30
3	A	406	MLA	O1A-C1	-2.08	1.23	1.30
3	B	604	MLA	O1A-C1	-2.07	1.24	1.30
2	A	401	5ID	C3'-C4'	2.06	1.58	1.53
8	B	606	6GI	O36-C35	-2.05	1.39	1.44
8	B	606	6GI	C31-C30	2.04	1.42	1.38
7	B	602	TAR	C2-C1	-2.03	1.49	1.52
8	B	606	6GI	C01-N06	2.00	1.44	1.39
6	A	408	EPE	C10-S	2.00	1.80	1.77

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	5ID	C5-C4-N3	-8.15	118.33	126.97
8	B	606	6GI	C33-O32-C29	5.64	125.50	116.13
8	B	606	6GI	O11-C10-C08	5.27	122.00	109.19
8	B	606	6GI	O36-C35-C34	-5.11	102.08	112.80
2	A	401	5ID	N3-C2-N1	-4.84	121.26	128.58
8	B	606	6GI	C26-N27-C20	4.43	108.92	104.81
8	B	606	6GI	C28-C25-C26	-4.31	117.30	122.47
2	A	401	5ID	C2-N3-C4	4.30	122.33	111.83
8	B	606	6GI	N06-C05-N07	4.12	112.89	110.64
6	A	408	EPE	C5-N4-C3	4.01	117.47	108.84
8	B	606	6GI	O36-C30-C29	-3.92	119.17	123.24
2	A	401	5ID	C4-N9-C8	3.80	109.65	108.08
8	B	606	6GI	C25-N19-C18	3.78	136.53	127.18
2	A	401	5ID	N3-C4-N9	3.78	133.59	127.17
8	B	606	6GI	C09-C08-N07	-3.77	107.42	110.65
8	B	606	6GI	O32-C33-C34	3.72	120.61	112.80
8	B	606	6GI	C10-O11-C12	3.71	124.28	117.63
8	B	606	6GI	N19-C20-N27	-3.66	109.36	113.57
8	B	606	6GI	C28-C25-N19	3.63	134.95	128.59
6	B	605	EPE	C7-N4-C3	3.62	120.88	111.24
7	B	602	TAR	O41-C4-C3	3.50	123.03	113.31
6	B	605	EPE	C5-N4-C3	3.46	116.30	108.84
2	A	401	5ID	C1'-N9-C8	-3.40	121.86	125.72
7	B	602	TAR	O4-C4-C3	-3.33	112.74	121.62
8	B	606	6GI	N19-C20-N21	3.25	124.76	121.91
3	A	406	MLA	O1A-C1-C2	3.10	124.12	114.51
8	B	606	6GI	C26-C25-N19	3.04	107.66	105.12
6	A	408	EPE	C7-N4-C5	3.01	119.25	111.24
8	B	606	6GI	C16-C15-C14	-2.97	114.62	118.30
8	B	606	6GI	C09-N06-C05	2.95	108.57	106.90
6	A	408	EPE	C7-N4-C3	2.93	119.04	111.24
8	B	606	6GI	O32-C29-C30	-2.84	120.30	123.24
6	B	605	EPE	C7-N4-C5	2.80	118.70	111.24
3	A	402	MLA	O1A-C1-C2	2.80	123.17	114.51
8	B	606	6GI	C14-C15-C18	2.76	125.74	120.72
3	B	603	MLA	O1A-C1-C2	2.75	123.02	114.51
6	A	408	EPE	O1S-S-C10	2.70	110.81	106.73
8	B	606	6GI	C17-C12-C13	-2.60	116.36	120.16
2	A	401	5ID	C6-C5-C4	2.52	117.63	115.74
3	A	406	MLA	O1B-C1-C2	-2.50	115.00	122.11
8	B	606	6GI	N23-C18-N19	2.20	110.76	107.04
4	A	405	SIN	O2-C1-O1	-2.18	117.73	123.33
2	A	401	5ID	O4'-C4'-C5'	2.17	113.81	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	MLA	O1B-C1-C2	-2.13	116.05	122.11
4	A	403	SIN	C2-C3-C4	-2.13	108.02	113.67
8	B	606	6GI	C01-N06-C09	-2.09	126.59	130.31
3	A	407	MLA	O1B-C1-C2	-2.06	116.25	122.11
3	A	402	MLA	O1B-C1-C2	-2.06	116.26	122.11
4	A	405	SIN	O2-C1-C2	2.05	120.49	114.00
8	B	606	6GI	C18-N19-C20	-2.04	117.52	124.85
4	A	403	SIN	O4-C4-O3	-2.02	118.14	123.33
6	B	605	EPE	O1S-S-C10	2.02	109.77	106.73
3	B	603	MLA	O3B-C3-C2	2.02	120.75	114.51
8	B	606	6GI	C31-C26-C25	2.01	122.01	120.16

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	408	EPE	C9-C10-S-O2S
6	A	408	EPE	C9-C10-S-O3S
6	B	605	EPE	N4-C7-C8-O8
6	B	605	EPE	C9-C10-S-O1S
6	B	605	EPE	C9-C10-S-O2S
6	B	605	EPE	C9-C10-S-O3S
7	B	602	TAR	C2-C3-C4-O41
4	A	403	SIN	C1-C2-C3-C4
7	B	602	TAR	C1-C2-C3-C4
7	B	602	TAR	O3-C3-C4-O4
7	B	602	TAR	O3-C3-C4-O41
7	B	602	TAR	C2-C3-C4-O4
7	B	602	TAR	O2-C2-C3-O3
8	B	606	6GI	C08-C10-O11-C12
8	B	606	6GI	C17-C12-O11-C10
7	B	602	TAR	C1-C2-C3-O3
7	B	602	TAR	O2-C2-C3-C4
8	B	606	6GI	C13-C12-O11-C10
7	B	602	TAR	O1-C1-C2-O2
7	B	602	TAR	O11-C1-C2-O2
6	A	408	EPE	S-C10-C9-N1
3	B	604	MLA	C1-C2-C3-O3B
8	B	606	6GI	C09-C08-C10-O11
3	B	604	MLA	C1-C2-C3-O3A
8	B	606	6GI	N07-C08-C10-O11
3	A	406	MLA	O1A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	406	MLA	O1B-C1-C2-C3
6	A	408	EPE	C9-C10-S-O1S
3	B	601	MLA	O1A-C1-C2-C3
3	A	407	MLA	C1-C2-C3-O3A
2	A	401	5ID	C2'-C1'-N9-C8
6	B	605	EPE	C8-C7-N4-C3
2	A	401	5ID	C2'-C1'-N9-C4
3	A	407	MLA	C1-C2-C3-O3B
3	B	601	MLA	O1B-C1-C2-C3
4	A	403	SIN	C2-C3-C4-O3
4	A	405	SIN	C2-C3-C4-O3
3	A	407	MLA	O1A-C1-C2-C3
4	A	403	SIN	C2-C3-C4-O4
4	A	405	SIN	C2-C3-C4-O4
3	A	407	MLA	O1B-C1-C2-C3
3	B	603	MLA	O1B-C1-C2-C3
4	A	403	SIN	O2-C1-C2-C3
4	A	403	SIN	O1-C1-C2-C3
3	B	604	MLA	O1A-C1-C2-C3

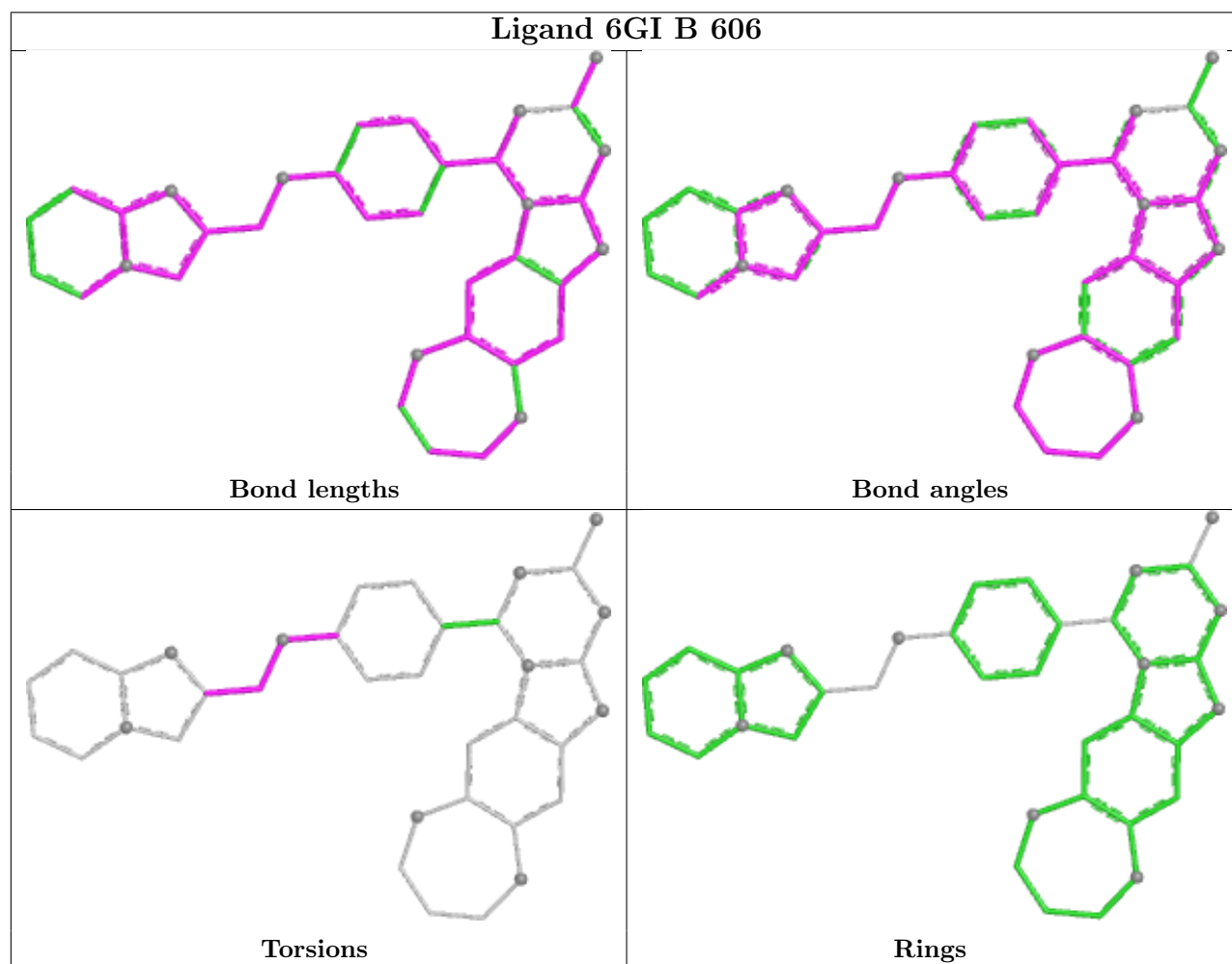
There are no ring outliers.

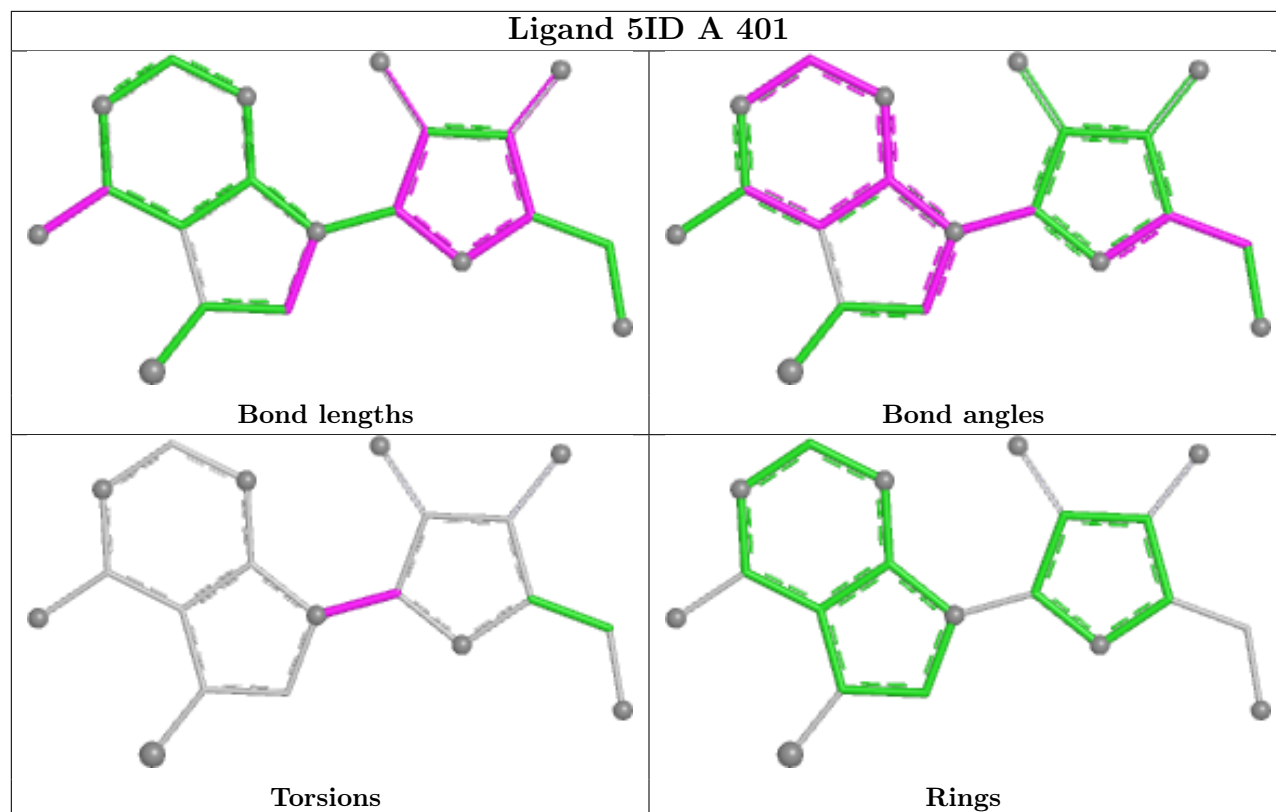
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	605	EPE	4	0
3	A	402	MLA	1	0
3	B	603	MLA	3	0
3	A	406	MLA	1	0
8	B	606	6GI	7	0
2	A	401	5ID	3	0
7	B	602	TAR	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	349/368 (94%)	0.69	36 (10%)	12 13	43, 63, 99, 118	0
1	B	345/368 (93%)	0.75	28 (8%)	18 20	42, 67, 99, 108	0
All	All	694/736 (94%)	0.72	64 (9%)	14 17	42, 65, 99, 118	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	LEU	5.8
1	A	11	PRO	4.7
1	A	254	CYS	4.4
1	A	331	PHE	3.8
1	B	357	GLY	3.6
1	A	188	VAL	3.6
1	A	18	VAL	3.6
1	A	256	ILE	3.3
1	B	255	ILE	3.3
1	A	181	THR	3.3
1	B	46	VAL	3.3
1	A	329	PHE	3.2
1	A	95	ILE	3.1
1	A	265	LEU	3.1
1	A	61	HIS	3.0
1	B	23	PRO	3.0
1	A	14	VAL	2.9
1	A	263	TYR	2.9
1	B	182	GLY	2.8
1	A	267	LEU	2.8
1	B	356	PRO	2.8
1	B	181	THR	2.7
1	A	333	MET	2.7
1	B	21	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	260	ALA	2.7
1	A	183	PHE	2.7
1	A	38	MET	2.7
1	A	264	LEU	2.6
1	B	35	ALA	2.6
1	B	269	HIS	2.6
1	B	200	LEU	2.5
1	A	92	ALA	2.5
1	B	14	VAL	2.5
1	B	120	HIS	2.5
1	A	13	MET	2.4
1	B	259	LYS	2.4
1	A	36	TYR	2.4
1	A	179	ASP	2.4
1	A	182	GLY	2.3
1	B	331	PHE	2.3
1	B	50	ARG	2.3
1	A	35	ALA	2.3
1	A	120	HIS	2.3
1	B	183	PHE	2.3
1	A	278	LEU	2.3
1	B	56	ILE	2.3
1	B	28	LEU	2.2
1	A	99	LYS	2.2
1	A	21	VAL	2.2
1	B	179	ASP	2.2
1	B	19	PHE	2.2
1	A	176	PRO	2.1
1	B	103	ILE	2.1
1	A	204	GLY	2.1
1	A	16	GLY	2.1
1	B	92	ALA	2.1
1	A	31	ILE	2.1
1	B	330	LYS	2.0
1	B	40	CYS	2.0
1	B	249	GLN	2.0
1	A	262	ASN	2.0
1	A	330	LYS	2.0
1	B	352	ALA	2.0
1	B	45	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	NEP	B	125	14/15	0.95	0.09	45,55,61,62	0
1	NEP	A	125	14/15	0.97	0.07	43,49,54,56	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

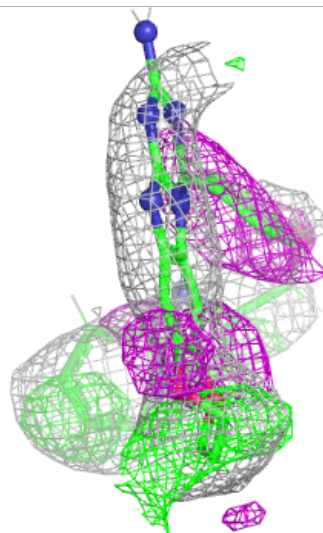
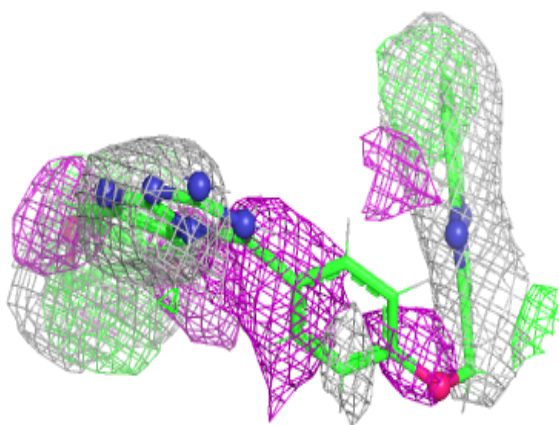
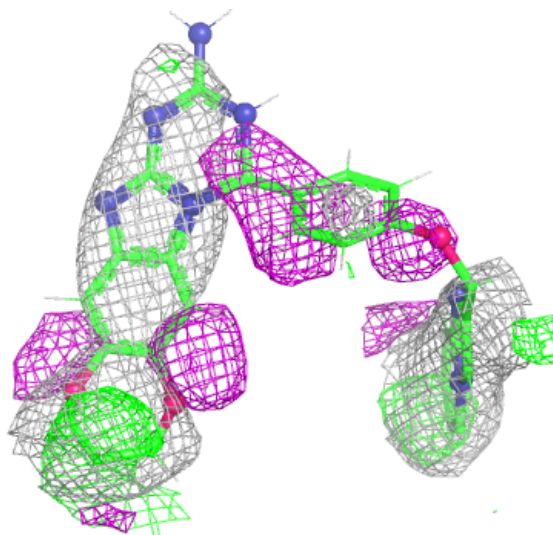
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MLA	B	601	7/7	0.54	0.19	63,75,95,95	0
3	MLA	A	407	7/7	0.61	0.19	56,68,72,74	0
3	MLA	B	603	7/7	0.62	0.20	67,75,95,95	0
8	6GI	B	606	36/36	0.67	0.22	42,87,116,129	0
3	MLA	B	604	7/7	0.69	0.19	58,70,78,78	0
4	SIN	A	405	8/8	0.74	0.14	64,76,88,88	0
6	EPE	B	605	15/15	0.76	0.17	69,85,97,102	0
3	MLA	A	402	7/7	0.77	0.13	63,71,80,82	0
4	SIN	A	403	8/8	0.79	0.14	76,90,103,103	0
3	MLA	A	406	7/7	0.80	0.15	70,74,89,89	0
6	EPE	A	408	15/15	0.82	0.12	75,102,115,117	0
7	TAR	B	602	10/10	0.87	0.14	51,73,89,93	0
5	NA	A	404	1/1	0.87	0.18	79,79,79,79	0
2	5ID	A	401	20/20	0.88	0.14	62,88,109,128	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.

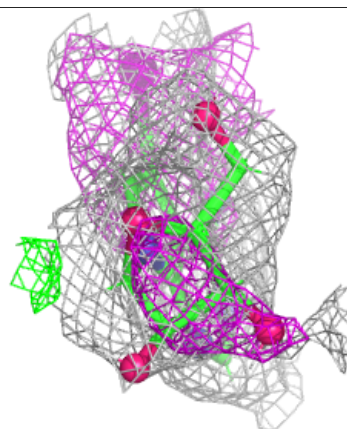
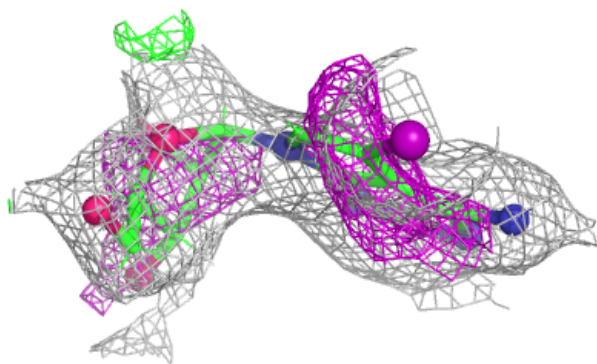
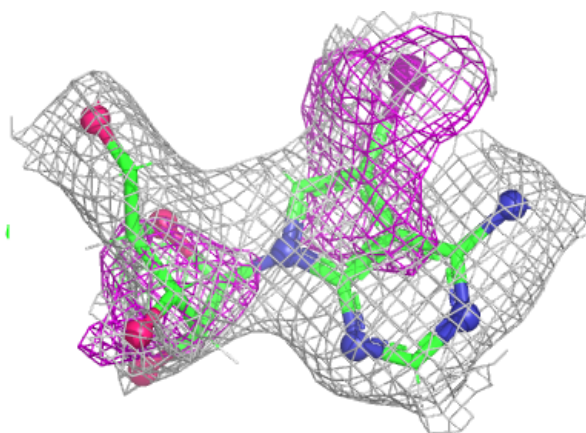
Electron density around 6GI B 606:

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



Electron density around 5ID A 401:

$2mF_o-DF_c$ (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.