



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:13 PM UTC

PDB ID : 7XC1 / pdb_00007xc1
Title : Crystal structure of ERK2 with an allosteric inhibitor 3
Authors : Yoshida, M.; Kinoshita, T.
Deposited on : 2022-03-22
Resolution : 2.09 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

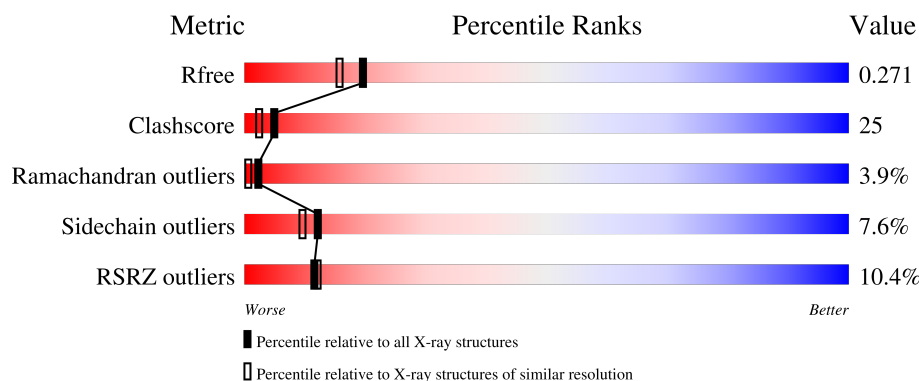
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	9% 63% 26% 6% 5%
1	B	368	11% 53% 35% 5% 6%

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
5	B8Z	A	405	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6118 atoms, of which 108 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.

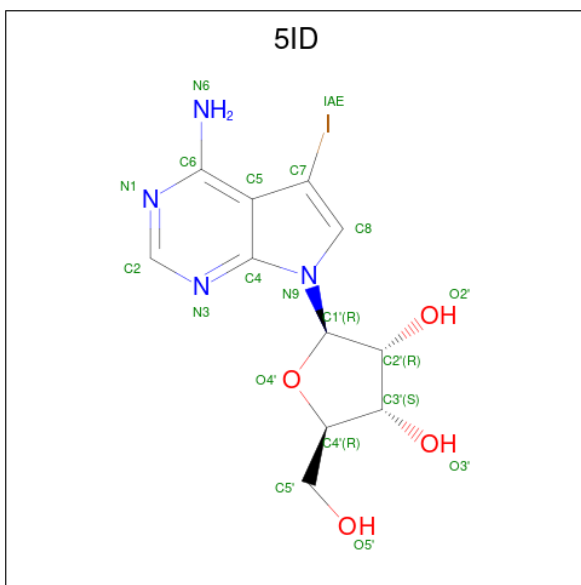
- Molecule 1 is a protein called Mitogen-activated protein kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	P	S	0	0	0
			2872	1840	491	525	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		
2	B	1	Total	C	H	I	N	O	0	0
			33	11	13	1	4	4		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

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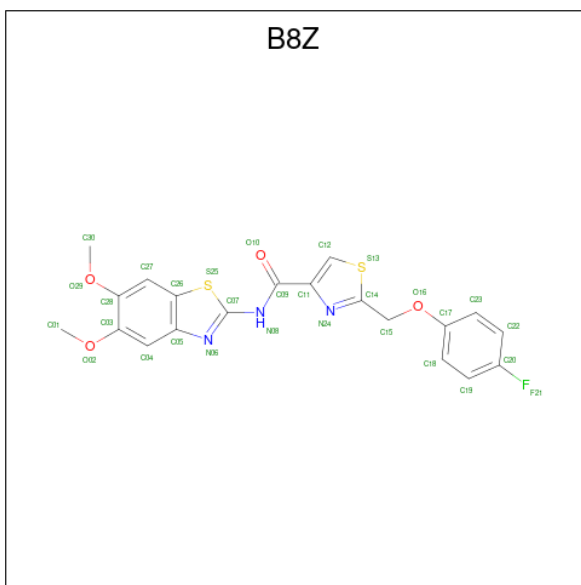
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



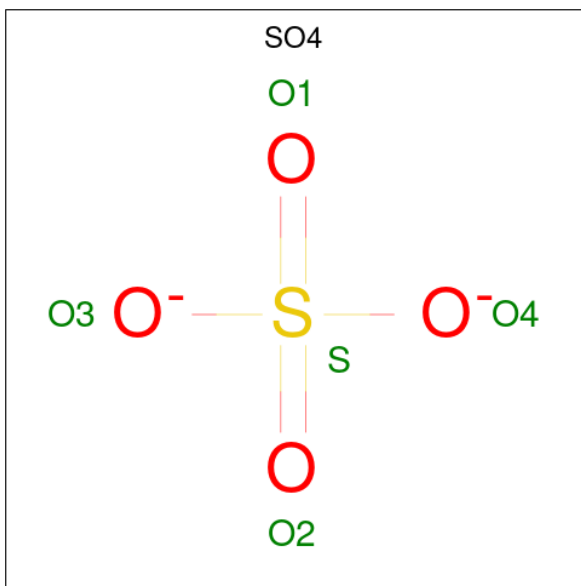
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is {N}-(5,6-dimethoxy-1,3-benzothiazol-2-yl)-2-[(4-fluoranylphenoxy)methyl]-1,3-thiazole-4-carboxamide (CCD ID: B8Z) (formula: $C_{20}H_{16}FN_3O_4S_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	F	H	N	O	S	0	0
			46	20	1	16	3	4	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	105	Total 105	O 105	0	0
7	B	73	Total 73	O 73	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.65Å 82.65Å 275.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.33 – 2.09 41.33 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.33-2.09) 99.9 (41.33-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.230 , 0.271 0.230 , 0.271	Depositor DCC
R_{free} test set	2882 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6118	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: SO4, EPE, B8Z, 5ID, NEP, GOL

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	0.37	0/2926	0.54	0/3962
1	B	0.37	0/2883	0.53	0/3905
All	All	0.37	0/5809	0.53	0/7867

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	172	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2872	0	2863	119	0
1	B	2831	0	2826	168	0
2	A	20	13	12	3	0
2	B	20	13	13	3	0
3	A	15	17	17	0	0
3	B	15	17	17	1	0
4	A	12	16	16	3	0
4	B	12	16	16	1	0
5	A	30	16	0	10	0
6	A	5	0	0	1	0
7	A	105	0	0	2	0
7	B	73	0	0	9	0
All	All	6010	108	5780	293	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 (293) 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:A:405:B8Z:O29	5:A:405:B8Z:C30	1.66	1.42
2:A:401:5ID:O4'	2:A:401:5ID:C1'	1.63	1.21
2:B:402:5ID:C1'	2:B:402:5ID:O4'	1.63	1.10
1:A:215:GLY:HA2	1:A:293:MET:HE3	1.46	0.96
1:B:297:ASN:HB3	1:B:300:LYS:HE3	1.48	0.95
1:B:78:PHE:O	1:B:79:ARG:HD3	1.69	0.93
1:A:330:LYS:HE2	1:A:330:LYS:HA	1.52	0.92
1:B:255:ILE:HB	1:B:261:ARG:HD2	1.52	0.89
1:A:252:LEU:O	1:A:261:ARG:NH2	2.05	0.88
1:B:297:ASN:H	1:B:300:LYS:HE3	1.38	0.88
1:A:30:TYR:HD2	1:A:38:MET:HE3	1.39	0.88
1:B:183:PHE:HZ	1:B:257:ASN:HB2	1.39	0.86
1:B:148:ARG:HD3	1:B:170:LEU:O	1.73	0.85
1:B:252:LEU:HD12	1:B:255:ILE:HD12	1.59	0.84
1:A:119:GLN:HG2	5:A:405:B8Z:C04	2.09	0.83
1:B:92:ALA:HB1	1:B:97:GLN:HG2	1.59	0.82
1:B:297:ASN:HB3	1:B:300:LYS:CE	2.12	0.80
1:B:21:VAL:HG21	1:B:28:LEU:HD11	1.64	0.79
1:B:255:ILE:HG22	1:B:257:ASN:O	1.83	0.79
5:A:405:B8Z:C30	5:A:405:B8Z:C28	2.59	0.79
1:A:90:ILE:HG13	1:A:102:TYR:HB2	1.64	0.79
1:B:261:ARG:HH12	1:B:265:LEU:HD11	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ASP:O	1:B:292:LYS:HD2	1.83	0.79
1:B:261:ARG:NH1	1:B:265:LEU:HD11	1.99	0.78
1:A:177:ASP:OD1	1:A:177:ASP:N	2.14	0.78
1:A:335:LEU:HD12	1:A:335:LEU:H	1.50	0.76
1:B:177:ASP:O	1:B:179:ASP:N	2.18	0.75
1:B:267:LEU:HD23	1:B:268:PRO:HD2	1.66	0.75
1:A:302:ILE:HA	4:A:404:GOL:H32	1.69	0.74
1:A:90:ILE:CG1	1:A:102:TYR:HB2	2.17	0.74
1:A:175:ASP:OD2	1:A:178:HIS:HB2	1.85	0.74
1:B:201:ASN:O	1:B:203:LYS:HG2	1.87	0.74
1:A:197:GLU:HG3	1:A:203:LYS:HE3	1.69	0.74
1:B:297:ASN:CB	1:B:300:LYS:HE3	2.16	0.74
1:B:255:ILE:HD12	1:B:261:ARG:HG3	1.70	0.74
1:B:347:ILE:O	1:B:351:THR:HG22	1.89	0.73
1:B:77:ARG:NH1	1:B:77:ARG:HB3	2.03	0.73
1:A:267:LEU:HD23	1:A:270:LYS:HZ1	1.53	0.73
1:A:246:SER:OG	1:A:267:LEU:HD21	1.89	0.72
1:A:252:LEU:O	1:A:261:ARG:NH1	2.22	0.72
1:B:200:LEU:O	1:B:257:ASN:HB2	1.88	0.72
1:A:175:ASP:CG	1:A:178:HIS:HB2	2.15	0.72
1:A:30:TYR:CD2	1:A:38:MET:HE3	2.25	0.71
1:A:37:GLY:HA3	1:A:55:LYS:O	1.91	0.71
1:B:118:THR:HG23	1:B:119:GLN:H	1.56	0.71
1:A:89:ILE:HG21	1:A:351:THR:HG22	1.72	0.70
1:B:91:ARG:NH1	1:B:351:THR:HG23	2.05	0.70
1:B:297:ASN:N	1:B:300:LYS:HE3	2.06	0.70
1:B:252:LEU:HD12	1:B:255:ILE:CD1	2.22	0.70
1:B:172:ARG:NH2	7:B:502:HOH:O	2.25	0.69
1:B:182:GLY:O	1:B:183:PHE:HB2	1.90	0.69
1:B:42:ALA:O	1:B:50:ARG:HG2	1.93	0.69
1:B:274:PRO:HD2	1:B:277:ARG:HG3	1.75	0.69
1:B:37:GLY:HA2	1:B:55:LYS:O	1.93	0.69
1:B:88:ASP:HB3	1:B:104:VAL:CG2	2.23	0.68
1:A:181:THR:O	1:A:181:THR:HG22	1.94	0.68
1:A:85:GLY:O	1:A:105:GLN:HG2	1.95	0.67
1:B:91:ARG:HH21	1:B:355:GLN:HG3	1.58	0.67
1:B:243:ILE:HD13	1:B:278:LEU:HD21	1.78	0.66
1:A:89:ILE:HG21	1:A:351:THR:CG2	2.25	0.66
1:A:14:VAL:HG13	1:A:38:MET:HE1	1.78	0.66
1:A:241:LEU:HD13	1:A:247:PRO:HD3	1.78	0.66
1:B:30:TYR:HA	1:B:40:CYS:SG	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASN:O	1:B:49:VAL:HG12	1.96	0.65
1:B:92:ALA:HB1	1:B:97:GLN:CG	2.26	0.65
1:B:241:LEU:HD22	1:B:247:PRO:HD3	1.79	0.65
1:B:92:ALA:CB	1:B:97:GLN:HG2	2.26	0.65
1:A:257:ASN:OD1	1:A:260:ALA:N	2.31	0.64
1:B:246:SER:OG	1:B:270:LYS:N	2.30	0.64
5:A:405:B8Z:S25	1:B:187:TYR:CD1	2.91	0.64
1:A:267:LEU:HD23	1:A:270:LYS:NZ	2.12	0.64
1:B:183:PHE:HZ	1:B:257:ASN:CB	2.10	0.64
1:A:267:LEU:HD13	1:A:267:LEU:O	1.97	0.63
1:B:59:PHE:CZ	1:B:98:MET:HE3	2.33	0.63
1:B:94:THR:HA	1:B:348:PHE:CZ	2.34	0.63
1:B:88:ASP:HA	1:B:354:PHE:CD1	2.34	0.62
1:A:261:ARG:HG3	1:A:265:LEU:CD1	2.29	0.62
1:A:252:LEU:O	1:A:261:ARG:CZ	2.46	0.62
1:A:261:ARG:HG3	1:A:265:LEU:HD13	1.81	0.62
1:B:267:LEU:CD2	1:B:268:PRO:HD2	2.29	0.62
1:B:31:ILE:HD11	1:B:41:SER:HB3	1.82	0.62
1:B:258:LEU:HD23	1:B:261:ARG:HD3	1.82	0.62
1:A:283:ASP:OD1	1:A:285:LYS:N	2.27	0.62
1:B:183:PHE:CZ	1:B:257:ASN:HB2	2.30	0.61
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.66	0.61
1:A:27:ASN:ND2	6:A:406:SO4:O4	2.34	0.61
1:B:35:ALA:N	7:B:504:HOH:O	2.33	0.60
1:A:31:ILE:HB	1:A:39:VAL:O	2.00	0.60
1:A:238:ASN:OD1	1:A:263:TYR:OH	2.19	0.60
1:B:88:ASP:HB3	1:B:104:VAL:HG21	1.83	0.60
1:A:252:LEU:HB3	1:A:261:ARG:CZ	2.32	0.59
1:B:91:ARG:HB2	1:B:98:MET:HG3	1.84	0.59
1:A:203:LYS:HD2	1:A:203:LYS:O	2.02	0.59
1:B:330:LYS:O	1:B:331:PHE:HB2	2.01	0.59
1:B:28:LEU:HA	1:B:42:ALA:HA	1.84	0.59
1:A:252:LEU:C	1:A:261:ARG:HH12	2.10	0.58
1:A:250:GLU:O	1:A:253:ASN:HB2	2.03	0.58
1:B:77:ARG:HG3	1:B:329:PHE:HE2	1.68	0.58
1:A:13:MET:HG2	1:A:14:VAL:N	2.19	0.58
1:A:186:GLU:O	4:A:403:GOL:H31	2.04	0.58
1:B:88:ASP:HA	1:B:354:PHE:CE1	2.38	0.58
1:B:29:SER:HB2	1:B:41:SER:OG	2.05	0.57
1:B:353:ARG:HG3	1:B:354:PHE:CD2	2.40	0.57
1:B:43:TYR:HA	1:B:50:ARG:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:O	1:A:267:LEU:HD12	2.05	0.57
1:A:66:GLN:O	1:A:70:ARG:HG3	2.05	0.56
1:B:87:ASN:HB2	1:B:104:VAL:HG23	1.87	0.56
1:B:46:VAL:HG13	1:B:47:ASN:OD1	2.05	0.56
1:B:95:ILE:HG22	1:B:344:LYS:HE2	1.87	0.56
1:B:108:MET:O	2:B:402:5ID:H2	2.06	0.56
1:A:12:GLU:OE1	1:A:12:GLU:HA	2.06	0.56
1:A:56:ILE:HG22	1:A:58:PRO:HD3	1.87	0.56
1:A:192:TRP:CD1	1:A:229:PRO:HA	2.41	0.55
1:B:91:ARG:NH2	1:B:355:GLN:HG3	2.21	0.55
1:B:283:ASP:OD1	1:B:285:LYS:HB2	2.06	0.55
1:A:332:ASP:C	1:A:333:MET:HG2	2.31	0.55
1:B:243:ILE:CD1	1:B:278:LEU:HD21	2.36	0.55
1:A:11:PRO:O	1:A:12:GLU:HB2	2.07	0.55
1:B:258:LEU:CD2	1:B:261:ARG:HD3	2.36	0.55
1:B:90:ILE:O	1:B:90:ILE:HD12	2.07	0.55
1:B:88:ASP:HB3	1:B:104:VAL:HG22	1.88	0.54
1:B:241:LEU:CD2	1:B:247:PRO:HD3	2.37	0.54
1:A:264:LEU:O	1:A:267:LEU:HB3	2.08	0.54
1:A:181:THR:HA	1:A:202:SER:HB3	1.89	0.54
1:B:66:GLN:HE22	3:B:401:EPE:H62	1.72	0.54
1:B:12:GLU:HG3	1:B:13:MET:SD	2.48	0.54
1:A:261:ARG:HD2	1:A:265:LEU:HD11	1.90	0.54
5:A:405:B8Z:C30	5:A:405:B8Z:C27	2.86	0.54
1:B:12:GLU:O	1:B:13:MET:HB2	2.07	0.54
5:A:405:B8Z:C01	1:B:184:LEU:HD22	2.36	0.53
1:A:257:ASN:HB3	1:A:260:ALA:CB	2.39	0.53
1:B:94:THR:HG22	1:B:97:GLN:NE2	2.22	0.53
1:A:19:PHE:O	1:A:21:VAL:N	2.40	0.53
1:B:142:SER:HG	1:B:325:ALA:H	1.57	0.53
1:B:94:THR:HG22	1:B:97:GLN:OE1	2.08	0.53
1:A:335:LEU:HA	1:A:338:LEU:HD13	1.90	0.53
1:B:297:ASN:HB3	1:B:300:LYS:HG2	1.91	0.52
1:A:59:PHE:HA	1:A:65:CYS:SG	2.48	0.52
1:B:94:THR:HG22	1:B:97:GLN:HE22	1.73	0.52
1:A:359:ARG:O	1:A:360:SER:HB2	2.09	0.52
1:A:19:PHE:C	1:A:21:VAL:H	2.15	0.52
1:B:13:MET:HE1	1:B:18:VAL:HG22	1.91	0.52
1:B:30:TYR:H	1:B:40:CYS:HB3	1.73	0.52
1:A:330:LYS:HA	1:A:330:LYS:CE	2.33	0.51
1:B:95:ILE:HG12	1:B:348:PHE:CG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:OG1	1:B:182:GLY:N	2.43	0.51
1:A:91:ARG:HD2	1:A:98:MET:SD	2.50	0.51
1:A:317:TYR:CZ	1:A:319:PRO:HG3	2.45	0.51
1:A:334:GLU:OE1	1:A:334:GLU:HA	2.09	0.51
1:B:238:ASN:ND2	7:B:508:HOH:O	2.43	0.51
1:A:22:GLY:HA2	1:A:23:PRO:C	2.36	0.51
1:B:77:ARG:HB3	1:B:77:ARG:CZ	2.40	0.51
1:B:95:ILE:CG2	1:B:344:LYS:HE2	2.41	0.51
1:B:61:HIS:HB3	4:B:404:GOL:O2	2.11	0.51
1:B:24:ARG:HE	1:B:44:ASP:CG	2.19	0.50
1:B:333:MET:HE1	1:B:346:LEU:HD11	1.92	0.50
1:A:175:ASP:HB3	1:A:178:HIS:HB3	1.93	0.50
1:B:243:ILE:HD13	1:B:278:LEU:CD2	2.41	0.50
1:B:264:LEU:O	1:B:267:LEU:HB2	2.12	0.50
1:B:26:THR:O	1:B:43:TYR:HB3	2.12	0.50
1:B:81:GLU:HG3	7:B:544:HOH:O	2.10	0.50
1:B:94:THR:HA	1:B:348:PHE:CE1	2.47	0.50
1:B:288:ASP:OD2	1:B:292:LYS:HE2	2.12	0.50
1:B:69:LEU:HD23	1:B:335:LEU:CD2	2.42	0.50
1:B:188:VAL:O	1:B:189:ALA:HB3	2.12	0.49
1:A:262:ASN:O	1:A:266:SER:OG	2.30	0.49
1:B:32:GLY:O	1:B:33:GLU:HG3	2.12	0.49
1:A:119:GLN:HG2	5:A:405:B8Z:C05	2.41	0.49
1:A:255:ILE:O	1:A:255:ILE:HG22	2.13	0.49
1:B:12:GLU:O	1:B:13:MET:CB	2.61	0.49
1:B:91:ARG:HD2	1:B:92:ALA:O	2.11	0.49
1:B:91:ARG:HH11	1:B:351:THR:HG23	1.76	0.48
1:A:215:GLY:CA	1:A:293:MET:HE3	2.31	0.48
1:B:98:MET:CE	1:B:344:LYS:HE3	2.43	0.48
1:B:199:MET:O	1:B:200:LEU:HB2	2.12	0.48
1:B:234:LEU:HD21	1:B:260:ALA:CB	2.43	0.48
1:B:241:LEU:HD12	1:B:264:LEU:HD22	1.95	0.48
1:A:71:GLU:OE2	7:A:501:HOH:O	2.20	0.48
1:A:163:LEU:HD23	1:A:163:LEU:C	2.38	0.48
1:B:274:PRO:HD2	1:B:277:ARG:CG	2.42	0.48
1:B:148:ARG:CD	1:B:170:LEU:O	2.54	0.48
1:B:234:LEU:HD21	1:B:260:ALA:HB1	1.95	0.48
1:A:105:GLN:OE1	2:A:401:5ID:IAE	3.02	0.48
1:A:246:SER:OG	1:A:269:HIS:HA	2.14	0.48
1:B:94:THR:HG22	1:B:97:GLN:CD	2.39	0.48
1:A:292:LYS:O	1:A:295:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HG13	1:A:38:MET:CE	2.42	0.47
1:A:337:ASP:O	1:A:338:LEU:HD12	2.15	0.47
1:B:214:VAL:CG1	1:B:293:MET:HE1	2.45	0.47
1:B:62:GLN:O	1:B:63:THR:CB	2.61	0.47
1:B:105:GLN:OE1	2:B:402:5ID:IAE	3.02	0.47
1:B:98:MET:HE2	1:B:344:LYS:HE3	1.97	0.47
1:B:297:ASN:O	1:B:300:LYS:HG2	2.14	0.47
1:B:353:ARG:HD2	1:B:354:PHE:CE2	2.49	0.47
1:A:13:MET:O	1:A:14:VAL:HB	2.15	0.46
1:A:91:ARG:HH11	1:A:91:ARG:CG	2.29	0.46
1:B:19:PHE:O	1:B:21:VAL:N	2.45	0.46
1:B:75:LEU:HD21	1:B:168:PHE:CD1	2.51	0.46
1:A:261:ARG:CD	1:A:265:LEU:HD11	2.46	0.46
1:B:43:TYR:HA	1:B:50:ARG:HG2	1.96	0.46
1:B:77:ARG:HB3	1:B:77:ARG:HH11	1.77	0.46
1:A:332:ASP:OD1	1:A:332:ASP:N	2.45	0.46
1:A:60:GLU:O	1:A:340:LYS:NZ	2.33	0.46
1:A:119:GLN:HG2	5:A:405:B8Z:N06	2.29	0.46
1:B:19:PHE:HD1	1:B:21:VAL:HG13	1.81	0.46
1:B:41:SER:OG	7:B:501:HOH:O	2.21	0.46
1:A:261:ARG:HD2	1:A:265:LEU:CD1	2.45	0.46
1:B:111:ASP:OD1	1:B:113:TYR:HB3	2.16	0.46
1:B:24:ARG:HD3	1:B:25:TYR:CZ	2.51	0.46
1:B:91:ARG:NH1	1:B:348:PHE:O	2.49	0.46
1:B:180:HIS:HB2	1:B:181:THR:H	1.53	0.45
1:A:177:ASP:O	1:A:178:HIS:C	2.59	0.45
1:A:30:TYR:HD2	1:A:38:MET:CE	2.19	0.45
1:A:22:GLY:HA2	1:A:24:ARG:N	2.32	0.45
1:A:283:ASP:OD1	1:A:283:ASP:C	2.59	0.45
1:A:252:LEU:HD23	1:A:255:ILE:HD12	1.99	0.45
1:A:306:GLN:OE1	4:A:404:GOL:H11	2.17	0.45
1:A:257:ASN:HB3	1:A:260:ALA:HB2	1.99	0.45
1:A:297:ASN:H	1:A:300:LYS:HZ3	1.62	0.45
1:B:121:LEU:HB3	1:B:126:ILE:HG13	1.98	0.45
1:B:310:HIS:CG	1:B:311:PRO:HD2	2.51	0.45
2:A:401:5ID:H5'1	2:A:401:5ID:N3	2.32	0.45
1:B:43:TYR:CD1	1:B:43:TYR:C	2.95	0.45
1:B:59:PHE:HA	1:B:65:CYS:SG	2.57	0.45
1:B:198:ILE:O	1:B:202:SER:HA	2.16	0.45
1:B:204:GLY:HA2	1:B:209:ILE:CD1	2.46	0.45
1:A:13:MET:O	1:A:14:VAL:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:HG2	1:A:135:ARG:HH12	1.82	0.44
1:A:257:ASN:HB3	1:A:260:ALA:HB3	1.99	0.44
1:A:181:THR:O	1:A:181:THR:CG2	2.63	0.44
1:B:151:LYS:NZ	7:B:511:HOH:O	2.46	0.44
1:A:175:ASP:HB3	1:A:178:HIS:CB	2.48	0.44
1:A:179:ASP:OD1	1:A:180:HIS:N	2.51	0.44
1:A:337:ASP:C	1:A:338:LEU:HD12	2.43	0.44
1:B:207:LYS:NZ	7:B:515:HOH:O	2.49	0.44
1:A:146:LEU:HD11	1:A:205:TYR:C	2.42	0.44
1:B:118:THR:HG23	1:B:119:GLN:N	2.29	0.44
1:A:13:MET:O	1:A:14:VAL:HG12	2.18	0.44
1:A:30:TYR:CE1	1:A:32:GLY:HA2	2.53	0.44
1:A:267:LEU:HD22	1:A:268:PRO:C	2.43	0.44
1:B:255:ILE:HG21	1:B:261:ARG:HB2	1.99	0.44
1:B:297:ASN:H	1:B:300:LYS:CE	2.19	0.44
1:A:297:ASN:HB3	1:A:300:LYS:HD3	2.00	0.43
1:B:43:TYR:CA	1:B:50:ARG:HG2	2.48	0.43
1:B:43:TYR:CB	1:B:50:ARG:HG2	2.48	0.43
1:B:198:ILE:C	1:B:199:MET:O	2.60	0.43
1:A:97:GLN:O	1:A:97:GLN:HG2	2.18	0.43
1:A:345:GLU:O	1:A:349:GLU:HG3	2.18	0.43
1:B:43:TYR:C	1:B:43:TYR:HD1	2.26	0.43
1:B:249:GLN:HA	1:B:252:LEU:HB3	2.01	0.43
1:A:81:GLU:CG	1:A:135:ARG:HH12	2.31	0.43
1:B:278:LEU:HD12	1:B:278:LEU:H	1.83	0.43
1:B:335:LEU:H	1:B:335:LEU:HD12	1.84	0.43
1:B:55:LYS:HE3	1:B:100:ASP:OD2	2.18	0.43
1:B:73:LYS:O	1:B:77:ARG:HG2	2.19	0.43
1:B:333:MET:O	1:B:333:MET:HG2	2.19	0.43
1:A:90:ILE:HG12	1:A:102:TYR:HB2	2.01	0.43
1:B:241:LEU:HD13	1:B:247:PRO:HD3	2.00	0.43
1:B:97:GLN:OE1	1:B:97:GLN:N	2.49	0.43
1:B:235:ASP:O	1:B:238:ASN:HB3	2.19	0.43
1:B:28:LEU:HD12	1:B:28:LEU:N	2.34	0.42
1:B:283:ASP:OD1	1:B:285:LYS:N	2.49	0.42
1:B:33:GLU:HA	1:B:38:MET:HA	2.01	0.42
1:B:141:HIS:CE1	1:B:207:LYS:HB3	2.54	0.42
1:B:252:LEU:HA	1:B:255:ILE:HD11	2.01	0.42
1:A:12:GLU:HB2	1:A:19:PHE:O	2.19	0.42
1:A:13:MET:CG	1:A:14:VAL:H	2.33	0.42
1:A:75:LEU:HD21	1:A:168:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:VAL:HG11	1:B:293:MET:HE1	2.02	0.42
1:B:252:LEU:O	1:B:261:ARG:NE	2.53	0.42
1:B:333:MET:CE	1:B:346:LEU:HD11	2.50	0.42
1:A:120:HIS:O	5:A:405:B8Z:N08	2.53	0.41
1:A:215:GLY:HA2	1:A:293:MET:CE	2.34	0.41
1:B:278:LEU:HD12	1:B:278:LEU:N	2.35	0.41
1:A:252:LEU:HB3	1:A:261:ARG:NH1	2.34	0.41
1:B:119:GLN:NE2	7:B:517:HOH:O	2.53	0.41
1:A:13:MET:HG2	1:A:14:VAL:H	1.85	0.41
1:A:54:LYS:HE3	1:A:56:ILE:HD11	2.03	0.41
1:B:237:LEU:HA	1:B:237:LEU:HD23	1.78	0.41
1:B:265:LEU:C	1:B:267:LEU:H	2.29	0.41
1:B:275:TRP:CD1	1:B:291:ASP:HB2	2.54	0.41
1:A:54:LYS:O	1:A:102:TYR:HA	2.20	0.41
1:B:13:MET:HE1	1:B:18:VAL:CG2	2.50	0.41
1:B:44:ASP:OD1	1:B:46:VAL:HG12	2.20	0.41
1:A:128:TYR:O	1:A:132:GLN:HG3	2.20	0.41
1:A:239:HIS:HD2	7:A:551:HOH:O	2.03	0.41
1:B:192:TRP:CD1	1:B:229:PRO:HA	2.56	0.41
1:B:200:LEU:O	1:B:257:ASN:CB	2.64	0.41
1:A:125:NEP:HE1	5:A:405:B8Z:C27	2.51	0.41
1:A:30:TYR:OH	1:A:33:GLU:HG2	2.21	0.40
1:B:227:ILE:O	1:B:227:ILE:HG12	2.21	0.40
1:B:34:GLY:HA3	7:B:504:HOH:O	2.21	0.40
1:A:11:PRO:O	1:A:12:GLU:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	348/368 (95%)	312 (90%)	27 (8%)	9 (3%)	4 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	343/368 (93%)	287 (84%)	38 (11%)	18 (5%)	1	0
All	All	691/736 (94%)	599 (87%)	65 (9%)	27 (4%)	2	0

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	35	ALA
1	B	63	THR
1	B	177	ASP
1	B	178	HIS
1	A	12	GLU
1	B	13	MET
1	B	14	VAL
1	B	22	GLY
1	B	183	PHE
1	A	20	ASP
1	B	30	TYR
1	B	202	SER
1	B	334	GLU
1	A	58	PRO
1	A	178	HIS
1	A	269	HIS
1	B	20	ASP
1	B	43	TYR
1	B	88	ASP
1	A	11	PRO
1	B	23	PRO
1	B	331	PHE
1	A	13	MET
1	B	245	GLY
1	B	182	GLY
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%)	289 (92%)	27 (8%)	10	7
1	B	312/323 (97%)	291 (93%)	21 (7%)	15	12
All	All	628/646 (97%)	580 (92%)	48 (8%)	12	9

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	17	GLN
1	A	19	PHE
1	A	21	VAL
1	A	36	TYR
1	A	56	ILE
1	A	76	LEU
1	A	90	ILE
1	A	96	GLU
1	A	117	LYS
1	A	118	THR
1	A	177	ASP
1	A	184	LEU
1	A	203	LYS
1	A	233	TYR
1	A	238	ASN
1	A	256	ILE
1	A	259	LYS
1	A	266	SER
1	A	267	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	A	359	ARG
1	B	19	PHE
1	B	26	THR
1	B	31	ILE
1	B	46	VAL
1	B	56	ILE
1	B	57	SER
1	B	63	THR
1	B	79	ARG

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Mol	Chain	Res	Type
1	B	91	ARG
1	B	116	LEU
1	B	118	THR
1	B	146	LEU
1	B	177	ASP
1	B	180	HIS
1	B	183	PHE
1	B	201	ASN
1	B	259	LYS
1	B	270	LYS
1	B	331	PHE
1	B	335	LEU
1	B	351	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	239	HIS
1	B	61	HIS
1	B	123	ASN
1	B	201	ASN
1	B	238	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	B	125	1	11,14,15	2.95	4 (36%)	8,20,22	2.28	2 (25%)
1	NEP	A	125	1	11,14,15	2.70	3 (27%)	8,20,22	2.62	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	B	125	1	-	3/5/12/14	0/1/1/1
1	NEP	A	125	1	-	2/5/12/14	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	125	NEP	P-O3P	7.50	1.57	1.46
1	A	125	NEP	P-O3P	6.75	1.56	1.46
1	B	125	NEP	P-O2P	-4.66	1.44	1.56
1	A	125	NEP	P-O2P	-4.11	1.45	1.56
1	B	125	NEP	CD2-CG	3.15	1.41	1.36
1	A	125	NEP	CD2-CG	3.15	1.41	1.36
1	B	125	NEP	CA-N	-2.05	1.42	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	NEP	O1P-P-O3P	-6.53	96.89	112.95
1	B	125	NEP	O1P-P-O3P	-5.87	98.52	112.95
1	A	125	NEP	O2P-P-O3P	3.41	121.35	112.95
1	B	125	NEP	O2P-P-O3P	2.60	119.34	112.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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](#)

10 ligands 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	$\# Z > 2$
3	EPE	B	401	-	15,15,15	0.94	1 (6%)	19,20,20	1.88	5 (26%)
4	GOL	B	403	-	5,5,5	1.25	0	5,5,5	1.50	1 (20%)
4	GOL	A	403	-	5,5,5	0.75	0	5,5,5	1.11	1 (20%)
2	5ID	B	402	-	21,22,22	3.47	8 (38%)	28,33,33	2.56	8 (28%)
4	GOL	B	404	-	5,5,5	0.45	0	5,5,5	0.88	0
2	5ID	A	401	-	21,22,22	3.53	7 (33%)	28,33,33	3.01	10 (35%)
4	GOL	A	404	-	5,5,5	1.10	0	5,5,5	1.41	1 (20%)
5	B8Z	A	405	-	33,33,33	3.79	13 (39%)	44,46,46	2.63	18 (40%)
6	SO4	A	406	-	4,4,4	0.34	0	6,6,6	0.11	0
3	EPE	A	402	-	15,15,15	0.89	1 (6%)	19,20,20	1.88	5 (26%)

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
3	EPE	B	401	-	-	5/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	403	-	-	2/4/4/4	-
4	GOL	A	403	-	-	2/4/4/4	-
2	5ID	B	402	-	-	0/6/22/22	0/3/3/3
4	GOL	B	404	-	-	2/4/4/4	-
2	5ID	A	401	-	-	3/6/22/22	0/3/3/3
4	GOL	A	404	-	-	1/4/4/4	-
5	B8Z	A	405	-	-	5/17/17/17	0/4/4/4
3	EPE	A	402	-	-	5/9/19/19	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	B8Z	C15-C14	11.02	1.57	1.49
5	A	405	B8Z	C07-S25	9.54	1.87	1.75
2	A	401	5ID	O4'-C1'	9.52	1.64	1.42
2	B	402	5ID	O4'-C1'	9.36	1.63	1.42
5	A	405	B8Z	O29-C30	8.36	1.66	1.42
2	B	402	5ID	O4'-C4'	-7.43	1.28	1.45
2	A	401	5ID	O4'-C4'	-7.30	1.28	1.45
5	A	405	B8Z	O02-C01	7.26	1.63	1.42
2	A	401	5ID	C2'-C1'	-7.16	1.31	1.53
2	B	402	5ID	C2'-C1'	-6.89	1.31	1.53
5	A	405	B8Z	O29-C28	5.00	1.45	1.37
5	A	405	B8Z	C09-N08	4.92	1.46	1.37
2	B	402	5ID	C6-N6	4.64	1.46	1.34
2	A	401	5ID	C6-N6	4.34	1.45	1.34
5	A	405	B8Z	C14-S13	4.12	1.79	1.72
2	A	401	5ID	O2'-C2'	3.98	1.52	1.43
5	A	405	B8Z	C07-N08	3.18	1.42	1.38
3	B	401	EPE	C10-S	3.11	1.81	1.77
2	B	402	5ID	O2'-C2'	3.07	1.50	1.43
5	A	405	B8Z	C05-N06	3.06	1.46	1.39
2	A	401	5ID	C8-N9	-2.91	1.33	1.38
3	A	402	EPE	C10-S	2.88	1.81	1.77
2	B	402	5ID	C8-N9	-2.85	1.33	1.38
5	A	405	B8Z	C11-N24	2.84	1.44	1.38
5	A	405	B8Z	C04-C03	2.77	1.43	1.38
2	A	401	5ID	O3'-C3'	-2.32	1.37	1.43
2	B	402	5ID	O3'-C3'	-2.23	1.37	1.43
5	A	405	B8Z	C26-S25	2.22	1.78	1.74
5	A	405	B8Z	C11-C09	2.14	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	5ID	C5-C4	-2.08	1.38	1.40

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	5ID	C5-C4-N3	-9.84	116.53	126.97
5	A	405	B8Z	C11-N24-C14	7.48	113.25	110.27
2	B	402	5ID	C5-C4-N3	-7.17	119.36	126.97
5	A	405	B8Z	N08-C07-N06	7.07	132.95	120.87
5	A	405	B8Z	S25-C07-N06	-6.88	108.79	117.06
2	B	402	5ID	C4-N9-C8	6.01	110.56	108.08
2	B	402	5ID	N3-C2-N1	-5.16	120.77	128.58
2	A	401	5ID	C1'-N9-C8	-4.92	120.14	125.72
5	A	405	B8Z	C26-S25-C07	4.87	92.84	88.33
2	A	401	5ID	N3-C2-N1	-4.77	121.36	128.58
2	A	401	5ID	N3-C4-N9	4.70	135.16	127.17
2	A	401	5ID	C2-N3-C4	4.64	123.16	111.83
3	B	401	EPE	C5-N4-C3	4.61	118.76	108.84
2	A	401	5ID	C6-C5-C4	4.46	119.08	115.74
3	A	402	EPE	C5-N4-C3	4.34	118.19	108.84
3	A	402	EPE	C7-N4-C5	4.14	122.28	111.24
2	B	402	5ID	C2-N3-C4	3.97	121.52	111.83
5	A	405	B8Z	C01-O02-C03	-3.68	112.11	117.51
3	B	401	EPE	C7-N4-C5	3.66	121.00	111.24
5	A	405	B8Z	O29-C28-C03	3.40	120.02	115.40
3	B	401	EPE	C7-N4-C3	3.37	120.23	111.24
2	A	401	5ID	C4-N9-C8	3.19	109.40	108.08
2	A	401	5ID	C3'-C2'-C1'	3.10	107.34	101.46
2	B	402	5ID	N3-C4-N9	3.09	132.42	127.17
3	A	402	EPE	C7-N4-C3	3.08	119.44	111.24
5	A	405	B8Z	S13-C14-N24	-3.02	112.14	114.68
5	A	405	B8Z	C30-O29-C28	-3.00	113.12	117.51
2	B	402	5ID	C5'-C4'-C3'	-2.89	108.27	115.10
4	B	403	GOL	C3-C2-C1	-2.83	101.41	111.80
3	A	402	EPE	O2S-S-C10	2.73	110.86	106.73
5	A	405	B8Z	C27-C26-S25	2.71	132.82	126.07
2	B	402	5ID	C6-C5-C4	2.58	117.67	115.74
5	A	405	B8Z	O10-C09-N08	-2.56	118.31	122.88
5	A	405	B8Z	C05-C26-S25	-2.49	106.06	109.75
4	A	404	GOL	C3-C2-C1	-2.46	102.78	111.80
3	A	402	EPE	C6-N1-C2	2.40	114.01	108.84
5	A	405	B8Z	C04-C05-N06	-2.38	124.19	129.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	B8Z	C07-N08-C09	2.37	127.32	123.78
2	B	402	5ID	O4'-C1'-N9	2.35	112.61	108.09
5	A	405	B8Z	S25-C07-N08	-2.34	117.78	121.87
5	A	405	B8Z	C05-N06-C07	2.32	114.15	108.66
5	A	405	B8Z	C12-C11-N24	-2.28	112.30	115.43
5	A	405	B8Z	O10-C09-C11	-2.27	115.47	121.15
4	A	403	GOL	C3-C2-C1	-2.19	103.77	111.80
2	A	401	5ID	C2'-C3'-C4'	2.15	106.77	102.61
2	A	401	5ID	C5-C6-N6	-2.11	120.61	123.40
3	B	401	EPE	C6-N1-C2	2.11	113.39	108.84
3	B	401	EPE	O1S-S-C10	2.08	109.86	106.73
5	A	405	B8Z	C04-C05-C26	-2.04	117.89	120.08

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	EPE	C8-C7-N4-C5
3	B	401	EPE	C9-C10-S-O1S
3	B	401	EPE	C9-C10-S-O3S
4	B	403	GOL	O1-C1-C2-C3
4	B	404	GOL	O1-C1-C2-C3
3	B	401	EPE	N4-C7-C8-O8
2	A	401	5ID	O4'-C4'-C5'-O5'
2	A	401	5ID	C3'-C4'-C5'-O5'
5	A	405	B8Z	C28-C03-O02-C01
5	A	405	B8Z	C04-C03-O02-C01
5	A	405	B8Z	S25-C07-N08-C09
3	A	402	EPE	C9-C10-S-O3S
4	A	403	GOL	O1-C1-C2-C3
4	A	403	GOL	O1-C1-C2-O2
4	B	404	GOL	O1-C1-C2-O2
3	B	401	EPE	C8-C7-N4-C5
3	A	402	EPE	C9-C10-S-O1S
3	A	402	EPE	C9-C10-S-O2S
3	B	401	EPE	C9-C10-S-O2S
3	A	402	EPE	S-C10-C9-N1
4	A	404	GOL	O2-C2-C3-O3
5	A	405	B8Z	C18-C17-O16-C15
2	A	401	5ID	O4'-C1'-N9-C8
5	A	405	B8Z	C23-C17-O16-C15
4	B	403	GOL	O1-C1-C2-O2

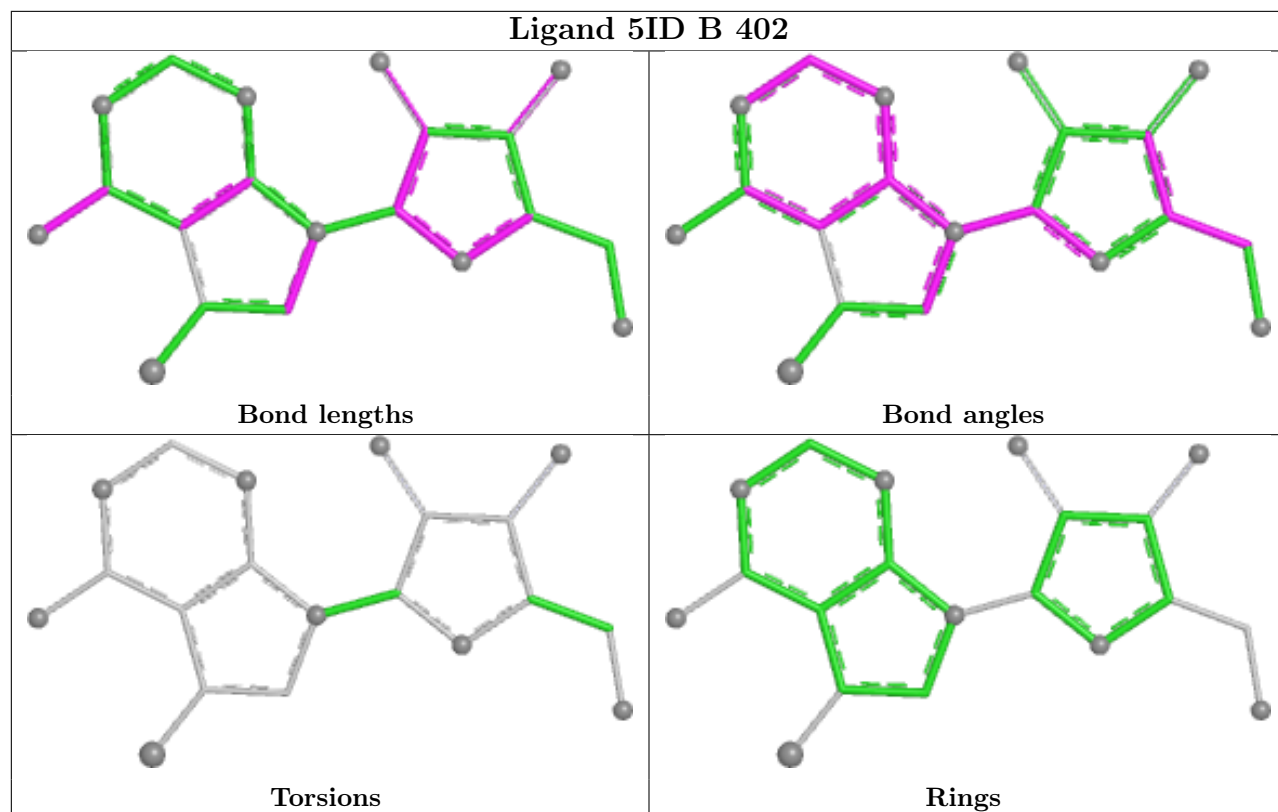
There are no ring outliers.

8 monomers are involved in 22 short contacts:

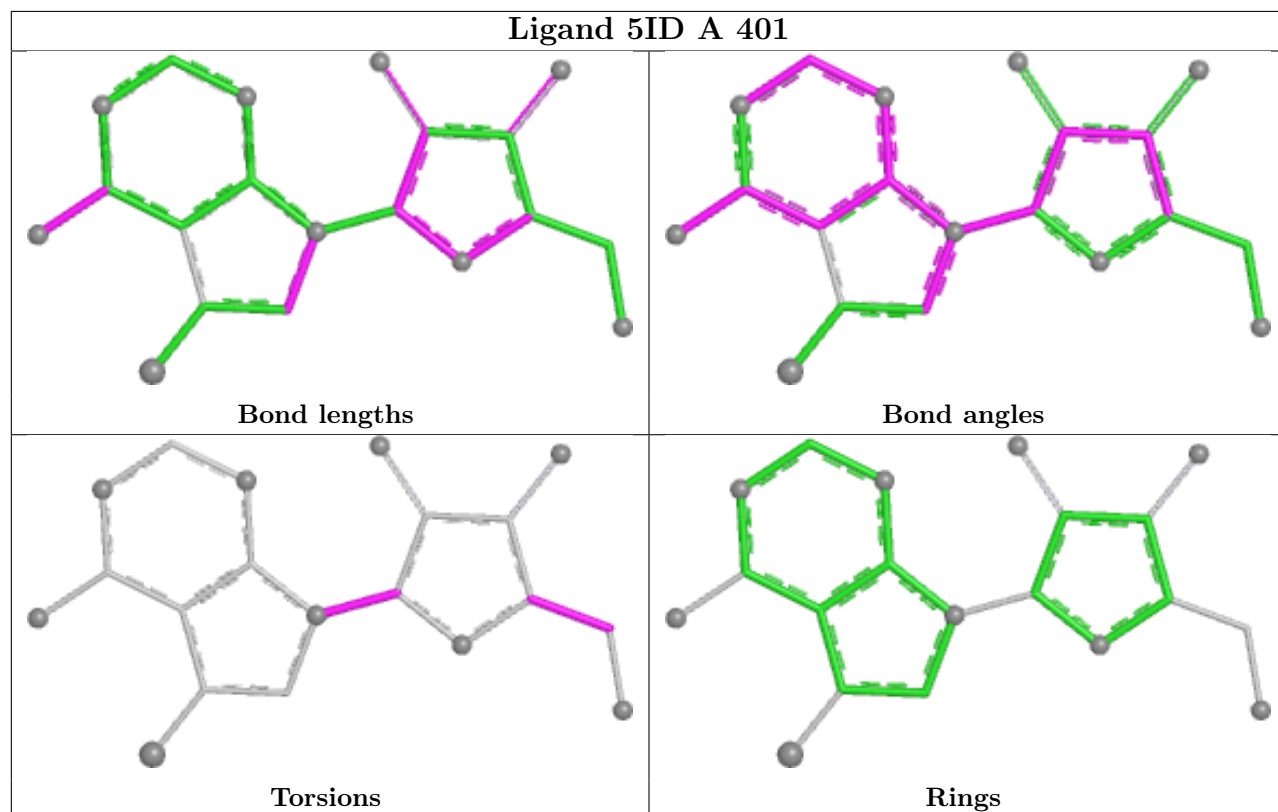
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	EPE	1	0
4	A	403	GOL	1	0
2	B	402	5ID	3	0
4	B	404	GOL	1	0
2	A	401	5ID	3	0
4	A	404	GOL	2	0
5	A	405	B8Z	10	0
6	A	406	SO4	1	0

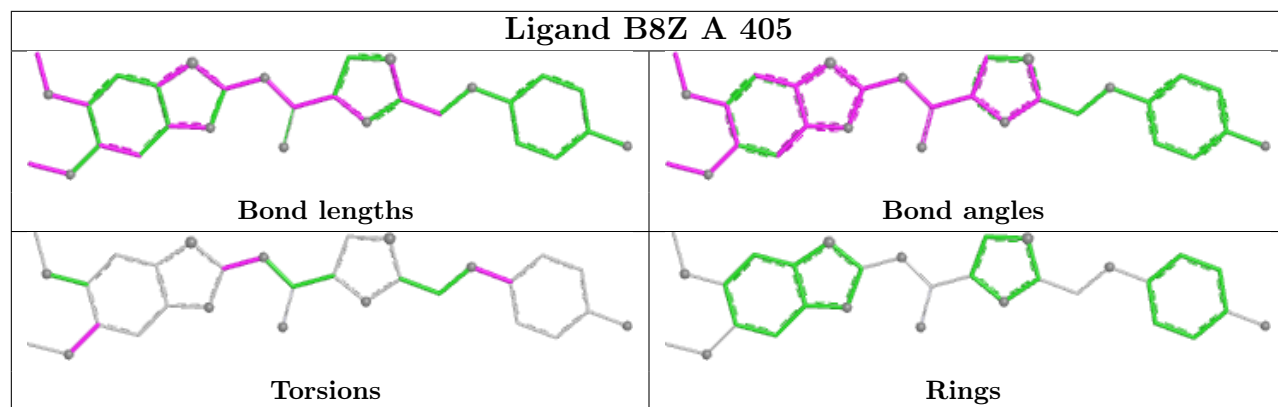
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 5ID B 402



Ligand 5ID A 401





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	350/368 (95%)	0.70	32 (9%) 15 15	39, 60, 96, 120	0
1	B	345/368 (93%)	0.86	40 (11%) 9 10	40, 65, 102, 113	0
All	All	695/736 (94%)	0.78	72 (10%) 11 12	39, 62, 100, 120	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	ILE	4.9
1	A	11	PRO	4.5
1	B	255	ILE	4.3
1	B	258	LEU	4.2
1	A	254	CYS	4.1
1	B	256	ILE	4.1
1	A	258	LEU	4.1
1	B	200	LEU	4.1
1	B	252	LEU	4.0
1	A	13	MET	3.5
1	A	267	LEU	3.5
1	B	356	PRO	3.5
1	A	181	THR	3.4
1	A	36	TYR	3.4
1	B	181	THR	3.3
1	B	357	GLY	3.3
1	B	329	PHE	3.2
1	A	14	VAL	3.1
1	A	203	LYS	3.0
1	A	182	GLY	2.9
1	B	14	VAL	2.9
1	B	43	TYR	2.9
1	A	10	GLY	2.9
1	B	36	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	180	HIS	2.8
1	B	46	VAL	2.8
1	A	255	ILE	2.8
1	A	120	HIS	2.8
1	B	331	PHE	2.7
1	B	21	VAL	2.7
1	B	35	ALA	2.7
1	A	61	HIS	2.6
1	A	260	ALA	2.6
1	B	50	ARG	2.6
1	B	273	VAL	2.6
1	B	45	ASN	2.6
1	B	183	PHE	2.6
1	A	39	VAL	2.5
1	B	30	TYR	2.5
1	A	263	TYR	2.5
1	B	263	TYR	2.5
1	B	23	PRO	2.5
1	B	90	ILE	2.5
1	B	269	HIS	2.4
1	A	92	ALA	2.3
1	B	18	VAL	2.3
1	B	93	PRO	2.3
1	A	28	LEU	2.3
1	A	19	PHE	2.3
1	A	90	ILE	2.2
1	A	264	LEU	2.2
1	B	19	PHE	2.2
1	B	265	LEU	2.2
1	B	61	HIS	2.2
1	B	120	HIS	2.2
1	B	209	ILE	2.2
1	B	260	ALA	2.2
1	B	94	THR	2.1
1	A	31	ILE	2.1
1	A	34	GLY	2.1
1	B	272	LYS	2.1
1	A	252	LEU	2.1
1	B	267	LEU	2.1
1	A	334	GLU	2.1
1	A	180	HIS	2.1
1	B	26	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	259	LYS	2.1
1	A	21	VAL	2.1
1	A	329	PHE	2.1
1	A	35	ALA	2.1
1	A	333	MET	2.0
1	B	92	ALA	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	0.96	0.08	46,47,54,57	0
1	NEP	A	125	14/15	0.97	0.06	40,48,55,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

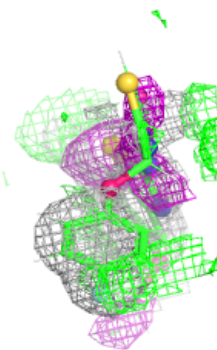
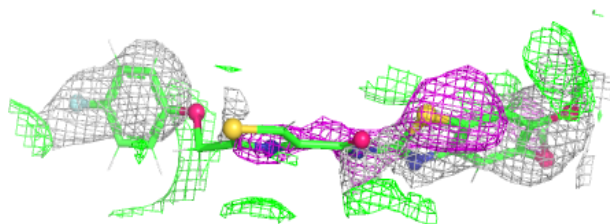
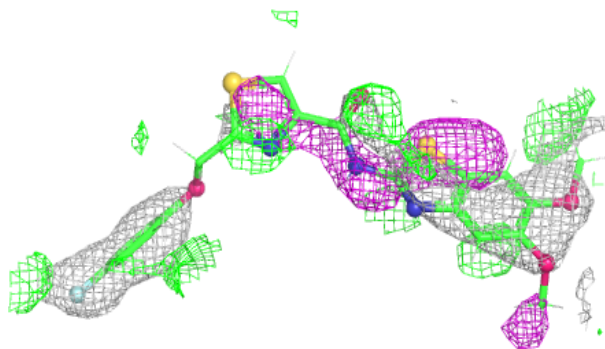
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	B8Z	A	405	30/30	0.60	0.24	61,76,96,103	46
4	GOL	B	404	6/6	0.73	0.14	75,90,95,97	0
4	GOL	A	403	6/6	0.74	0.15	59,71,89,96	0
4	GOL	A	404	6/6	0.76	0.12	63,76,88,88	0
6	SO4	A	406	5/5	0.79	0.10	84,88,100,102	0
4	GOL	B	403	6/6	0.84	0.11	60,81,93,97	0
2	5ID	A	401	20/20	0.90	0.13	64,88,107,125	0
3	EPE	A	402	15/15	0.91	0.10	67,92,110,121	0
3	EPE	B	401	15/15	0.92	0.11	56,83,104,117	0
2	5ID	B	402	20/20	0.94	0.12	65,90,115,119	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.

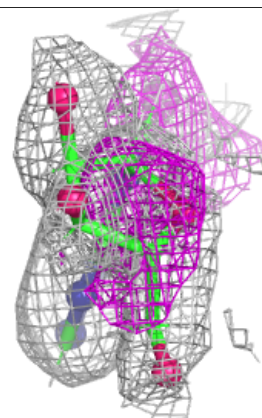
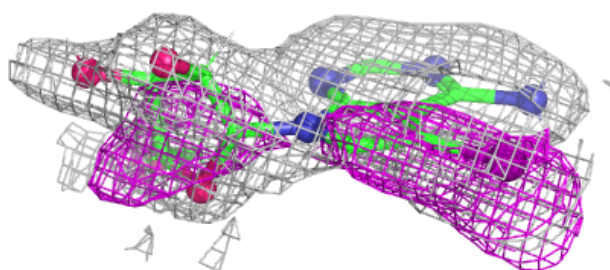
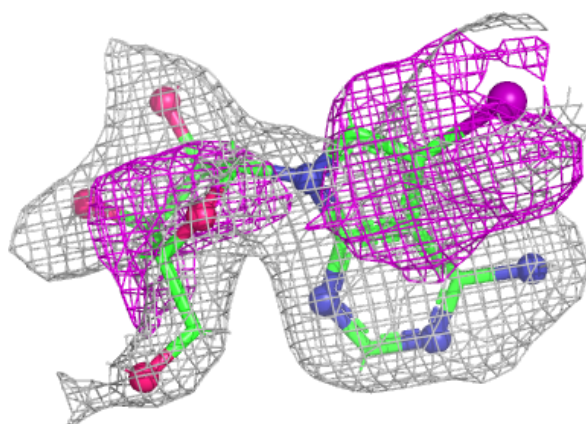
Electron density around B8Z A 405:

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

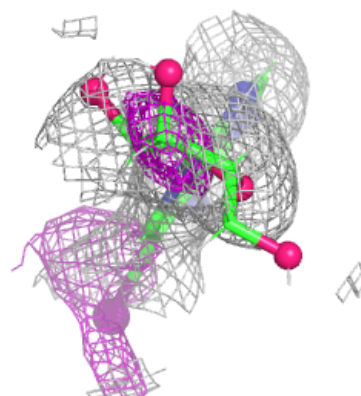
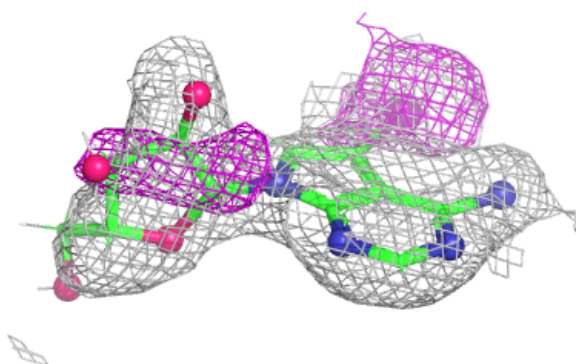
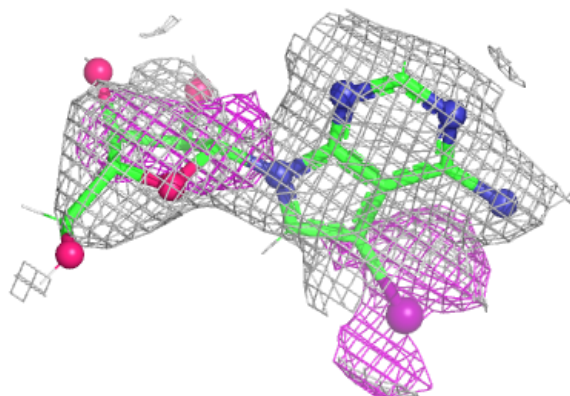


Electron density around 5ID A 401:

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

**Electron density around 5ID B 402:**

$2mF_o-DF_c$ (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.