



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:54 AM UTC

PDB ID : 2B1G / pdb_00002b1g
Title : Crystal structures of transition state analogue inhibitors of inosine monophosphate cyclohydrolase
Authors : Xu, L.; Chong, Y.; Hwang, I.; D'Onofrio, A.; Amore, K.; Beardsley, G.P.; Li, C.; Olson, A.J.; Boger, D.L.; Wilson, I.A.
Deposited on : 2005-09-15
Resolution : 2.10 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

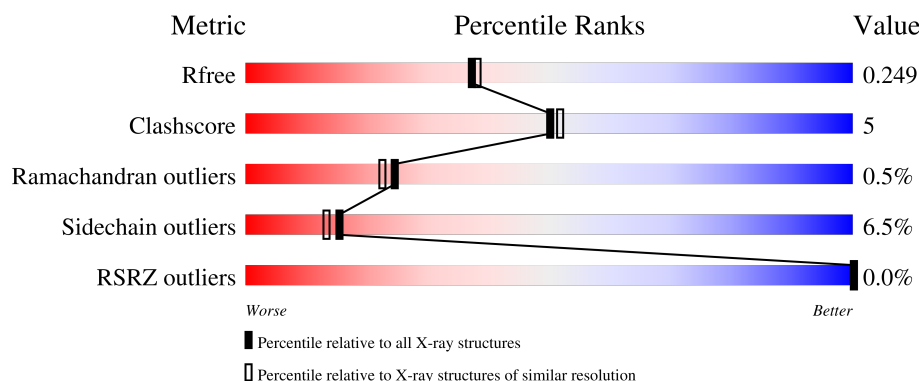
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	593	
1	B	593	
1	C	593	
1	D	593	

2 Entry composition [i](#)

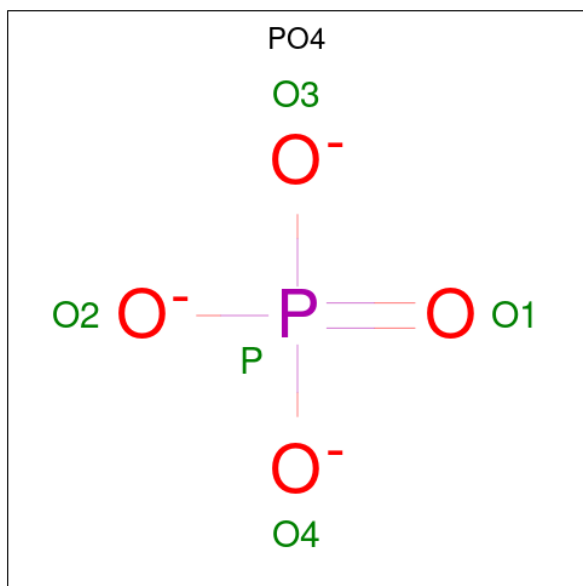
There are 5 unique types of molecules in this entry. The entry contains 18526 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional purine biosynthesis protein PURH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	0
			4511	2843	800	849	19			
1	B	590	Total	C	N	O	S	0	0	0
			4511	2843	800	849	19			
1	C	590	Total	C	N	O	S	0	0	0
			4511	2843	800	849	19			
1	D	590	Total	C	N	O	S	0	0	0
			4511	2843	800	849	19			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

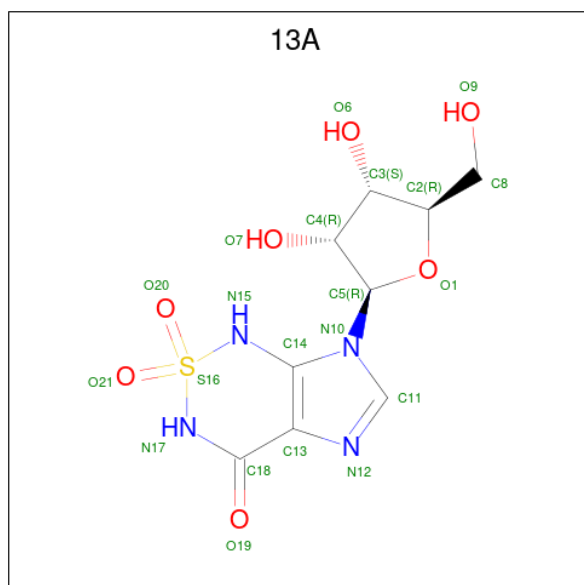


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0

- Molecule 4 is 7-(3,4-DIHYDROXY-5R-HYDROXYMETHYLTETRAHYDROFURAN-2-YL)-2,2-DIOXO-1,2R,3R,7-TETRAHYDRO-2L6-IMIDAZO[4,5-C][1,2,6]THIADIAZIN-4S-ONE (CCD ID: 13A) (formula: C₉H₁₂N₄O₇S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 21 9 4 7 1	0	0
4	D	1	Total C N O S 21 9 4 7 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	121	Total O 121 121	0	0
5	B	93	Total O 93 93	0	0

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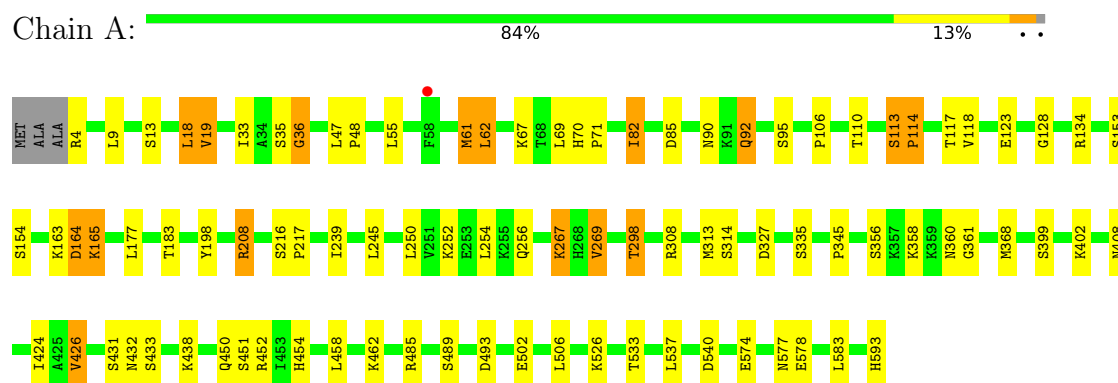
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	100	Total 100	O 100	0	0
5	D	112	Total 112	O 112	0	0

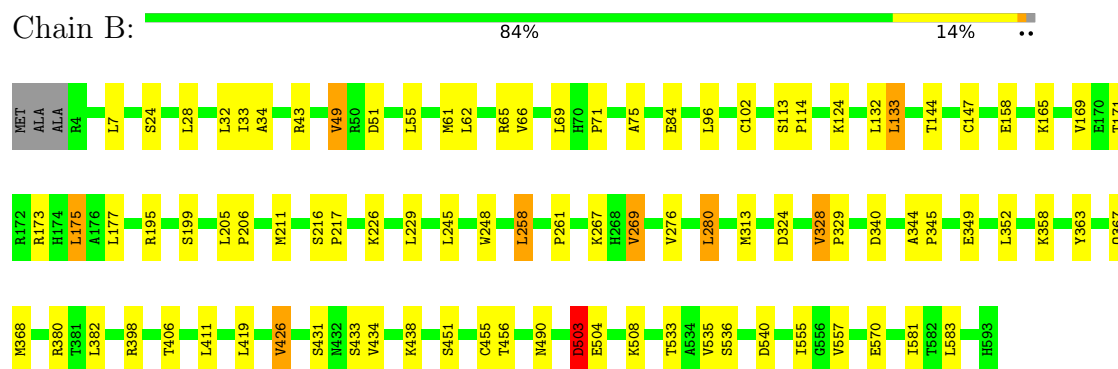
3 Residue-property plots

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.

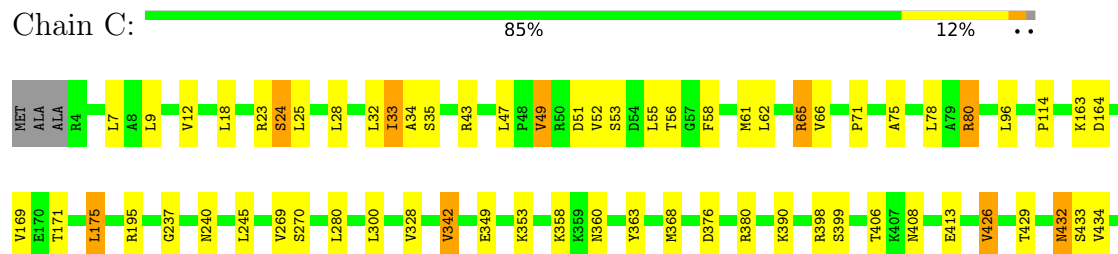
- Molecule 1: Bifunctional purine biosynthesis protein PURH



- Molecule 1: Bifunctional purine biosynthesis protein PURH



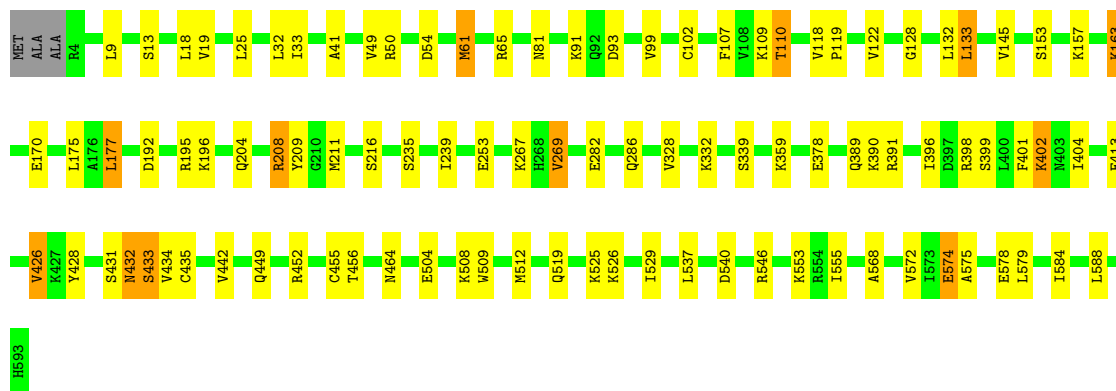
- Molecule 1: Bifunctional purine biosynthesis protein PURH





- Molecule 1: Bifunctional purine biosynthesis protein PURH

Chain D: 83% 15% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.20Å 62.00Å 196.60Å 80.80° 81.50° 90.00°	Depositor
Resolution (Å)	41.89 – 2.10 41.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (41.89-2.10) 76.5 (41.89-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.248 0.198 , 0.249	Depositor DCC
R_{free} test set	3151 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 19.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.427 for h,-k,h-l 0.026 for -h,k,k-l 0.022 for -h,-k,-h-k+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18526	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: K, PO4, 13A

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	0.73	1/4595 (0.0%)	0.95	2/6230 (0.0%)
1	B	0.69	0/4595	0.92	3/6230 (0.0%)
1	C	0.72	1/4595 (0.0%)	0.92	1/6230 (0.0%)
1	D	0.79	1/4595 (0.0%)	0.94	2/6230 (0.0%)
All	All	0.73	3/18380 (0.0%)	0.93	8/24920 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	93	ASP	CG-OD1	6.19	1.37	1.25
1	C	328	VAL	CA-CB	5.79	1.57	1.54
1	A	118	VAL	CA-CB	5.04	1.56	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	VAL	CB-CA-C	-7.36	98.91	110.69
1	B	113	SER	CA-C-N	7.18	128.81	119.84
1	B	113	SER	C-N-CA	7.18	128.81	119.84
1	A	113	SER	CA-C-N	7.12	128.74	119.84
1	A	113	SER	C-N-CA	7.12	128.74	119.84
1	B	431	SER	N-CA-C	5.60	117.92	110.53
1	D	433	SER	N-CA-C	5.19	117.14	108.99
1	D	110	THR	N-CA-C	5.19	116.62	111.07

There are no chirality outliers.

There are no planarity outliers.

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	4511	0	4559	61	0
1	B	4511	0	4561	49	0
1	C	4511	0	4561	42	0
1	D	4511	0	4560	53	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	21	0	10	3	0
4	D	21	0	12	2	0
5	A	121	0	0	5	0
5	B	93	0	0	0	0
5	C	100	0	0	1	0
5	D	112	0	0	4	0
All	All	18526	0	18263	194	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 5.

All (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:SER:HB3	1:A:114:PRO:HD2	1.41	1.00
1:D:390:LYS:HE3	1:D:391:ARG:O	1.59	1.00
1:A:208:ARG:HD3	1:A:208:ARG:H	1.37	0.89
1:A:298:THR:HG21	1:A:327:ASP:OD2	1.75	0.86
1:A:252:LYS:O	1:A:256:GLN:HG3	1.78	0.83
1:D:432:ASN:C	1:D:432:ASN:HD22	1.83	0.83
1:A:92:GLN:HG2	1:B:61:MET:HE1	1.63	0.80
1:D:378:GLU:HG2	5:D:1047:HOH:O	1.83	0.79
1:A:113:SER:CB	1:A:114:PRO:HD2	2.13	0.79
1:C:24:SER:O	1:C:28:LEU:HD23	1.83	0.78
1:C:432:ASN:C	1:C:432:ASN:HD22	1.92	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:NZ	1:A:267:LYS:HB3	2.01	0.76
1:B:43:ARG:HG3	1:B:49:VAL:HG13	1.67	0.76
1:D:107:PHE:HA	1:D:110:THR:HG22	1.69	0.75
1:C:33:ILE:HD13	1:C:55:LEU:HD22	1.73	0.71
1:A:106:PRO:O	1:A:110:THR:OG1	2.09	0.71
1:A:267:LYS:HG3	1:A:314:SER:O	1.92	0.69
1:D:432:ASN:HD21	1:D:449:GLN:HB2	1.56	0.69
1:D:33:ILE:HG22	1:D:50:ARG:HB2	1.76	0.68
1:B:438:LYS:NZ	1:B:533:THR:O	2.24	0.67
1:C:426:VAL:HG13	1:C:540:ASP:HB3	1.75	0.67
1:D:390:LYS:CE	1:D:391:ARG:O	2.39	0.67
1:D:504:GLU:O	1:D:508:LYS:HG3	1.95	0.67
1:C:62:LEU:O	1:C:65:ARG:HB2	1.96	0.66
1:A:61:MET:HG3	1:A:62:LEU:HD22	1.77	0.66
1:A:208:ARG:HD3	1:A:208:ARG:N	2.09	0.66
1:D:432:ASN:C	1:D:432:ASN:ND2	2.55	0.65
1:C:53:SER:HA	1:C:56:THR:CG2	2.26	0.65
1:D:107:PHE:O	1:D:110:THR:HG22	1.97	0.65
1:A:426:VAL:HG13	1:A:540:ASP:HB3	1.78	0.65
1:B:158:GLU:OE1	1:B:171:THR:HG21	1.96	0.65
1:D:398:ARG:NH2	1:D:413:GLU:OE2	2.29	0.65
1:A:113:SER:HB3	1:A:114:PRO:CD	2.23	0.64
1:D:434:VAL:CG2	1:D:537:LEU:HD11	2.29	0.63
1:C:23:ARG:HG2	1:C:47:LEU:HD21	1.82	0.62
1:A:593:HIS:HB2	1:B:211:MET:HE1	1.81	0.62
1:A:267:LYS:HB3	1:A:267:LYS:HZ1	1.64	0.61
1:C:53:SER:HA	1:C:56:THR:HG22	1.82	0.61
1:C:66:VAL:HG12	1:C:66:VAL:O	2.01	0.61
1:A:208:ARG:H	1:A:208:ARG:CD	2.13	0.60
1:B:426:VAL:HG13	1:B:540:ASP:HB3	1.83	0.60
1:D:435:CYS:SG	1:D:442:VAL:HG22	2.42	0.60
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.67	0.59
1:B:43:ARG:CG	1:B:49:VAL:HG13	2.34	0.58
1:A:4:ARG:HD2	5:A:1047:HOH:O	2.03	0.58
1:D:404:ILE:HG12	1:D:584:ILE:CD1	2.35	0.57
1:C:432:ASN:HD21	1:C:455:CYS:HB2	1.69	0.57
1:C:380:ARG:NH2	5:C:1103:HOH:O	2.37	0.57
1:B:229:LEU:HD13	1:B:368:MET:HE2	1.88	0.56
1:C:434:VAL:CG1	1:C:537:LEU:HD11	2.35	0.56
1:C:80:ARG:HD3	1:D:65:ARG:NH2	2.20	0.56
1:C:593:HIS:HB2	1:D:211:MET:HE1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:SER:HB2	1:A:402:LYS:HE3	1.87	0.56
1:D:398:ARG:HH22	1:D:413:GLU:CD	2.15	0.55
1:D:107:PHE:CA	1:D:110:THR:HG22	2.36	0.55
1:D:401:PHE:HA	1:D:584:ILE:HG21	1.88	0.55
1:A:313:MET:HE2	1:A:493:ASP:HB3	1.88	0.55
1:C:398:ARG:NH2	1:C:413:GLU:OE1	2.39	0.55
1:C:464:ASN:ND2	1:C:555:ILE:HD13	2.21	0.54
1:B:33:ILE:HD13	1:B:55:LEU:HD22	1.90	0.54
1:B:313:MET:HE3	1:B:490:ASN:ND2	2.23	0.54
1:B:434:VAL:HG22	1:B:455:CYS:SG	2.47	0.54
1:D:434:VAL:HG11	1:D:456:THR:HA	1.90	0.54
1:C:56:THR:OG1	1:C:58:PHE:HB2	2.08	0.54
1:D:25:LEU:HD22	1:D:99:VAL:HG11	1.90	0.54
1:A:55:LEU:HD21	5:A:1121:HOH:O	2.08	0.53
1:A:356:SER:O	1:A:361:GLY:HA2	2.08	0.53
1:D:553:LYS:HE3	1:D:579:LEU:O	2.09	0.52
1:C:237:GLY:O	1:C:240:ASN:HB2	2.10	0.52
1:B:216:SER:HB2	1:B:217:PRO:HA	1.92	0.52
1:D:574:GLU:O	1:D:578:GLU:HG2	2.10	0.52
1:C:171:THR:HG22	1:C:175:LEU:CD2	2.41	0.51
1:D:118:VAL:HB	1:D:119:PRO:HD3	1.92	0.51
1:D:253:GLU:OE2	1:D:428:TYR:OH	2.27	0.51
1:A:18:LEU:CD1	1:A:19:VAL:H	2.24	0.51
1:D:389:GLN:O	5:D:1047:HOH:O	2.19	0.51
1:A:71:PRO:HD3	1:B:69:LEU:O	2.11	0.50
1:B:71:PRO:O	1:B:75:ALA:HB3	2.12	0.50
1:C:560:ILE:HB	1:C:583:LEU:HD23	1.92	0.50
1:D:107:PHE:C	1:D:110:THR:HG22	2.37	0.50
1:D:192:ASP:O	1:D:196:LYS:HG3	2.12	0.50
1:A:250:LEU:C	1:A:250:LEU:HD23	2.37	0.49
1:D:464:ASN:HD22	1:D:555:ILE:HD13	1.76	0.49
1:A:537:LEU:C	1:A:537:LEU:HD23	2.37	0.49
1:D:211:MET:SD	1:D:239:ILE:HD11	2.53	0.49
1:A:71:PRO:HA	1:B:66:VAL:HG11	1.95	0.49
1:C:566:SER:C	1:C:568:ALA:H	2.21	0.49
1:C:574:GLU:O	1:C:578:GLU:HG3	2.13	0.49
1:A:208:ARG:NH2	5:A:1036:HOH:O	2.46	0.48
1:A:345:PRO:HA	1:A:368:MET:O	2.14	0.48
1:D:208:ARG:HG2	1:D:209:TYR:H	1.78	0.48
1:B:43:ARG:HG3	1:B:49:VAL:CG1	2.40	0.47
1:C:358:LYS:HB3	1:C:363:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HD23	1:A:424:ILE:HD12	1.97	0.47
1:B:248:TRP:HZ3	1:B:345:PRO:HD3	1.79	0.47
1:B:258:LEU:HD23	1:B:276:VAL:HG11	1.95	0.47
1:D:339:SER:O	1:D:359:LYS:HE2	2.15	0.47
1:D:431:SER:HB3	1:D:432:ASN:HA	1.95	0.47
1:A:82:ILE:HD12	1:A:85:ASP:H	1.80	0.47
1:B:328:VAL:N	1:B:329:PRO:HD2	2.30	0.47
1:D:128:GLY:HA3	4:D:601:13A:C18	2.45	0.47
1:B:102:CYS:HB3	1:B:133:LEU:HD13	1.97	0.46
1:D:434:VAL:HG12	1:D:455:CYS:SG	2.55	0.46
1:D:399:SER:HA	1:D:402:LYS:HD3	1.97	0.46
1:A:164:ASP:O	1:A:165:LYS:HG2	2.15	0.46
1:B:406:THR:HG23	1:B:583:LEU:HB3	1.98	0.46
1:D:107:PHE:HA	1:D:110:THR:CG2	2.41	0.46
1:B:535:VAL:HB	1:B:557:VAL:HA	1.97	0.46
1:B:7:LEU:HD13	1:B:33:ILE:HD12	1.98	0.46
1:A:128:GLY:HA3	4:A:600:13A:C18	2.46	0.46
1:B:102:CYS:O	1:B:147:CYS:HA	2.16	0.45
1:A:35:SER:O	1:A:36:GLY:C	2.58	0.45
1:D:546:ARG:HB2	5:D:1054:HOH:O	2.16	0.45
1:B:434:VAL:HG21	1:B:456:THR:HA	1.99	0.45
1:A:431:SER:HB3	1:A:432:ASN:HA	1.98	0.45
1:B:344:ALA:O	1:B:367:GLN:HA	2.17	0.45
1:B:7:LEU:HD13	1:B:33:ILE:CD1	2.47	0.45
1:A:408:ASN:HD21	1:A:577:ASN:HA	1.82	0.45
1:D:426:VAL:HG13	1:D:540:ASP:HB3	1.99	0.45
1:B:248:TRP:CZ3	1:B:345:PRO:HD3	2.52	0.45
1:C:171:THR:O	1:C:175:LEU:HD22	2.17	0.44
1:D:525:LYS:O	1:D:529:ILE:HG12	2.16	0.44
1:C:51:ASP:OD1	1:C:52:VAL:N	2.50	0.44
1:D:163:LYS:H	1:D:163:LYS:HD2	1.82	0.44
1:D:432:ASN:HB2	1:D:452:ARG:NH2	2.32	0.44
1:A:128:GLY:HA3	4:A:600:13A:C13	2.47	0.44
1:C:504:GLU:O	1:C:508:LYS:HG3	2.17	0.44
1:C:61:MET:HG3	1:C:62:LEU:HG	2.00	0.44
1:A:245:LEU:HD23	1:A:368:MET:HE1	2.00	0.44
1:B:245:LEU:CD2	1:B:368:MET:HE1	2.48	0.44
1:B:419:LEU:HD23	1:B:536:SER:HB3	2.00	0.44
1:D:128:GLY:HA3	4:D:601:13A:C13	2.48	0.44
1:A:335:SER:HA	1:A:358:LYS:HD2	2.00	0.44
1:B:62:LEU:O	1:B:65:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:SER:CB	1:A:114:PRO:CD	2.89	0.43
1:A:267:LYS:NZ	1:A:267:LYS:CB	2.79	0.43
1:A:438:LYS:HE2	1:A:533:THR:O	2.19	0.43
1:B:34:ALA:O	1:B:51:ASP:HA	2.18	0.43
1:A:239:ILE:HG12	5:A:1034:HOH:O	2.18	0.43
1:B:345:PRO:HA	1:B:368:MET:O	2.19	0.43
1:B:71:PRO:O	1:B:75:ALA:CB	2.67	0.43
1:B:504:GLU:O	1:B:508:LYS:HG3	2.18	0.43
1:C:9:LEU:HD13	1:C:33:ILE:HG12	2.01	0.43
1:A:208:ARG:HG3	1:A:208:ARG:NH1	2.32	0.43
1:B:24:SER:O	1:B:28:LEU:HG	2.18	0.43
1:D:509:TRP:HA	1:D:512:MET:HE2	2.01	0.43
1:D:546:ARG:HG3	1:D:575:ALA:HB2	2.00	0.43
1:C:270:SER:HB3	1:C:429:THR:HG23	2.01	0.42
1:D:391:ARG:N	5:D:1047:HOH:O	2.52	0.42
1:A:154:SER:HB2	5:A:1049:HOH:O	2.19	0.42
1:A:47:LEU:HA	1:A:48:PRO:HD3	1.94	0.42
1:A:69:LEU:O	1:B:71:PRO:HD3	2.19	0.42
1:A:177:LEU:HD11	1:B:195:ARG:HG3	2.01	0.42
1:B:261:PRO:HG3	1:B:324:ASP:OD2	2.20	0.42
1:C:12:VAL:HG21	1:C:18:LEU:HD13	2.01	0.42
1:C:566:SER:C	1:C:568:ALA:N	2.75	0.42
1:D:568:ALA:O	1:D:572:VAL:HG23	2.19	0.42
1:A:18:LEU:HD13	1:A:19:VAL:N	2.35	0.42
1:C:245:LEU:CD2	1:C:368:MET:HE1	2.50	0.42
1:D:328:VAL:CG1	1:D:332:LYS:HE3	2.50	0.42
1:B:144:THR:HG23	1:B:175:LEU:HD23	2.02	0.42
1:C:195:ARG:HG3	1:D:177:LEU:HD21	2.02	0.42
1:D:145:VAL:O	1:D:175:LEU:HB3	2.20	0.42
1:C:33:ILE:CD1	1:C:55:LEU:HD22	2.46	0.42
1:D:102:CYS:HB3	1:D:133:LEU:HD13	2.01	0.42
1:C:43:ARG:HG3	1:C:49:VAL:HG13	2.00	0.42
1:C:464:ASN:HD22	1:C:555:ILE:HD13	1.85	0.41
1:A:18:LEU:HD13	1:A:19:VAL:H	1.85	0.41
1:A:216:SER:HB2	1:A:217:PRO:HA	2.01	0.41
1:A:574:GLU:O	1:A:578:GLU:HG2	2.19	0.41
1:C:406:THR:HG23	1:C:583:LEU:HB3	2.02	0.41
1:C:426:VAL:CG1	1:C:540:ASP:HB3	2.48	0.41
1:A:67:LYS:NZ	4:A:600:13A:H82	2.35	0.41
1:A:198:TYR:CZ	1:B:173:ARG:HG2	2.55	0.41
1:A:450:GLN:HB3	1:B:267:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ASP:HB3	1:B:504:GLU:H	1.55	0.41
1:A:432:ASN:HB2	1:A:452:ARG:NH2	2.35	0.41
1:C:34:ALA:O	1:C:51:ASP:HA	2.20	0.41
1:C:376:ASP:HB3	1:C:390:LYS:HD2	2.02	0.41
1:D:195:ARG:HG2	1:D:204:GLN:HB2	2.03	0.41
1:B:358:LYS:HB2	1:B:363:TYR:HB2	2.03	0.41
1:D:128:GLY:O	1:D:132:LEU:HG	2.21	0.41
1:B:205:LEU:HA	1:B:206:PRO:HD3	1.91	0.41
1:C:71:PRO:O	1:C:75:ALA:HB3	2.20	0.41
1:A:134:ARG:HD2	1:A:183:THR:HG21	2.02	0.41
1:A:485:ARG:HG2	1:A:485:ARG:HH11	1.85	0.41
1:B:280:LEU:N	1:B:280:LEU:HD23	2.36	0.40
1:C:461:ASP:O	1:C:464:ASN:HB2	2.21	0.40
1:A:308:ARG:O	1:A:308:ARG:HG2	2.20	0.40
1:B:62:LEU:O	1:B:65:ARG:CG	2.69	0.40
1:B:165:LYS:N	1:B:165:LYS:HD2	2.36	0.40
1:A:70:HIS:CG	1:A:71:PRO:HD2	2.56	0.40
1:B:426:VAL:CG1	1:B:540:ASP:HB3	2.51	0.40
1:A:250:LEU:HD23	1:A:250:LEU:O	2.22	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	588/593 (99%)	565 (96%)	19 (3%)	4 (1%)	18	15
1	B	588/593 (99%)	574 (98%)	11 (2%)	3 (0%)	24	22
1	C	588/593 (99%)	565 (96%)	21 (4%)	2 (0%)	36	36
1	D	588/593 (99%)	568 (97%)	17 (3%)	3 (0%)	24	22
All	All	2352/2372 (99%)	2272 (97%)	68 (3%)	12 (0%)	24	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLY
1	A	61	MET
1	A	114	PRO
1	B	503	ASP
1	D	41	ALA
1	D	61	MET
1	B	114	PRO
1	D	269	VAL
1	A	269	VAL
1	C	114	PRO
1	B	269	VAL
1	C	269	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	484/485 (100%)	452 (93%)	32 (7%)	15	13
1	B	484/485 (100%)	454 (94%)	30 (6%)	16	14
1	C	484/485 (100%)	454 (94%)	30 (6%)	16	14
1	D	484/485 (100%)	450 (93%)	34 (7%)	14	11
All	All	1936/1940 (100%)	1810 (94%)	126 (6%)	15	13

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	SER
1	A	18	LEU
1	A	19	VAL
1	A	33	ILE
1	A	62	LEU
1	A	82	ILE
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	92	GLN
1	A	95	SER
1	A	117	THR
1	A	123	GLU
1	A	153	SER
1	A	163	LYS
1	A	164	ASP
1	A	165	LYS
1	A	208	ARG
1	A	267	LYS
1	A	269	VAL
1	A	298	THR
1	A	360	ASN
1	A	426	VAL
1	A	433	SER
1	A	451	SER
1	A	454	HIS
1	A	458	LEU
1	A	462	LYS
1	A	489	SER
1	A	502	GLU
1	A	506	LEU
1	A	526	LYS
1	A	583	LEU
1	B	32	LEU
1	B	49	VAL
1	B	84	GLU
1	B	96	LEU
1	B	124	LYS
1	B	132	LEU
1	B	133	LEU
1	B	169	VAL
1	B	175	LEU
1	B	177	LEU
1	B	199	SER
1	B	226	LYS
1	B	258	LEU
1	B	269	VAL
1	B	280	LEU
1	B	328	VAL
1	B	340	ASP
1	B	349	GLU

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Mol	Chain	Res	Type
1	B	352	LEU
1	B	380	ARG
1	B	382	LEU
1	B	398	ARG
1	B	411	LEU
1	B	426	VAL
1	B	433	SER
1	B	451	SER
1	B	503	ASP
1	B	555	ILE
1	B	570	GLU
1	B	581	ILE
1	C	7	LEU
1	C	24	SER
1	C	25	LEU
1	C	32	LEU
1	C	33	ILE
1	C	35	SER
1	C	49	VAL
1	C	65	ARG
1	C	78	LEU
1	C	80	ARG
1	C	96	LEU
1	C	163	LYS
1	C	164	ASP
1	C	169	VAL
1	C	175	LEU
1	C	280	LEU
1	C	300	LEU
1	C	342	VAL
1	C	349	GLU
1	C	353	LYS
1	C	360	ASN
1	C	399	SER
1	C	408	ASN
1	C	426	VAL
1	C	432	ASN
1	C	433	SER
1	C	451	SER
1	C	520	LEU
1	C	583	LEU
1	C	588	LEU

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Mol	Chain	Res	Type
1	D	9	LEU
1	D	13	SER
1	D	18	LEU
1	D	19	VAL
1	D	32	LEU
1	D	49	VAL
1	D	54	ASP
1	D	61	MET
1	D	81	ASN
1	D	91	LYS
1	D	109	LYS
1	D	122	VAL
1	D	133	LEU
1	D	153	SER
1	D	157	LYS
1	D	163	LYS
1	D	170	GLU
1	D	177	LEU
1	D	208	ARG
1	D	216	SER
1	D	235	SER
1	D	267	LYS
1	D	269	VAL
1	D	282	GLU
1	D	286	GLN
1	D	396	ILE
1	D	402	LYS
1	D	426	VAL
1	D	432	ASN
1	D	433	SER
1	D	519	GLN
1	D	526	LYS
1	D	574	GLU
1	D	588	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	185	GLN
1	A	246	ASN
1	A	256	GLN

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Mol	Chain	Res	Type
1	A	367	GLN
1	A	408	ASN
1	A	464	ASN
1	A	490	ASN
1	A	585	HIS
1	B	90	ASN
1	B	92	GLN
1	B	464	ASN
1	B	490	ASN
1	B	494	GLN
1	C	74	HIS
1	C	86	ASN
1	C	90	ASN
1	C	92	GLN
1	C	204	GLN
1	C	219	GLN
1	C	246	ASN
1	C	386	GLN
1	C	432	ASN
1	C	464	ASN
1	C	548	ASN
1	C	587	ASN
1	D	386	GLN
1	D	432	ASN
1	D	454	HIS
1	D	464	ASN
1	D	490	ASN
1	D	494	GLN
1	D	585	HIS
1	D	587	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
2	PO4	A	801	-	4,4,4	1.55	1 (25%)	6,6,6	1.36	2 (33%)
4	13A	A	600	-	21,23,23	4.89	10 (47%)	25,36,36	6.23	13 (52%)
2	PO4	C	901	-	4,4,4	1.65	1 (25%)	6,6,6	0.95	0
4	13A	D	601	-	21,23,23	4.83	8 (38%)	25,36,36	6.16	16 (64%)

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	13A	A	600	-	-	2/6/36/36	0/2/3/3
4	13A	D	601	-	-	0/6/36/36	0/2/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	13A	O20-S16	15.60	1.64	1.43
4	D	601	13A	O20-S16	15.34	1.64	1.43
4	D	601	13A	O21-S16	11.14	1.58	1.43
4	A	600	13A	O21-S16	10.86	1.58	1.43
4	A	600	13A	C14-N15	6.86	1.48	1.36
4	D	601	13A	C14-N15	6.77	1.47	1.36
4	D	601	13A	C13-C18	4.89	1.62	1.44
4	A	600	13A	C13-C18	4.78	1.62	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	601	13A	C11-N12	4.51	1.45	1.32
4	A	600	13A	C11-N12	4.39	1.44	1.32
4	D	601	13A	C13-C14	3.62	1.44	1.38
4	A	600	13A	C13-C14	3.52	1.44	1.38
4	A	600	13A	O6-C3	-3.31	1.34	1.43
4	D	601	13A	C11-N10	3.18	1.44	1.37
2	C	901	PO4	P-O1	2.96	1.57	1.50
4	A	600	13A	C11-N10	2.95	1.44	1.37
2	A	801	PO4	P-O1	2.85	1.57	1.50
4	A	600	13A	C8-C2	2.26	1.59	1.51
4	D	601	13A	C8-C2	2.07	1.58	1.51
4	A	600	13A	O1-C2	2.03	1.49	1.45

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	13A	O20-S16-O21	-16.61	98.64	118.87
4	D	601	13A	O20-S16-O21	-15.70	99.76	118.87
4	D	601	13A	O9-C8-C2	14.68	161.31	111.33
4	A	600	13A	O9-C8-C2	13.65	157.81	111.33
4	D	601	13A	C13-C14-N10	13.35	112.42	106.25
4	A	600	13A	C13-C14-N10	11.63	111.63	106.25
4	A	600	13A	C8-C2-C3	10.99	141.04	115.10
4	A	600	13A	C11-N10-C14	-10.16	98.10	106.67
4	D	601	13A	C11-N10-C14	-10.07	98.18	106.67
4	D	601	13A	O1-C2-C8	-6.20	96.11	109.22
4	A	600	13A	C5-N10-C11	6.07	143.96	126.73
4	D	601	13A	C11-N12-C13	-5.31	94.81	104.26
4	A	600	13A	C11-N12-C13	-5.29	94.84	104.26
4	A	600	13A	C18-C13-N12	-4.85	121.46	130.29
4	D	601	13A	C5-N10-C11	4.67	140.01	126.73
4	A	600	13A	N10-C11-N12	4.40	121.56	113.40
4	D	601	13A	N10-C11-N12	4.25	121.28	113.40
4	D	601	13A	O1-C5-C4	4.22	115.64	106.62
4	D	601	13A	C18-C13-N12	-4.16	122.71	130.29
4	D	601	13A	O7-C4-C3	3.84	124.14	111.82
4	A	600	13A	C14-C13-N12	3.54	113.86	109.26
4	D	601	13A	O1-C2-C3	3.47	112.03	105.15
4	D	601	13A	C14-C13-N12	3.11	113.30	109.26
4	A	600	13A	O1-C2-C8	-3.11	102.65	109.22
4	D	601	13A	C8-C2-C3	-2.57	109.03	115.10
4	D	601	13A	O1-C5-N10	2.46	113.94	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	13A	O19-C18-C13	-2.24	120.61	126.53
2	A	801	PO4	O3-P-O2	2.18	114.70	107.91
2	A	801	PO4	O3-P-O1	-2.17	103.27	110.95
4	D	601	13A	C2-O1-C5	-2.14	104.75	109.47
4	A	600	13A	O1-C5-N10	2.01	112.92	108.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	13A	C3-C2-C8-O9
4	A	600	13A	O1-C2-C8-O9

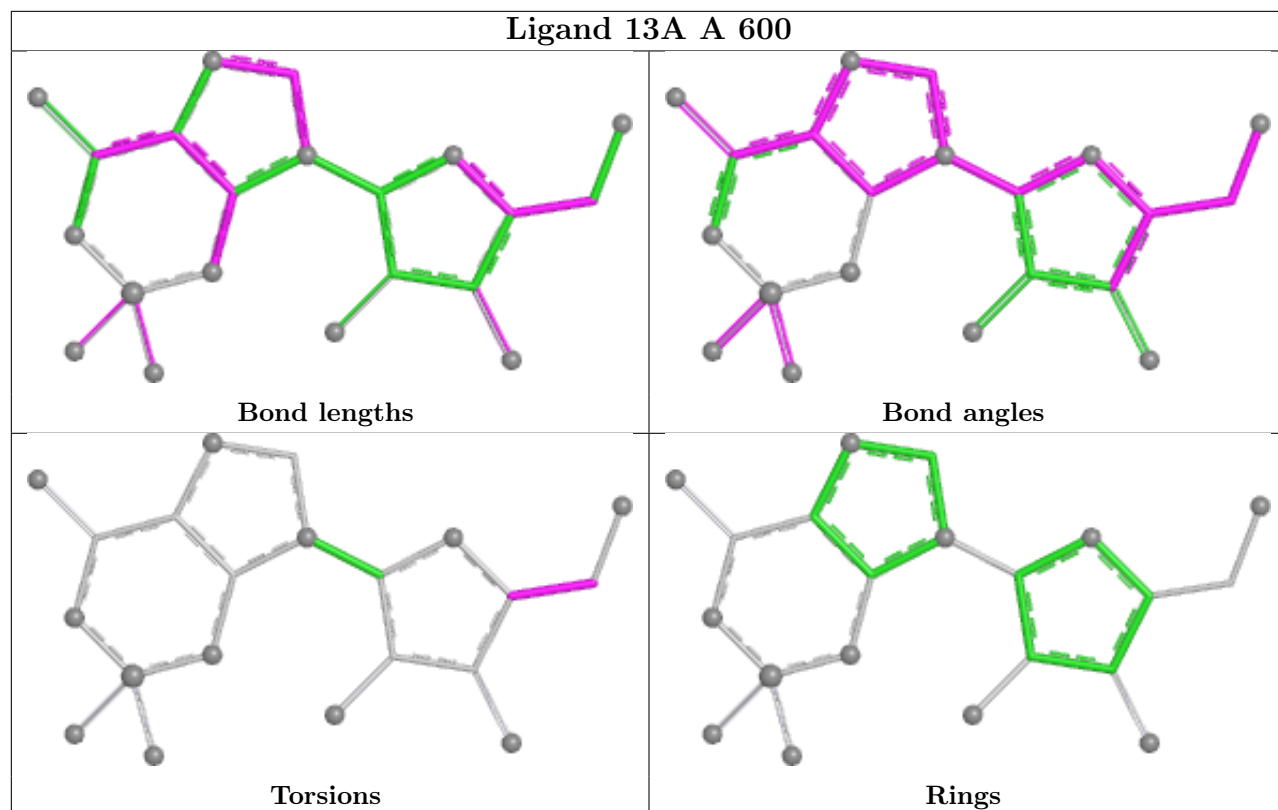
There are no ring outliers.

2 monomers are involved in 5 short contacts:

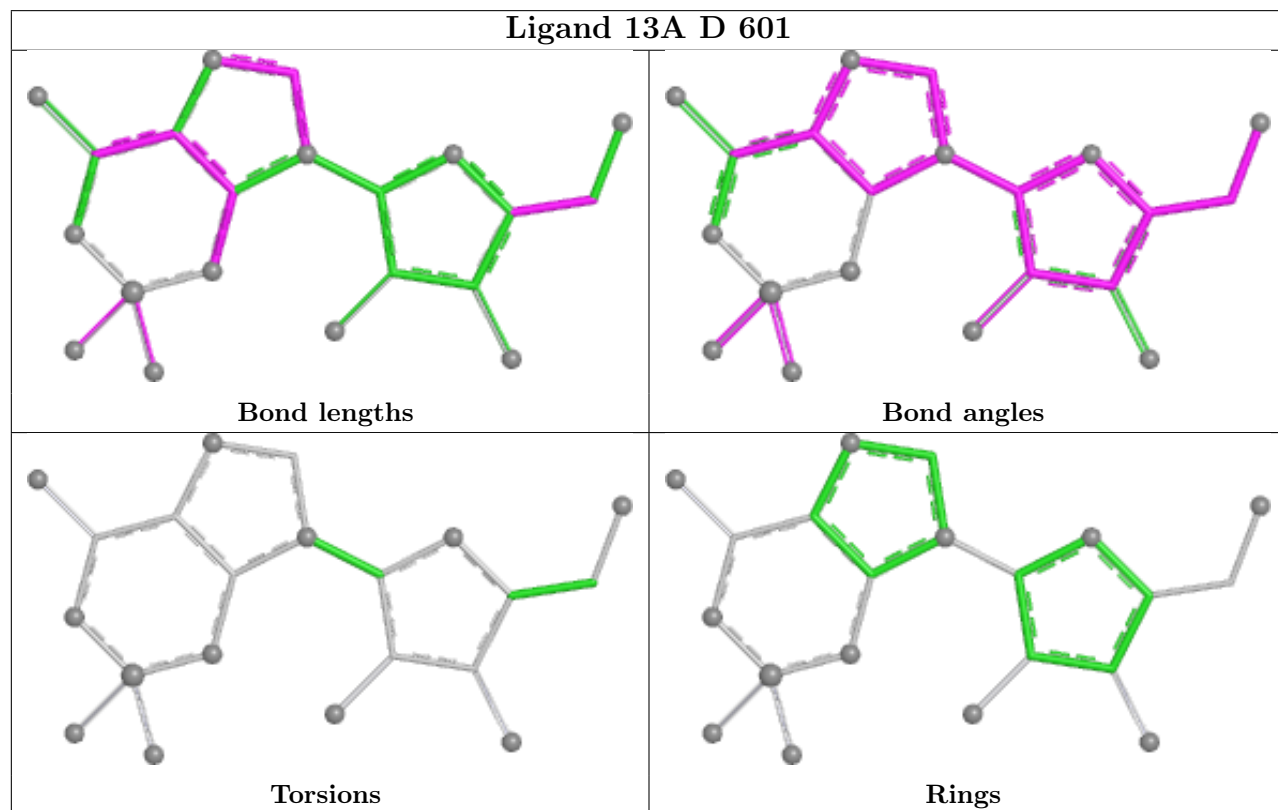
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	13A	3	0
4	D	601	13A	2	0

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 13A A 600



Ligand 13A D 601



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	590/593 (99%)	-1.08	1 (0%) 91 92	23, 41, 91, 116	0
1	B	590/593 (99%)	-1.13	0 100 100	28, 46, 71, 90	0
1	C	590/593 (99%)	-1.17	0 100 100	27, 44, 69, 91	0
1	D	590/593 (99%)	-1.06	0 100 100	23, 40, 94, 122	0
All	All	2360/2372 (99%)	-1.11	1 (0%) 100 100	23, 43, 85, 122	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	PHE	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	13A	D	601	21/21	0.97	0.06	77,78,79,79	0

Continued on next page...

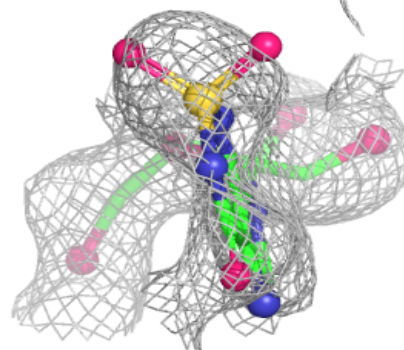
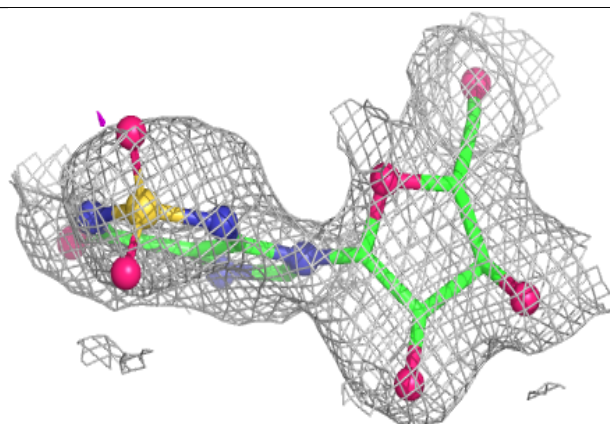
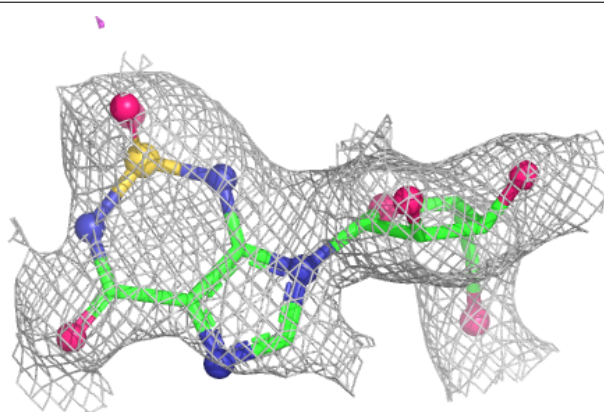
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	C	901	5/5	0.98	0.05	68,69,69,70	0
4	13A	A	600	21/21	0.98	0.05	73,75,77,78	0
2	PO4	A	801	5/5	0.98	0.05	66,67,67,68	0
3	K	C	1003	1/1	1.00	0.05	33,33,33,33	0
3	K	D	1004	1/1	1.00	0.04	26,26,26,26	0
3	K	A	1001	1/1	1.00	0.02	27,27,27,27	0
3	K	B	1002	1/1	1.00	0.01	33,33,33,33	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.

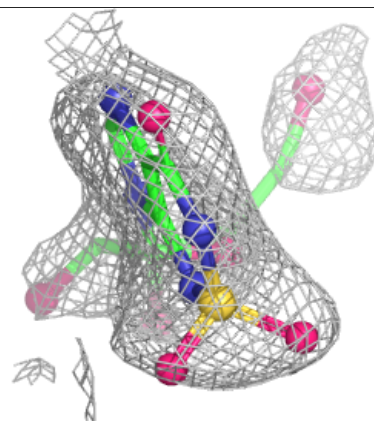
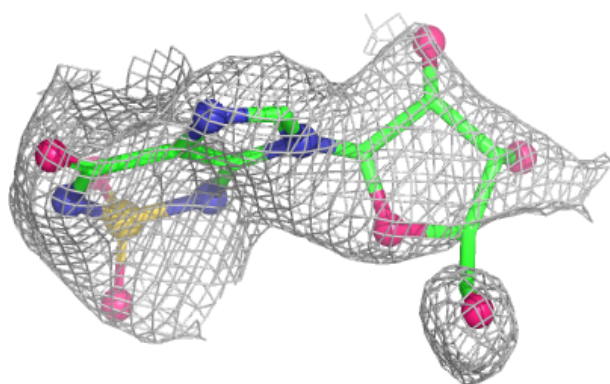
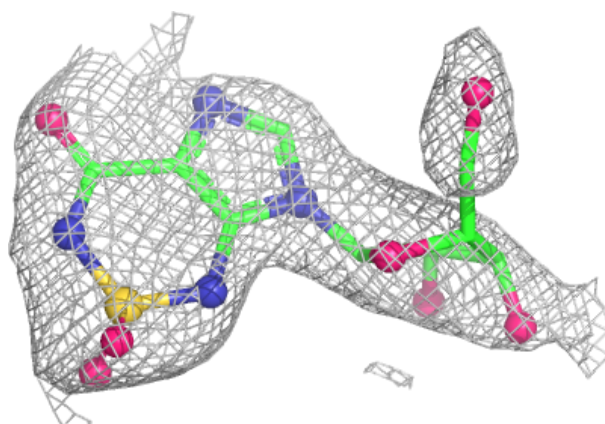
Electron density around 13A D 601:

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 13A A 600:

$2mF_o-DF_c$ (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.