



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:54 PM UTC

PDB ID : 1Y1Q / pdb_00001y1q
Title : Crystal Structure of the Uridine Phosphorylase from Salmonella Typhimurium
in Complex with Uridine-5p-monophosphate and Sulfate Ion at 2.35Å Resolution
Authors : Gabdoulkhakov, A.G.; Dontsova, M.V.; Kachalova, G.S.; Betzel, C.; Ealick,
S.E.; Mikhailov, A.M.
Deposited on : 2004-11-19
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](#) ①) were used in the production of this report:

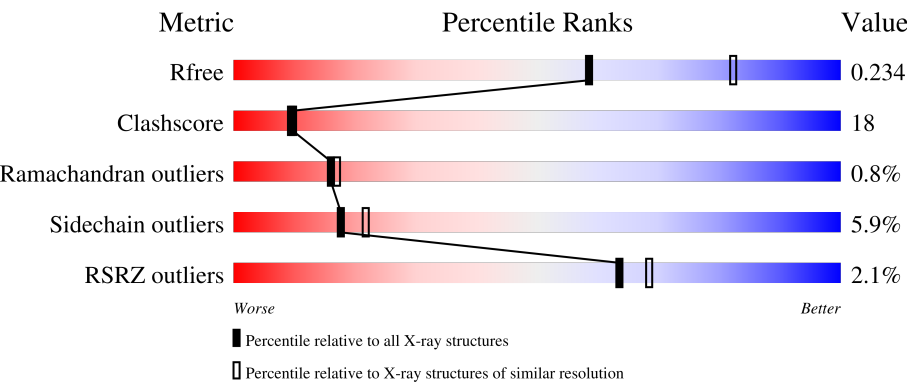
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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	253	4% 69%25% . .
1	B	253	% 59%32% . 6%
1	C	253	2% 60%30%5%5%
1	D	253	2% 60%32%5% .
1	E	253	2% 62%29% . 6%

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Mol	Chain	Length	Quality of chain
1	F	253	% 62% 32% .

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	U5P	C	8003	-	-	X	-

2 Entry composition [i](#)

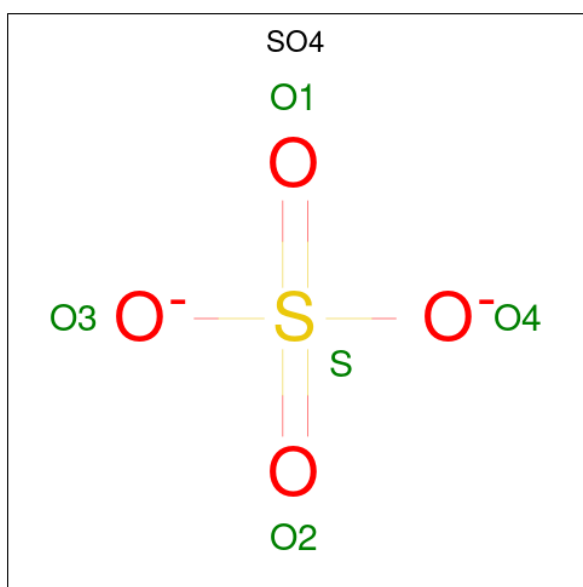
There are 4 unique types of molecules in this entry. The entry contains 11160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

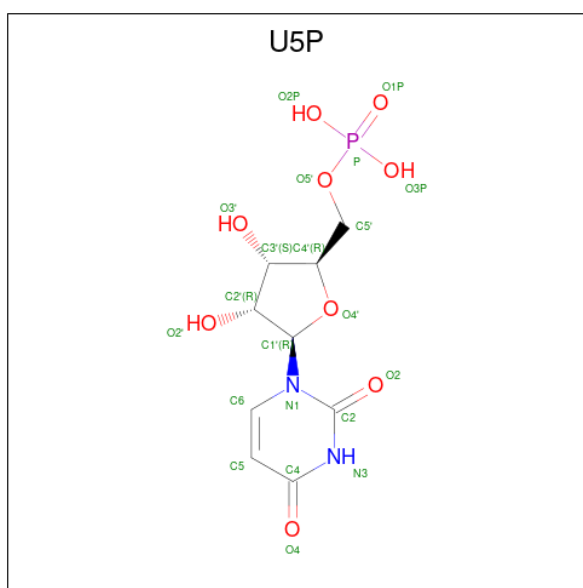
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	B	239	Total	C	N	O	S	0	0	0
			1789	1121	315	342	11			
1	C	240	Total	C	N	O	S	0	0	0
			1798	1126	317	344	11			
1	D	245	Total	C	N	O	S	0	0	0
			1836	1149	323	352	12			
1	E	238	Total	C	N	O	S	0	0	0
			1782	1117	314	340	11			
1	F	244	Total	C	N	O	S	0	0	0
			1830	1146	322	351	11			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: C₉H₁₃N₂O₉P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O P 21 9 2 9 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	34	Total O 34 34	0	0
4	C	30	Total O 30 30	0	0
4	D	35	Total O 35 35	0	0
4	E	35	Total O 35 35	0	0

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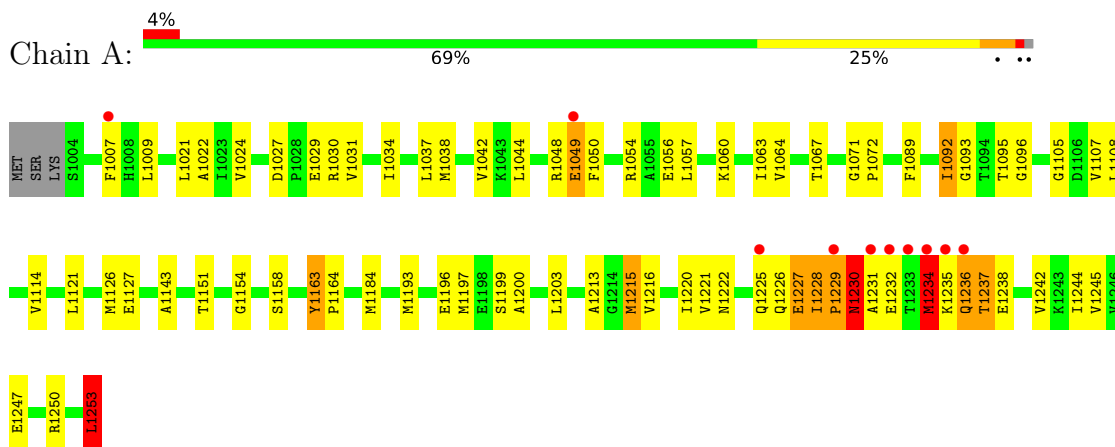
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	41	Total	O	0	0
			41	41		

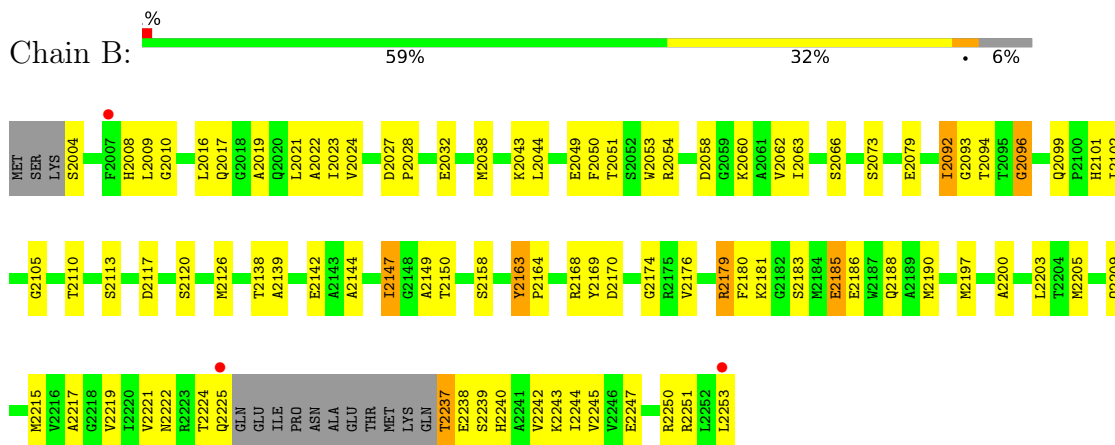
3 Residue-property plots

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.

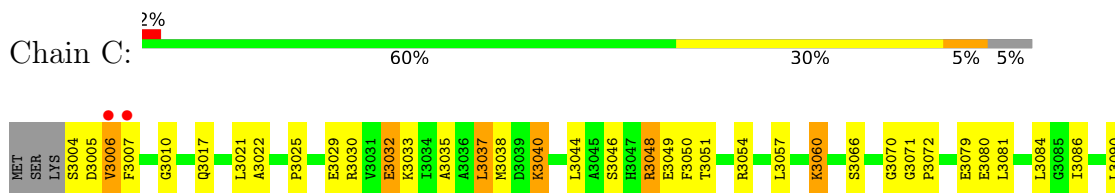
• Molecule 1: Uridine phosphorylase

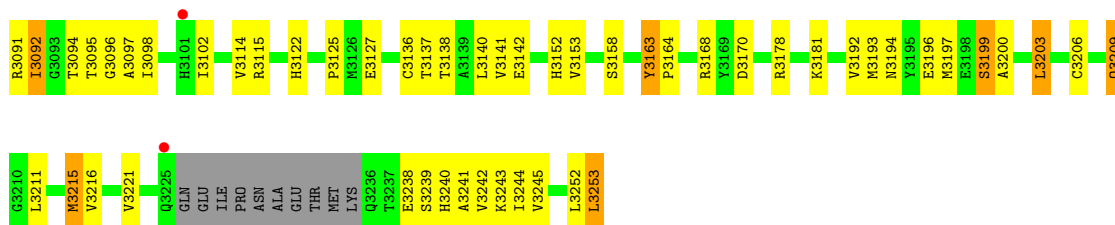


• Molecule 1: Uridine phosphorylase

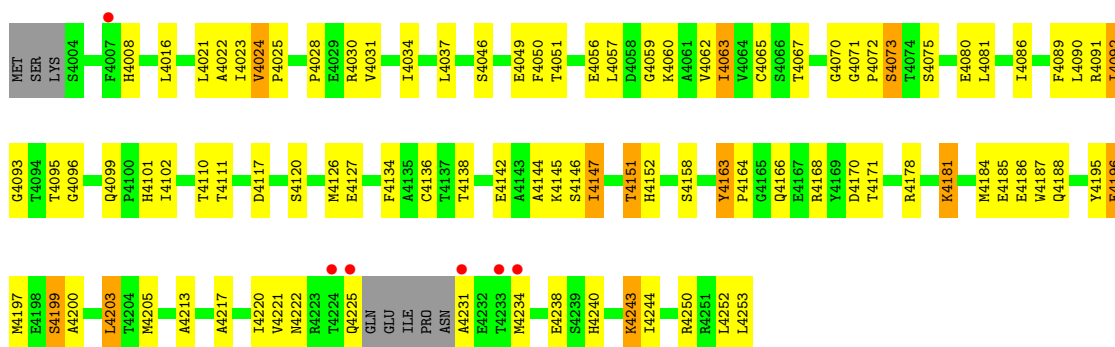


• Molecule 1: Uridine phosphorylase

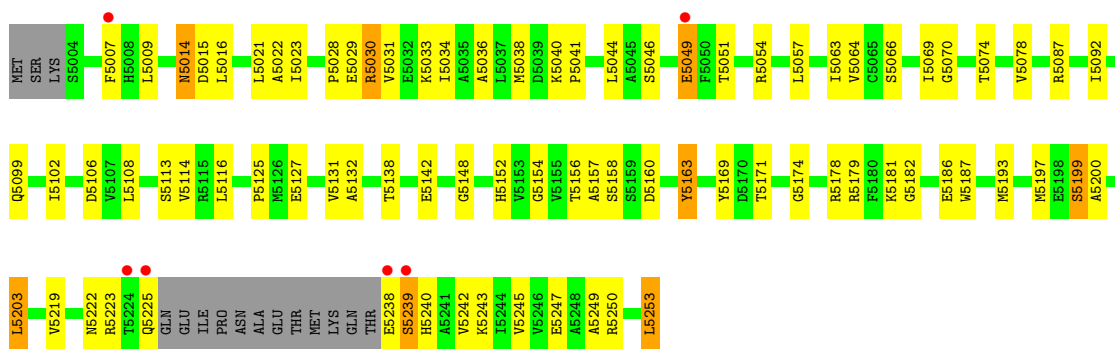




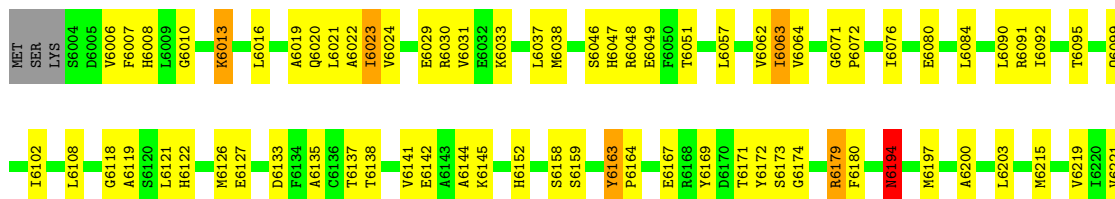
• Molecule 1: Uridine phosphorylase

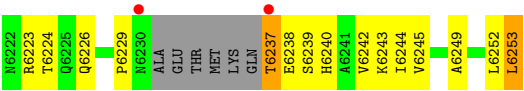


• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.37Å 123.73Å 134.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.66 – 2.35 28.66 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.6 (28.66-2.35) 98.5 (28.66-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.02 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.234 0.194 , 0.234	Depositor DCC
R_{free} test set	3020 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11160	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: U5P, SO4

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	0.44	0/1907	1.05	13/2584 (0.5%)
1	B	0.42	0/1817	0.98	7/2461 (0.3%)
1	C	0.42	0/1826	0.94	7/2473 (0.3%)
1	D	0.42	0/1864	1.02	8/2523 (0.3%)
1	E	0.45	0/1810	0.97	6/2451 (0.2%)
1	F	0.43	0/1859	0.95	6/2519 (0.2%)
All	All	0.43	0/11083	0.99	47/15011 (0.3%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4024	VAL	N-CA-C	9.87	117.92	108.15
1	A	1236	GLN	N-CA-C	-9.80	100.82	113.17
1	B	2024	VAL	N-CA-C	8.68	116.74	108.15
1	A	1197	MET	N-CA-C	7.55	123.59	112.94
1	E	5197	MET	N-CA-C	6.85	121.62	112.30
1	D	4070	GLY	N-CA-C	6.74	121.17	112.68
1	E	5023	ILE	N-CA-C	-6.48	99.09	108.36
1	E	5199	SER	N-CA-C	6.35	117.86	111.07
1	C	3050	PHE	N-CA-C	6.25	119.38	107.75
1	A	1009	LEU	N-CA-C	6.15	118.96	111.82
1	A	1050	PHE	N-CA-C	6.15	119.18	107.75
1	A	1237	THR	N-CA-C	-6.10	104.69	111.71
1	C	3070	GLY	N-CA-C	6.08	119.09	112.29
1	A	1234	MET	N-CA-C	-5.91	105.33	112.54
1	A	1253	LEU	N-CA-C	5.81	127.27	111.00
1	C	3199	SER	N-CA-C	5.79	117.59	111.28
1	C	3048	ARG	CB-CA-C	-5.77	109.90	116.54
1	B	2023	ILE	N-CA-C	-5.70	100.21	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5070	GLY	N-CA-C	5.69	119.85	112.68
1	D	4050	PHE	N-CA-C	5.68	118.59	107.57
1	B	2008	HIS	N-CA-C	5.56	120.56	113.55
1	A	1231	ALA	CB-CA-C	-5.54	110.17	116.54
1	F	6048	ARG	CB-CA-C	-5.54	110.17	116.54
1	A	1007	PHE	N-CA-C	5.45	119.19	112.54
1	D	4197	MET	N-CA-C	5.42	119.67	112.30
1	D	4151	THR	N-CA-C	5.40	118.80	110.42
1	F	6023	ILE	N-CA-C	-5.38	101.78	108.89
1	B	2197	MET	N-CA-C	5.37	122.38	113.89
1	A	1228	ILE	CA-C-N	5.37	126.55	119.84
1	A	1228	ILE	C-N-CA	5.37	126.55	119.84
1	F	6224	THR	N-CA-C	-5.35	106.71	113.18
1	C	3007	PHE	N-CA-C	5.34	122.17	110.80
1	C	3114	VAL	N-CA-C	-5.34	101.79	108.84
1	D	4110	THR	N-CA-C	5.28	117.35	108.96
1	F	6197	MET	N-CA-C	5.26	120.86	113.02
1	A	1114	VAL	N-CA-C	-5.25	100.77	108.54
1	E	5007	PHE	N-CA-C	5.25	117.91	111.82
1	A	1151	THR	N-CA-C	5.20	117.88	109.40
1	B	2094	THR	N-CA-C	-5.16	101.46	109.72
1	F	6194	ASN	N-CA-C	5.16	115.35	108.38
1	E	5009	LEU	N-CA-C	5.15	117.79	111.82
1	C	3197	MET	N-CA-C	5.15	119.30	112.30
1	F	6095	THR	N-CA-C	5.13	116.33	108.42
1	B	2113	SER	N-CA-C	5.13	116.98	109.24
1	D	4199	SER	N-CA-C	5.11	117.75	111.82
1	B	2096	GLY	N-CA-C	-5.09	105.22	112.55
1	D	4023	ILE	N-CA-C	-5.07	101.11	108.36

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	1877	0	1887	64	0
1	B	1789	0	1800	63	0
1	C	1798	0	1808	75	0
1	D	1836	0	1848	77	0
1	E	1782	0	1793	61	0
1	F	1830	0	1838	64	0
2	A	10	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	C	21	0	11	8	0
4	A	32	0	0	0	0
4	B	34	0	0	2	0
4	C	30	0	0	0	0
4	D	35	0	0	1	0
4	E	35	0	0	0	0
4	F	41	0	0	3	0
All	All	11160	0	10985	385	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 18.

All (385) 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:1049:GLU:HG3	1:E:5049:GLU:HG2	1.09	1.09
1:D:4144:ALA:HA	1:D:4244:ILE:HD12	1.43	1.00
1:A:1049:GLU:HG3	1:E:5049:GLU:CG	1.93	0.98
1:C:3163:TYR:HB2	1:C:3164:PRO:HD3	1.47	0.95
1:A:1049:GLU:CG	1:E:5049:GLU:HG2	1.97	0.92
1:C:3022:ALA:HB2	1:C:3086:ILE:HD13	1.52	0.91
1:B:2049:GLU:HG3	1:D:4049:GLU:HG3	1.53	0.89
1:B:2049:GLU:CG	1:D:4049:GLU:HG3	2.03	0.88
1:F:6099:GLN:HB2	1:F:6102:ILE:HD13	1.56	0.87
1:A:1199:SER:HB3	1:A:1215:MET:HE2	1.57	0.86
1:C:3199:SER:HB3	1:C:3215:MET:HE2	1.58	0.85
1:A:1220:ILE:O	1:A:1229:PRO:HG3	1.76	0.85
1:E:5250:ARG:HA	1:E:5253:LEU:HD22	1.57	0.85
1:B:2105:GLY:HA2	1:B:2237:THR:HB	1.61	0.82
1:D:4030:ARG:O	1:D:4034:ILE:HG12	1.79	0.82
1:F:6194:ASN:N	1:F:6194:ASN:HD22	1.77	0.82
1:A:1238:GLU:O	1:A:1242:VAL:HG23	1.79	0.81
1:A:1049:GLU:OE1	1:E:5069:ILE:HD12	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3049:GLU:HG2	1:F:6049:GLU:HB3	1.63	0.80
1:A:1027:ASP:HB3	1:A:1030:ARG:HG2	1.62	0.79
1:A:1121:LEU:HD21	1:A:1126:MET:HE2	1.63	0.78
1:C:3158:SER:HB3	1:C:3200:ALA:HB2	1.65	0.78
1:A:1048:ARG:HD3	1:E:5069:ILE:HD11	1.64	0.78
1:D:4181:LYS:NZ	1:D:4181:LYS:HB3	1.96	0.78
1:F:6144:ALA:HA	1:F:6244:ILE:HD12	1.64	0.78
1:C:3239:SER:HB3	1:C:3243:LYS:HE3	1.66	0.77
1:A:1230:ASN:H	1:A:1230:ASN:ND2	1.82	0.77
1:B:2158:SER:HB3	1:B:2200:ALA:HB2	1.67	0.77
1:F:6240:HIS:O	1:F:6244:ILE:HG12	1.86	0.76
1:D:4037:LEU:HD21	1:D:4243:LYS:HE2	1.67	0.76
1:A:1230:ASN:HD22	1:A:1230:ASN:N	1.83	0.75
1:A:1242:VAL:O	1:A:1245:VAL:HG12	1.88	0.74
1:C:3040:LYS:HZ3	1:C:3040:LYS:HB2	1.53	0.73
1:D:4145:LYS:HD2	1:D:4146:SER:N	2.03	0.73
1:F:6158:SER:HB3	1:F:6200:ALA:HB2	1.69	0.73
1:D:4240:HIS:O	1:D:4244:ILE:HG12	1.88	0.73
1:D:4092:ILE:HD13	1:D:4093:GLY:N	2.05	0.72
1:E:5247:GLU:O	1:E:5250:ARG:HG2	1.90	0.72
1:C:3095:THR:HA	3:C:8003:U5P:H5	1.70	0.72
1:A:1037:LEU:HD22	1:A:1242:VAL:HG12	1.71	0.71
1:E:5099:GLN:HB2	1:E:5102:ILE:HD12	1.73	0.71
1:C:3092:ILE:HD11	1:C:3241:ALA:HB1	1.72	0.70
1:B:2147:ILE:HD11	1:B:2149:ALA:CB	2.21	0.70
1:A:1230:ASN:O	1:A:1234:MET:HB2	1.92	0.69
1:C:3137:THR:O	1:C:3141:VAL:HG23	1.93	0.69
1:D:4231:ALA:HA	1:D:4234:MET:HE3	1.74	0.69
1:E:5125:PRO:HB2	1:E:5127:GLU:OE2	1.93	0.69
1:B:2222:ASN:HB3	1:B:2225:GLN:HB2	1.74	0.68
1:B:2058:ASP:OD1	1:B:2250:ARG:HD2	1.92	0.68
1:E:5138:THR:O	1:E:5142:GLU:HG3	1.93	0.68
1:C:3152:HIS:HB3	1:C:3193:MET:HE2	1.76	0.68
1:C:3163:TYR:HA	1:C:3168:ARG:HD2	1.76	0.67
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.76	0.67
1:D:4057:LEU:HB3	1:D:4253:LEU:HD11	1.76	0.67
1:F:6239:SER:O	1:F:6243:LYS:HG3	1.95	0.67
1:D:4134:PHE:O	1:D:4138:THR:HG23	1.96	0.66
1:C:3044:LEU:HD21	1:C:3054:ARG:NH1	2.11	0.66
1:D:4147:ILE:HD11	1:D:4243:LYS:HG2	1.76	0.66
1:E:5021:LEU:HD23	1:E:5022:ALA:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3040:LYS:HB2	1:C:3040:LYS:NZ	2.12	0.65
1:F:6099:GLN:HB2	1:F:6102:ILE:CD1	2.25	0.65
1:B:2093:GLY:O	1:B:2217:ALA:HA	1.96	0.65
1:C:3095:THR:CA	3:C:8003:U5P:H5	2.28	0.64
1:C:3079:GLU:OE1	1:F:6171:THR:HB	1.96	0.64
1:A:1230:ASN:ND2	1:A:1230:ASN:N	2.41	0.64
1:D:4086:ILE:HD12	1:D:4086:ILE:H	1.62	0.64
1:E:5030:ARG:HD3	1:E:5238:GLU:CD	2.23	0.64
1:F:6249:ALA:O	1:F:6253:LEU:HD13	1.97	0.64
1:B:2147:ILE:HD11	1:B:2149:ALA:HB2	1.80	0.63
1:D:4163:TYR:HA	1:D:4168:ARG:HG3	1.80	0.63
1:F:6038:MET:HE1	1:F:6062:VAL:HB	1.78	0.63
1:A:1031:VAL:HG13	1:A:1064:VAL:HG12	1.81	0.63
1:A:1230:ASN:H	1:A:1230:ASN:HD22	1.44	0.63
1:D:4086:ILE:HD12	1:D:4086:ILE:N	2.13	0.62
1:C:3240:HIS:O	1:C:3244:ILE:HG13	1.99	0.62
1:A:1154:GLY:C	1:A:1193:MET:HE2	2.24	0.62
1:E:5158:SER:HB3	1:E:5200:ALA:HB2	1.81	0.61
1:E:5044:LEU:HD11	1:E:5054:ARG:HB2	1.82	0.61
1:B:2092:ILE:HD13	1:B:2093:GLY:N	2.15	0.61
1:E:5030:ARG:HD3	1:E:5238:GLU:OE2	2.00	0.61
1:C:3017:GLN:HG3	1:C:3054:ARG:NE	2.15	0.61
1:D:4181:LYS:HB3	1:D:4181:LYS:HZ3	1.63	0.61
1:B:2179:ARG:HD2	4:B:9133:HOH:O	1.99	0.61
1:F:6091:ARG:HH21	1:F:6215:MET:HE1	1.66	0.60
1:B:2247:GLU:O	1:B:2250:ARG:HB3	2.01	0.60
1:F:6194:ASN:HD22	1:F:6194:ASN:H	1.48	0.60
1:F:6038:MET:HE3	1:F:6057:LEU:HB2	1.84	0.59
1:C:3152:HIS:C	1:C:3193:MET:HE1	2.27	0.58
1:D:4163:TYR:HB2	1:D:4164:PRO:CD	2.33	0.58
1:F:6108:LEU:HD22	1:F:6152:HIS:HB2	1.86	0.58
1:C:3096:GLY:N	3:C:8003:U5P:H5	2.18	0.58
1:A:1027:ASP:HB3	1:A:1030:ARG:CG	2.33	0.58
1:D:4178:ARG:HA	1:D:4181:LYS:HG3	1.86	0.57
1:E:5030:ARG:NE	1:E:5238:GLU:HG2	2.19	0.57
1:A:1229:PRO:HB2	1:A:1235:LYS:HE2	1.85	0.57
1:C:3046:SER:OG	1:C:3051:THR:HG22	2.04	0.57
1:B:2188:GLN:NE2	1:B:2224:THR:HG21	2.20	0.57
1:F:6145:LYS:C	1:F:6145:LYS:HD3	2.30	0.57
1:F:6194:ASN:N	1:F:6194:ASN:ND2	2.48	0.57
1:A:1092:ILE:HD13	1:A:1093:GLY:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3081:LEU:HB3	1:C:3086:ILE:HD12	1.86	0.56
1:F:6007:PHE:HD2	1:F:6008:HIS:CE1	2.24	0.56
1:C:3152:HIS:HB3	1:C:3193:MET:CE	2.35	0.56
1:F:6121:LEU:HD21	1:F:6126:MET:HE2	1.88	0.56
1:B:2239:SER:O	1:B:2243:LYS:HG3	2.06	0.56
1:A:1143:ALA:HB1	1:A:1247:GLU:HB3	1.88	0.56
1:D:4093:GLY:O	1:D:4217:ALA:HA	2.06	0.56
1:C:3096:GLY:H	3:C:8003:U5P:H5	1.70	0.55
1:C:3163:TYR:CB	1:C:3164:PRO:HD3	2.31	0.55
1:E:5222:ASN:HB3	1:E:5225:GLN:HB2	1.87	0.55
1:C:3238:GLU:O	1:C:3242:VAL:HG23	2.06	0.55
1:D:4046:SER:OG	1:D:4051:THR:HG22	2.06	0.55
1:C:3004:SER:OG	1:C:3010:GLY:HA2	2.06	0.55
1:F:6021:LEU:C	1:F:6021:LEU:HD23	2.32	0.55
1:A:1092:ILE:HD13	1:A:1092:ILE:C	2.32	0.55
1:D:4184:MET:O	1:D:4188:GLN:HG3	2.07	0.55
1:F:6030:ARG:HA	1:F:6033:LYS:HD3	1.89	0.55
1:D:4168:ARG:HD3	4:D:9149:HOH:O	2.05	0.55
1:F:6240:HIS:HA	1:F:6243:LYS:HE2	1.88	0.55
1:B:2060:LYS:HD3	1:B:2253:LEU:HB3	1.89	0.54
1:B:2139:ALA:HA	1:B:2251:ARG:HD2	1.89	0.54
1:C:3122:HIS:HE1	1:F:6159:SER:HB2	1.73	0.54
1:E:5046:SER:OG	1:E:5051:THR:HG22	2.07	0.54
1:F:6226:GLN:NE2	1:F:6229:PRO:HA	2.22	0.54
1:E:5033:LYS:O	1:E:5036:ALA:HB3	2.07	0.54
1:A:1230:ASN:HB2	1:A:1234:MET:HB2	1.89	0.54
1:B:2147:ILE:CD1	1:B:2149:ALA:H	2.21	0.54
1:C:3199:SER:HB3	1:C:3215:MET:CE	2.33	0.54
1:A:1029:GLU:C	1:A:1030:ARG:HE	2.17	0.53
1:D:4186:GLU:OE2	1:E:5178:ARG:HB2	2.09	0.53
1:B:2138:THR:O	1:B:2142:GLU:HG2	2.08	0.53
1:B:2096:GLY:HA2	1:B:2221:VAL:O	2.08	0.53
1:E:5178:ARG:HA	1:E:5181:LYS:HE3	1.91	0.53
1:C:3092:ILE:HD11	1:C:3241:ALA:CB	2.38	0.53
1:D:4067:THR:O	1:D:4073:SER:HB3	2.08	0.53
1:D:4151:THR:HG22	1:D:4152:HIS:N	2.24	0.53
1:F:6137:THR:O	1:F:6141:VAL:HG23	2.09	0.53
1:C:3006:VAL:HG12	1:C:3006:VAL:O	2.09	0.52
1:C:3092:ILE:CD1	1:C:3241:ALA:HB1	2.39	0.52
1:A:1232:GLU:O	1:A:1235:LYS:HB2	2.09	0.52
1:F:6023:ILE:O	1:F:6064:VAL:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2019:ALA:HB3	1:B:2063:ILE:HD13	1.91	0.52
1:F:6016:LEU:HD11	1:F:6084:LEU:HB3	1.89	0.52
1:A:1049:GLU:HG3	1:E:5049:GLU:CB	2.40	0.52
1:D:4144:ALA:HA	1:D:4244:ILE:CD1	2.28	0.52
1:E:5239:SER:O	1:E:5243:LYS:HG3	2.09	0.52
1:F:6144:ALA:HA	1:F:6244:ILE:CD1	2.38	0.52
1:E:5028:PRO:HA	1:E:5066:SER:HB3	1.92	0.52
1:A:1107:VAL:HG21	1:A:1244:ILE:HD12	1.90	0.52
1:B:2250:ARG:HG2	1:B:2250:ARG:HH11	1.74	0.52
1:B:2022:ALA:HA	1:B:2063:ILE:O	2.10	0.52
1:C:3153:VAL:N	1:C:3193:MET:HE1	2.24	0.52
1:D:4021:LEU:C	1:D:4021:LEU:HD23	2.35	0.52
1:F:6016:LEU:HA	1:F:6063:ILE:HD11	1.92	0.52
1:C:3091:ARG:HB3	1:C:3215:MET:HG2	1.92	0.51
1:E:5154:GLY:C	1:E:5193:MET:HE2	2.34	0.51
1:C:3239:SER:HB3	1:C:3243:LYS:CE	2.40	0.51
1:A:1044:LEU:HD11	1:A:1054:ARG:HB2	1.93	0.51
3:C:8003:U5P:H2'	4:F:9094:HOH:O	2.10	0.51
1:D:4081:LEU:HB3	1:D:4086:ILE:HD13	1.92	0.51
1:D:4220:ILE:HB	1:D:4234:MET:HG2	1.92	0.51
1:C:3136:CYS:HA	1:C:3252:LEU:HD11	1.91	0.51
1:F:6200:ALA:HB3	4:F:9159:HOH:O	2.11	0.51
1:C:3209:GLN:HG2	1:F:6173:SER:HB3	1.93	0.51
1:B:2009:LEU:HD22	1:B:2050:PHE:HB3	1.92	0.51
1:F:6019:ALA:CB	1:F:6063:ILE:HD13	2.41	0.51
1:E:5031:VAL:HG13	1:E:5064:VAL:HG12	1.92	0.50
1:E:5238:GLU:HG3	1:E:5242:VAL:HG21	1.93	0.50
1:D:4117:ASP:OD1	1:D:4120:SER:HB2	2.10	0.50
1:D:4158:SER:HB3	1:D:4200:ALA:HB2	1.93	0.50
1:A:1222:ASN:HB3	1:A:1225:GLN:HG3	1.94	0.50
1:C:3095:THR:HA	3:C:8003:U5P:C5	2.41	0.50
1:F:6221:VAL:HG23	1:F:6226:GLN:HE21	1.76	0.50
1:D:4025:PRO:HD2	1:D:4065:CYS:O	2.12	0.50
1:E:5030:ARG:CZ	1:E:5238:GLU:HG2	2.42	0.50
1:E:5169:TYR:O	1:E:5174:GLY:HA2	2.12	0.50
1:B:2169:TYR:O	1:B:2174:GLY:HA2	2.11	0.50
1:E:5016:LEU:HA	1:E:5063:ILE:HD11	1.94	0.50
1:D:4181:LYS:HB3	1:D:4181:LYS:HZ2	1.75	0.49
1:F:6119:ALA:O	1:F:6122:HIS:HB2	2.12	0.49
1:A:1038:MET:HG2	1:A:1057:LEU:HD13	1.95	0.49
1:D:4196:GLU:CD	1:D:4199:SER:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3163:TYR:HB2	1:C:3164:PRO:CD	2.30	0.49
1:A:1158:SER:HA	1:A:1196:GLU:O	2.12	0.49
1:B:2144:ALA:O	1:B:2147:ILE:HD13	2.13	0.49
1:F:6090:LEU:HD11	1:F:6252:LEU:HD12	1.95	0.49
1:A:1089:PHE:O	1:A:1213:ALA:HA	2.13	0.49
1:C:3060:LYS:HB2	1:C:3060:LYS:NZ	2.28	0.49
1:F:6024:VAL:HG23	1:F:6024:VAL:O	2.13	0.48
1:D:4142:GLU:O	1:D:4145:LYS:HE3	2.13	0.48
1:C:3178:ARG:HA	1:C:3181:LYS:HE3	1.96	0.48
1:D:4057:LEU:CD2	1:D:4250:ARG:HG2	2.43	0.48
1:B:2163:TYR:HA	1:B:2168:ARG:HD3	1.95	0.48
1:E:5015:ASP:O	1:E:5054:ARG:HD3	2.13	0.48
1:A:1060:LYS:HA	1:A:1060:LYS:HD3	1.64	0.48
1:C:3029:GLU:O	1:C:3033:LYS:HE2	2.12	0.48
1:F:6010:GLY:HA3	1:F:6047:HIS:CD2	2.49	0.48
1:A:1107:VAL:HG21	1:A:1244:ILE:CD1	2.44	0.48
1:E:5099:GLN:HB2	1:E:5102:ILE:CD1	2.43	0.48
1:A:1037:LEU:CD2	1:A:1242:VAL:HG12	2.41	0.48
1:D:4147:ILE:O	1:D:4147:ILE:CG2	2.61	0.48
1:E:5040:LYS:N	1:E:5041:PRO:CD	2.77	0.48
1:A:1247:GLU:O	1:A:1250:ARG:HB2	2.13	0.48
1:B:2021:LEU:C	1:B:2021:LEU:HD23	2.39	0.48
1:C:3080:GLU:O	1:C:3084:LEU:HG	2.13	0.48
1:A:1030:ARG:HE	1:A:1030:ARG:N	2.12	0.47
1:B:2179:ARG:HG2	1:B:2180:PHE:CD1	2.48	0.47
1:D:4060:LYS:HB2	1:D:4253:LEU:HD13	1.96	0.47
1:B:2183:SER:O	1:B:2186:GLU:HB2	2.14	0.47
1:D:4136:CYS:HA	1:D:4252:LEU:HD11	1.96	0.47
1:B:2028:PRO:HB3	1:B:2051:THR:HG23	1.97	0.47
1:B:2222:ASN:CB	1:B:2225:GLN:HB2	2.43	0.47
1:B:2163:TYR:HB2	1:B:2164:PRO:CD	2.45	0.47
1:E:5074:THR:O	1:E:5078:VAL:HG23	2.15	0.47
1:B:2147:ILE:HD13	1:B:2149:ALA:H	1.80	0.47
1:C:3096:GLY:HA2	1:C:3221:VAL:O	2.15	0.47
1:D:4016:LEU:CD1	1:D:4086:ILE:HD11	2.44	0.47
1:D:4199:SER:O	1:D:4203:LEU:HB2	2.14	0.47
1:E:5114:VAL:HB	1:E:5157:ALA:HA	1.97	0.47
1:F:6033:LYS:H	1:F:6033:LYS:HD2	1.79	0.47
1:B:2044:LEU:HD11	1:B:2054:ARG:HB2	1.96	0.47
1:E:5014:ASN:HD22	1:E:5014:ASN:HA	1.58	0.46
1:D:4095:THR:OG1	1:D:4096:GLY:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5106:ASP:O	1:E:5219:VAL:HG23	2.15	0.46
1:B:2163:TYR:O	1:B:2168:ARG:HG3	2.14	0.46
1:D:4022:ALA:HA	1:D:4063:ILE:O	2.15	0.46
1:C:3125:PRO:HB2	1:C:3127:GLU:OE1	2.16	0.46
1:F:6242:VAL:O	1:F:6245:VAL:HG12	2.16	0.46
1:F:6006:VAL:HG11	1:F:6080:GLU:HB3	1.98	0.46
1:A:1221:VAL:HG23	1:A:1229:PRO:HD2	1.96	0.46
2:A:7003:SO4:O4	1:D:4111:THR:HB	2.16	0.46
1:B:2176:VAL:O	1:B:2181:LYS:HG3	2.14	0.46
1:E:5199:SER:O	1:E:5203:LEU:HB2	2.15	0.46
1:B:2032:GLU:HG3	1:B:2053:TRP:CH2	2.49	0.46
1:E:5242:VAL:O	1:E:5245:VAL:HG12	2.16	0.46
1:D:4030:ARG:HD2	1:D:4238:GLU:OE2	2.16	0.46
1:F:6179:ARG:HG2	1:F:6180:PHE:CE1	2.50	0.46
1:B:2043:LYS:HD2	1:B:2053:TRP:NE1	2.30	0.46
1:D:4089:PHE:O	1:D:4213:ALA:HA	2.16	0.46
1:F:6013:LYS:HE3	1:F:6084:LEU:HA	1.98	0.46
1:F:6223:ARG:HG3	1:F:6223:ARG:HH11	1.80	0.46
1:D:4231:ALA:CA	1:D:4234:MET:HE3	2.42	0.46
1:E:5238:GLU:O	1:E:5242:VAL:HG23	2.16	0.46
1:B:2038:MET:SD	1:B:2062:VAL:HG21	2.56	0.45
1:B:2147:ILE:HD11	1:B:2149:ALA:HB3	1.96	0.45
1:C:3006:VAL:O	1:C:3006:VAL:CG1	2.64	0.45
1:D:4037:LEU:HD21	1:D:4243:LYS:CE	2.40	0.45
1:C:3096:GLY:O	1:C:3194:ASN:HB2	2.17	0.45
1:D:4024:VAL:HG23	1:D:4024:VAL:O	2.16	0.45
1:D:4092:ILE:HD13	1:D:4092:ILE:C	2.42	0.45
1:B:2021:LEU:HD23	1:B:2022:ALA:N	2.32	0.45
1:D:4091:ARG:HG3	1:D:4091:ARG:HH11	1.82	0.45
1:C:3021:LEU:C	1:C:3021:LEU:HD23	2.42	0.45
1:C:3097:ALA:HA	1:C:3194:ASN:HB3	1.98	0.45
1:D:4142:GLU:CA	1:D:4145:LYS:HE3	2.46	0.45
1:F:6021:LEU:HD23	1:F:6022:ALA:N	2.32	0.45
1:C:3017:GLN:HG3	1:C:3054:ARG:CD	2.46	0.45
1:C:3097:ALA:HB1	1:C:3102:ILE:HD12	1.99	0.45
1:E:5029:GLU:O	1:E:5033:LYS:HE2	2.16	0.45
1:F:6033:LYS:HD2	1:F:6033:LYS:N	2.32	0.45
1:A:1234:MET:C	1:A:1236:GLN:H	2.24	0.45
1:C:3140:LEU:HD22	1:C:3216:VAL:HB	1.99	0.45
1:D:4185:GLU:HA	1:D:4188:GLN:OE1	2.17	0.45
1:A:1095:THR:HG21	1:A:1108:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3091:ARG:HG3	1:C:3091:ARG:NH1	2.32	0.44
1:C:3094:THR:O	3:C:8003:U5P:H5'2	2.17	0.44
1:A:1096:GLY:HA2	1:A:1221:VAL:O	2.17	0.44
1:B:2004:SER:N	4:B:9201:HOH:O	2.49	0.44
1:B:2019:ALA:CB	1:B:2063:ILE:HD13	2.47	0.44
1:F:6167:GLU:HG2	1:F:6169:TYR:CE1	2.52	0.44
1:C:3071:GLY:N	1:C:3072:PRO:CD	2.81	0.44
1:D:4099:GLN:HG2	1:D:4101:HIS:CE1	2.53	0.44
1:F:6076:ILE:O	1:F:6080:GLU:HG3	2.17	0.44
1:A:1024:VAL:HB	1:A:1067:THR:CG2	2.48	0.44
1:A:1072:PRO:HA	1:E:5160:ASP:O	2.17	0.44
1:B:2099:GLN:HB3	1:B:2101:HIS:CE1	2.52	0.44
1:B:2179:ARG:HG2	1:B:2180:PHE:CE1	2.53	0.44
1:B:2110:THR:OG1	1:B:2215:MET:HE2	2.18	0.44
1:C:3199:SER:HB2	1:C:3203:LEU:HD22	2.00	0.44
1:E:5031:VAL:HG13	1:E:5064:VAL:CG1	2.48	0.44
1:E:5249:ALA:O	1:E:5253:LEU:HD13	2.17	0.44
1:A:1220:ILE:O	1:A:1229:PRO:CG	2.58	0.44
1:C:3090:LEU:HD11	1:C:3252:LEU:HD12	1.99	0.44
1:D:4075:SER:HA	1:D:4205:MET:SD	2.58	0.44
1:D:4090:LEU:HD11	1:D:4252:LEU:HD12	1.99	0.44
1:B:2242:VAL:O	1:B:2245:VAL:HG12	2.18	0.44
1:C:3206:CYS:HB3	1:C:3211:LEU:O	2.18	0.44
1:B:2102:ILE:CG2	1:B:2219:VAL:HG21	2.48	0.43
1:C:3025:PRO:O	1:C:3066:SER:HA	2.18	0.43
1:C:3138:THR:O	1:C:3142:GLU:HG3	2.18	0.43
1:B:2185:GLU:HA	1:B:2188:GLN:OE1	2.18	0.43
1:D:4091:ARG:HG3	1:D:4091:ARG:NH1	2.33	0.43
1:D:4166:GLN:HG2	1:D:4195:TYR:CD1	2.53	0.43
1:A:1163:TYR:HB2	1:A:1164:PRO:CD	2.48	0.43
1:F:6102:ILE:CG2	1:F:6219:VAL:HG21	2.48	0.43
1:F:6163:TYR:HB2	1:F:6164:PRO:CD	2.48	0.43
1:A:1030:ARG:O	1:A:1034:ILE:HD13	2.18	0.43
1:A:1071:GLY:N	1:A:1072:PRO:CD	2.82	0.43
1:E:5108:LEU:CD2	1:E:5152:HIS:HB2	2.48	0.43
1:D:4127:GLU:CD	1:D:4127:GLU:H	2.27	0.43
1:A:1105:GLY:HA2	1:A:1237:THR:OG1	2.19	0.43
1:E:5108:LEU:HD23	1:E:5152:HIS:HB2	2.01	0.43
1:D:4102:ILE:HG12	1:D:4152:HIS:CD2	2.53	0.43
1:E:5038:MET:HG2	1:E:5057:LEU:HD13	1.99	0.43
1:F:6046:SER:OG	1:F:6051:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:GLN:OE1	1:A:1227:GLU:HG2	2.19	0.43
1:D:4028:PRO:O	1:D:4031:VAL:HG23	2.19	0.43
1:F:6029:GLU:C	1:F:6030:ARG:HD2	2.44	0.43
1:B:2102:ILE:HG22	1:B:2219:VAL:HG21	2.00	0.43
1:B:2250:ARG:HG2	1:B:2250:ARG:NH1	2.33	0.43
1:D:4049:GLU:CD	1:D:4049:GLU:H	2.27	0.43
1:B:2186:GLU:O	1:B:2190:MET:HG3	2.19	0.43
1:D:4063:ILE:HD11	1:D:4065:CYS:HB2	2.01	0.43
1:F:6031:VAL:HG13	1:F:6064:VAL:HG12	2.00	0.43
1:C:3196:GLU:HA	3:C:8003:U5P:C1'	2.49	0.42
1:E:5187:TRP:HA	1:E:5187:TRP:CE3	2.54	0.42
1:F:6049:GLU:H	1:F:6049:GLU:HG2	1.58	0.42
1:E:5113:SER:HA	1:E:5156:THR:O	2.19	0.42
1:F:6057:LEU:HB3	1:F:6253:LEU:HD21	1.99	0.42
1:E:5087:ARG:HG3	1:E:5087:ARG:HH11	1.84	0.42
1:F:6019:ALA:HB3	1:F:6063:ILE:HD13	2.02	0.42
1:D:4008:HIS:HD2	1:D:4080:GLU:OE2	2.03	0.42
1:D:4071:GLY:N	1:D:4072:PRO:CD	2.82	0.42
1:E:5116:LEU:HB2	1:E:5158:SER:O	2.19	0.42
1:F:6169:TYR:O	1:F:6174:GLY:HA2	2.19	0.42
1:A:1049:GLU:HG3	1:E:5049:GLU:HB3	2.02	0.42
1:A:1127:GLU:HG3	1:D:4126:MET:HE3	2.02	0.42
1:C:3091:ARG:HG3	1:C:3091:ARG:HH11	1.84	0.42
1:D:4102:ILE:O	1:D:4222:ASN:ND2	2.52	0.42
1:E:5158:SER:HB3	1:E:5200:ALA:CB	2.48	0.42
1:F:6038:MET:HG2	1:F:6057:LEU:HD13	2.01	0.42
1:B:2049:GLU:O	1:B:2066:SER:OG	2.35	0.42
1:C:3040:LYS:NZ	1:C:3040:LYS:CB	2.81	0.42
1:C:3049:GLU:HG2	1:F:6049:GLU:CB	2.43	0.42
1:B:2126:MET:SD	1:C:3127:GLU:HG3	2.59	0.42
1:B:2205:MET:O	1:B:2209:GLN:HG3	2.19	0.42
1:D:4147:ILE:O	1:D:4147:ILE:HG23	2.19	0.42
1:D:4016:LEU:HD13	1:D:4086:ILE:HD11	2.02	0.41
1:D:4037:LEU:CD2	1:D:4243:LYS:HE2	2.42	0.41
1:A:1108:LEU:O	1:A:1216:VAL:HA	2.20	0.41
1:B:2028:PRO:HB3	1:B:2051:THR:CG2	2.50	0.41
1:A:1021:LEU:C	1:A:1021:LEU:HD23	2.45	0.41
1:A:1229:PRO:HB2	1:A:1235:LYS:CE	2.50	0.41
1:A:1250:ARG:HA	1:A:1253:LEU:HD22	2.02	0.41
1:C:3033:LYS:O	1:C:3037:LEU:HD12	2.20	0.41
1:E:5127:GLU:OE2	1:E:5127:GLU:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4187:TRP:HA	1:D:4187:TRP:CE3	2.55	0.41
1:E:5182:GLY:O	1:E:5186:GLU:HG3	2.20	0.41
1:B:2016:LEU:O	1:B:2017:GLN:HB2	2.21	0.41
1:E:5238:GLU:HG3	1:E:5242:VAL:CG2	2.50	0.41
1:A:1022:ALA:HA	1:A:1063:ILE:O	2.19	0.41
1:B:2079:GLU:OE1	1:D:4171:THR:HB	2.21	0.41
1:C:3035:ALA:HA	1:C:3038:MET:HE3	2.02	0.41
1:C:3211:LEU:HD21	1:F:6172:TYR:CE1	2.55	0.41
1:E:5034:ILE:HG12	1:E:5242:VAL:HG13	2.02	0.41
1:E:5163:TYR:CD2	1:E:5171:THR:HG22	2.56	0.41
1:A:1199:SER:O	1:A:1200:ALA:C	2.64	0.41
1:B:2117:ASP:OD1	1:B:2120:SER:HB3	2.21	0.41
1:C:3098:ILE:HD11	1:C:3192:VAL:HB	2.03	0.41
1:C:3239:SER:O	1:C:3243:LYS:HG3	2.21	0.41
1:E:5033:LYS:H	1:E:5033:LYS:CD	2.34	0.41
1:E:5131:VAL:HG22	1:E:5132:ALA:O	2.20	0.41
1:F:6237:THR:O	1:F:6240:HIS:HB2	2.20	0.41
1:A:1031:VAL:HG13	1:A:1064:VAL:CG1	2.51	0.41
1:B:2004:SER:OG	1:B:2010:GLY:HA2	2.21	0.41
1:B:2240:HIS:O	1:B:2244:ILE:HG13	2.21	0.41
1:C:3048:ARG:HD3	4:F:9105:HOH:O	2.19	0.41
1:C:3158:SER:CB	1:C:3200:ALA:HB2	2.45	0.41
1:C:3095:THR:OG1	1:C:3096:GLY:N	2.54	0.40
1:D:4056:GLU:OE2	1:D:4059:GLY:HA2	2.21	0.40
1:A:1196:GLU:HG2	1:A:1215:MET:HE1	2.03	0.40
1:A:1228:ILE:HA	1:A:1229:PRO:HD2	1.86	0.40
1:B:2027:ASP:HA	1:B:2028:PRO:HD3	1.94	0.40
1:C:3032:GLU:HG3	1:C:3033:LYS:N	2.36	0.40
1:F:6133:ASP:OD1	1:F:6135:ALA:N	2.54	0.40
1:F:6138:THR:O	1:F:6142:GLU:HG3	2.22	0.40
1:A:1163:TYR:HB2	1:A:1164:PRO:HD3	2.04	0.40
1:D:4057:LEU:HD21	1:D:4250:ARG:HG2	2.03	0.40
1:B:2163:TYR:CB	1:B:2164:PRO:CD	2.99	0.40
1:C:3057:LEU:O	1:C:3253:LEU:HD21	2.22	0.40
1:D:4187:TRP:HA	1:D:4187:TRP:HE3	1.87	0.40
1:E:5021:LEU:HD23	1:E:5021:LEU:C	2.47	0.40
1:F:6071:GLY:N	1:F:6072:PRO:CD	2.84	0.40
1:D:4145:LYS:HD2	1:D:4145:LYS:C	2.46	0.40
1:F:6006:VAL:HB	1:F:6080:GLU:OE1	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	248/253 (98%)	235 (95%)	10 (4%)	3 (1%)	10	9
1	B	235/253 (93%)	225 (96%)	9 (4%)	1 (0%)	30	34
1	C	236/253 (93%)	218 (92%)	17 (7%)	1 (0%)	30	34
1	D	241/253 (95%)	228 (95%)	11 (5%)	2 (1%)	16	17
1	E	234/253 (92%)	218 (93%)	13 (6%)	3 (1%)	9	8
1	F	240/253 (95%)	227 (95%)	11 (5%)	2 (1%)	16	17
All	All	1434/1518 (94%)	1351 (94%)	71 (5%)	12 (1%)	16	17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4163	TYR
1	A	1229	PRO
1	A	1230	ASN
1	A	1163	TYR
1	B	2163	TYR
1	C	3163	TYR
1	E	5163	TYR
1	E	5223	ARG
1	F	6163	TYR
1	D	4221	VAL
1	E	5148	GLY
1	F	6118	GLY

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	199/202 (98%)	188 (94%)	11 (6%)	19	24
1	B	189/202 (94%)	179 (95%)	10 (5%)	20	25
1	C	190/202 (94%)	175 (92%)	15 (8%)	11	12
1	D	194/202 (96%)	183 (94%)	11 (6%)	18	23
1	E	188/202 (93%)	179 (95%)	9 (5%)	23	29
1	F	194/202 (96%)	182 (94%)	12 (6%)	16	19
All	All	1154/1212 (95%)	1086 (94%)	68 (6%)	18	22

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1042	VAL
1	A	1049	GLU
1	A	1056	GLU
1	A	1092	ILE
1	A	1184	MET
1	A	1203	LEU
1	A	1215	MET
1	A	1227	GLU
1	A	1230	ASN
1	A	1234	MET
1	A	1253	LEU
1	B	2073	SER
1	B	2092	ILE
1	B	2147	ILE
1	B	2150	THR
1	B	2170	ASP
1	B	2179	ARG
1	B	2185	GLU
1	B	2203	LEU
1	B	2237	THR
1	B	2238	GLU
1	C	3005	ASP
1	C	3006	VAL
1	C	3030	ARG
1	C	3032	GLU
1	C	3037	LEU
1	C	3040	LYS
1	C	3060	LYS

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Mol	Chain	Res	Type
1	C	3092	ILE
1	C	3115	ARG
1	C	3170	ASP
1	C	3203	LEU
1	C	3209	GLN
1	C	3215	MET
1	C	3245	VAL
1	C	3253	LEU
1	D	4062	VAL
1	D	4063	ILE
1	D	4073	SER
1	D	4092	ILE
1	D	4147	ILE
1	D	4170	ASP
1	D	4181	LYS
1	D	4196	GLU
1	D	4203	LEU
1	D	4225	GLN
1	D	4243	LYS
1	E	5014	ASN
1	E	5030	ARG
1	E	5049	GLU
1	E	5092	ILE
1	E	5179	ARG
1	E	5203	LEU
1	E	5239	SER
1	E	5240	HIS
1	E	5253	LEU
1	F	6013	LYS
1	F	6020	GLN
1	F	6037	LEU
1	F	6063	ILE
1	F	6092	ILE
1	F	6127	GLU
1	F	6179	ARG
1	F	6194	ASN
1	F	6203	LEU
1	F	6237	THR
1	F	6238	GLU
1	F	6253	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1188	GLN
1	A	1225	GLN
1	A	1230	ASN
1	A	1240	HIS
1	B	2020	GLN
1	B	2152	HIS
1	C	3020	GLN
1	C	3047	HIS
1	C	3209	GLN
1	C	3225	GLN
1	D	4008	HIS
1	D	4020	GLN
1	D	4047	HIS
1	D	4099	GLN
1	D	4225	GLN
1	D	4240	HIS
1	E	5014	ASN
1	E	5047	HIS
1	E	5209	GLN
1	F	6014	ASN
1	F	6020	GLN
1	F	6047	HIS
1	F	6188	GLN
1	F	6194	ASN
1	F	6226	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
2	SO4	A	7003	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	E	7001	-	4,4,4	0.36	0	6,6,6	0.07	0
3	U5P	C	8003	-	22,22,22	0.39	0	32,33,33	0.39	0
2	SO4	A	7004	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	F	7005	-	4,4,4	0.37	0	6,6,6	0.14	0

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	U5P	C	8003	-	-	2/10/26/26	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	8003	U5P	O4'-C4'-C5'-O5'
3	C	8003	U5P	C4'-C5'-O5'-P

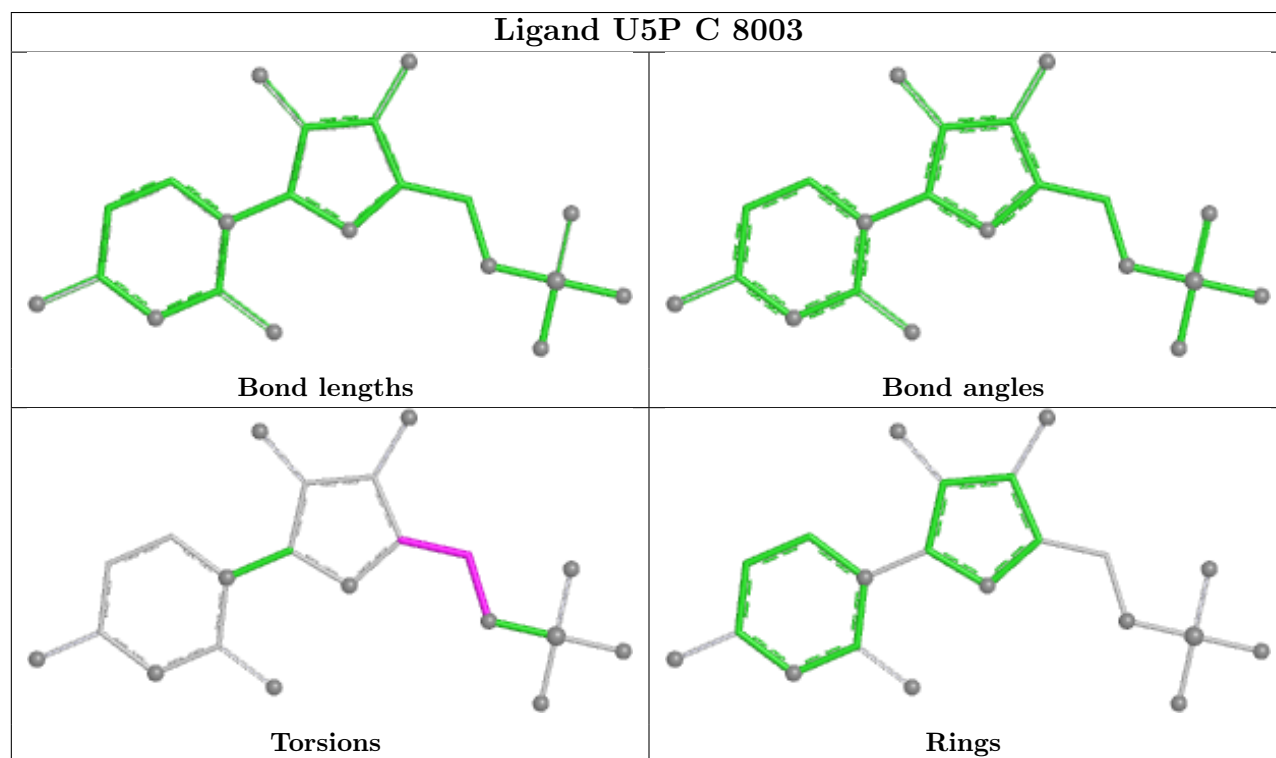
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	7003	SO4	1	0
3	C	8003	U5P	8	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	250/253 (98%)	-0.24	10 (4%) 42 48	8, 23, 61, 91	0
1	B	239/253 (94%)	-0.09	3 (1%) 75 79	10, 29, 54, 87	0
1	C	240/253 (94%)	-0.05	4 (1%) 69 74	13, 29, 59, 104	0
1	D	245/253 (96%)	-0.13	6 (2%) 59 66	10, 25, 54, 128	0
1	E	238/253 (94%)	-0.20	6 (2%) 58 64	7, 24, 52, 96	0
1	F	244/253 (96%)	-0.19	2 (0%) 82 86	12, 26, 52, 96	0
All	All	1456/1518 (95%)	-0.15	31 (2%) 63 68	7, 26, 56, 128	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4231	ALA	7.2
1	B	2007	PHE	5.8
1	E	5225	GLN	5.7
1	F	6237	THR	5.3
1	A	1234	MET	4.5
1	D	4007	PHE	4.1
1	A	1229	PRO	4.1
1	D	4234	MET	3.9
1	A	1235	LYS	3.5
1	E	5007	PHE	3.5
1	F	6230	ASN	3.4
1	E	5239	SER	3.3
1	A	1233	THR	3.2
1	D	4233	THR	3.1
1	C	3007	PHE	3.0
1	B	2225	GLN	2.7
1	E	5224	THR	2.7
1	A	1225	GLN	2.5
1	D	4224	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1236	GLN	2.5
1	A	1231	ALA	2.4
1	E	5238	GLU	2.4
1	C	3101	HIS	2.3
1	A	1232	GLU	2.2
1	A	1049	GLU	2.2
1	C	3225	GLN	2.2
1	E	5049	GLU	2.2
1	D	4225	GLN	2.2
1	A	1007	PHE	2.1
1	C	3006	VAL	2.0
1	B	2253	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

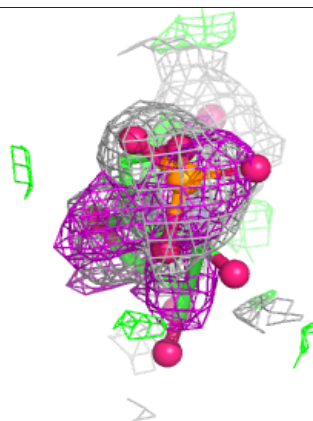
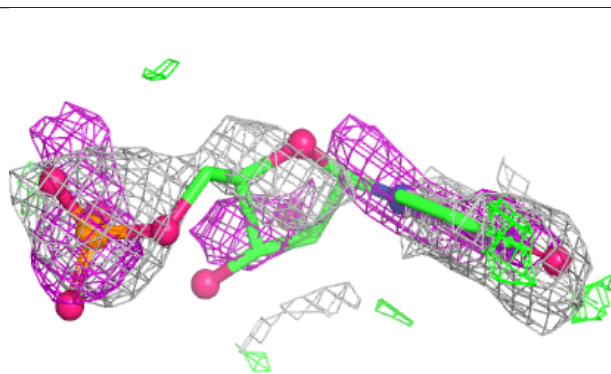
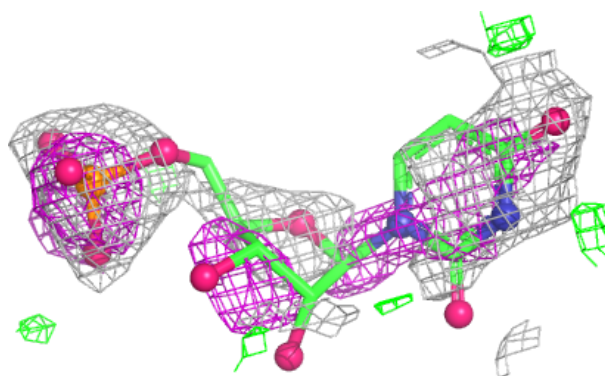
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	U5P	C	8003	21/21	0.78	0.16	35,58,71,71	0
2	SO4	A	7003	5/5	0.89	0.15	109,124,126,126	0
2	SO4	A	7004	5/5	0.95	0.13	14,60,71,89	0
2	SO4	F	7005	5/5	0.96	0.10	36,54,58,81	0
2	SO4	E	7001	5/5	0.97	0.11	26,50,67,74	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 U5P C 8003:

$2mF_o - DF_c$ (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.