



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:51 AM UTC

PDB ID : 6I5F / pdb_00006i5f
Title : Crystal structure of DNA-free E.coli MutS P839E dimer mutant
Authors : Bhairosing-Kok, D.; Groothuizen, F.S.; Fish, A.; Dharadhar, S.; Winterwerp, H.H.K.; Sixma, T.K.
Deposited on : 2018-11-13
Resolution : 2.60 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

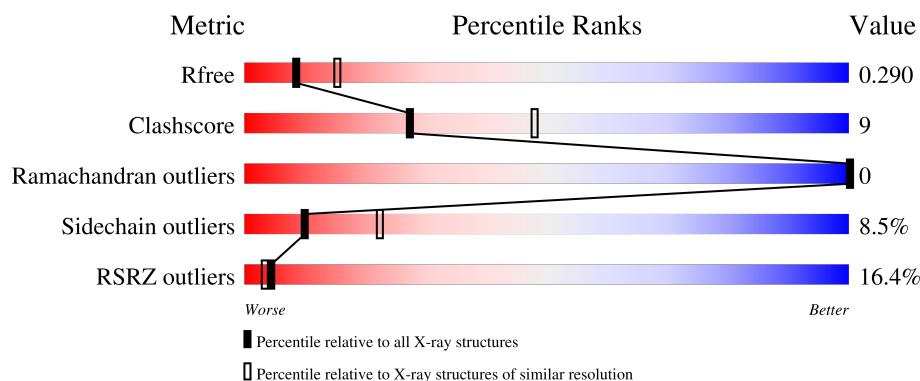
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	853	14% 66% 20% • 11%
1	B	853	16% 68% 19% • 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12451 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.

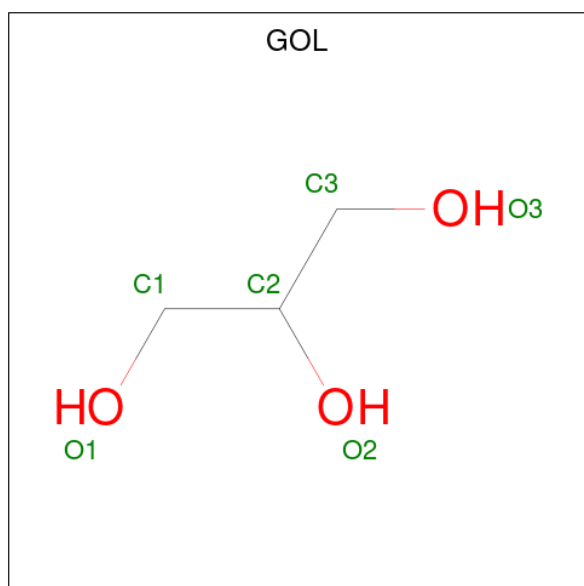
- Molecule 1 is a protein called DNA mismatch repair protein MutS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	760	Total	C	N	O	S	0	0	0
			6000	3782	1065	1124	29			
1	B	777	Total	C	N	O	S	0	1	0
			6134	3861	1093	1151	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	839	GLU	PRO	engineered mutation	UNP P23909
B	839	GLU	PRO	engineered mutation	UNP P23909

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



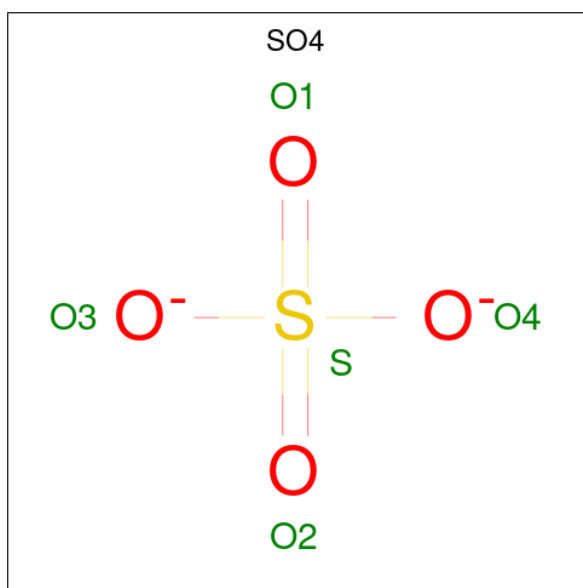
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

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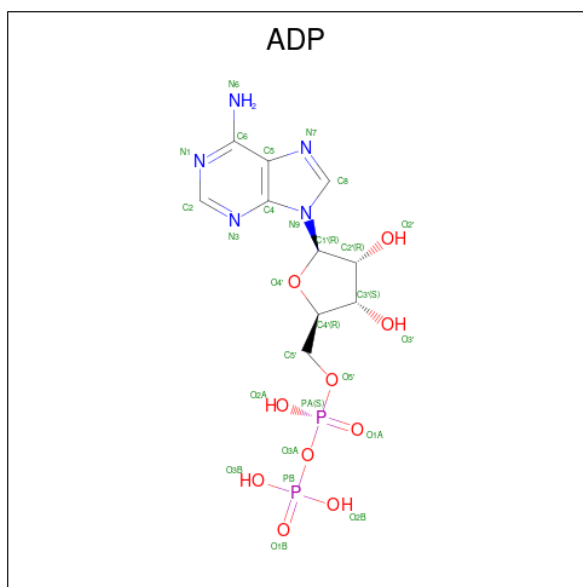
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 27 10 5 10 2	0	0
4	B	1	Total C N O P 27 10 5 10 2	0	0

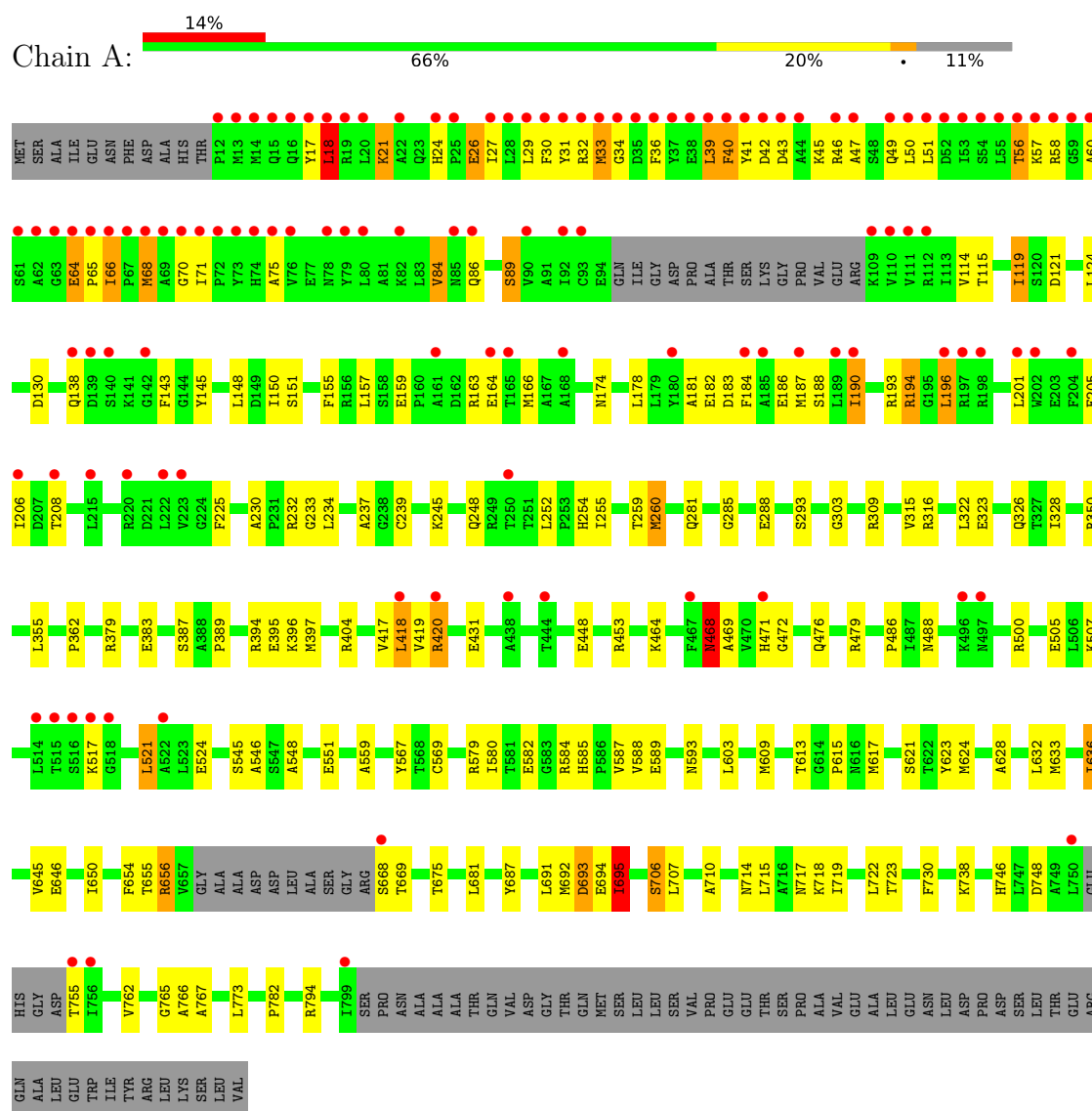
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total 76	O 76	0	0
5	B	64	Total 64	O 64	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: DNA mismatch repair protein MutS



• Molecule 1: DNA mismatch repair protein MutS





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.38Å 113.53Å 158.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.61 – 2.60 71.61 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (71.61-2.60) 97.6 (71.61-2.60)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.62Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.206 , 0.257 0.230 , 0.290	Depositor DCC
R_{free} test set	3051 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.030 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12451	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: ADP, SO4, 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	0.93	2/6099 (0.0%)	1.44	58/8251 (0.7%)
1	B	0.91	7/6248 (0.1%)	1.48	42/8454 (0.5%)
All	All	0.92	9/12347 (0.1%)	1.46	100/16705 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	6
All	All	0	8

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	494	THR	C-N	8.25	1.44	1.33
1	B	624	MET	SD-CE	-6.94	1.62	1.79
1	A	181	ALA	C-N	-6.91	1.24	1.33
1	B	154[A]	ARG	N-CA	6.45	1.54	1.46
1	B	154[B]	ARG	N-CA	6.45	1.54	1.46
1	B	154[A]	ARG	CA-C	6.29	1.60	1.52
1	B	154[B]	ARG	CA-C	6.29	1.60	1.52
1	B	376	PRO	C-O	-5.61	1.17	1.24
1	A	178	LEU	C-N	5.45	1.41	1.33

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154[A]	ARG	CA-CB-CG	25.40	164.90	114.10
1	B	154[B]	ARG	CA-CB-CG	25.40	164.90	114.10
1	A	64	GLU	CB-CA-C	9.06	122.92	108.87
1	B	154[A]	ARG	CA-C-O	8.46	130.16	120.60
1	B	154[B]	ARG	CA-C-O	8.46	130.16	120.60
1	A	468	ASN	CA-CB-CG	7.57	120.17	112.60
1	A	654	PHE	CA-CB-CG	7.52	121.32	113.80
1	A	43	ASP	N-CA-C	-7.14	103.57	111.36
1	B	163	ARG	N-CA-C	-7.06	103.66	111.36
1	A	695	ILE	N-CA-CB	6.93	118.09	110.53
1	A	42	ASP	CB-CA-C	6.87	119.96	110.06
1	A	469	ALA	CA-C-N	6.82	129.71	120.77
1	A	469	ALA	C-N-CA	6.82	129.71	120.77
1	B	155	PHE	CA-CB-CG	6.76	120.56	113.80
1	B	183	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	225	PHE	N-CA-C	-6.52	105.36	113.38
1	B	419	VAL	N-CA-C	-6.50	106.35	113.43
1	A	30	PHE	CA-C-N	6.42	129.99	120.87
1	A	30	PHE	C-N-CA	6.42	129.99	120.87
1	B	794	ARG	CA-C-N	6.32	128.75	120.28
1	B	794	ARG	C-N-CA	6.32	128.75	120.28
1	A	181	ALA	CA-C-N	6.28	128.70	120.28
1	A	181	ALA	C-N-CA	6.28	128.70	120.28
1	B	30	PHE	CA-CB-CG	6.23	120.03	113.80
1	B	205	GLU	CA-C-N	6.17	128.86	120.77
1	B	205	GLU	C-N-CA	6.17	128.86	120.77
1	A	693	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	163	ARG	CA-C-N	6.09	128.45	120.28
1	B	163	ARG	C-N-CA	6.09	128.45	120.28
1	B	327	THR	CA-C-N	6.09	128.46	120.60
1	B	327	THR	C-N-CA	6.09	128.46	120.60
1	A	121	ASP	CA-C-N	6.09	128.72	120.38
1	A	121	ASP	C-N-CA	6.09	128.72	120.38
1	B	748	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	18	LEU	CA-C-N	5.88	128.44	120.38
1	A	18	LEU	C-N-CA	5.88	128.44	120.38
1	A	710	ALA	CA-C-N	5.84	128.39	120.44
1	A	710	ALA	C-N-CA	5.84	128.39	120.44
1	B	154[A]	ARG	CB-CA-C	5.83	120.50	110.77
1	B	154[B]	ARG	CB-CA-C	5.83	120.50	110.77
1	A	288	GLU	CB-CG-CD	5.79	122.44	112.60
1	A	130	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	717	ASN	CA-CB-CG	5.72	118.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	GLY	N-CA-C	5.68	119.44	111.14
1	A	174	ASN	CA-CB-CG	5.64	118.25	112.60
1	B	142	GLY	N-CA-C	5.64	118.38	110.38
1	A	546	ALA	CA-C-N	5.62	128.09	120.44
1	A	546	ALA	C-N-CA	5.62	128.09	120.44
1	A	636	ILE	N-CA-CB	5.58	119.46	112.26
1	B	529	GLU	CA-C-N	5.56	128.76	120.31
1	B	529	GLU	C-N-CA	5.56	128.76	120.31
1	B	754	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	706	SER	CA-C-N	5.55	127.66	120.44
1	A	706	SER	C-N-CA	5.55	127.66	120.44
1	B	206	ILE	N-CA-C	5.51	115.96	110.23
1	A	65	PRO	N-CA-C	5.50	120.12	111.38
1	A	303	GLY	CA-C-N	5.48	127.89	120.38
1	A	303	GLY	C-N-CA	5.48	127.89	120.38
1	A	448	GLU	CA-C-N	5.47	127.87	120.44
1	A	448	GLU	C-N-CA	5.47	127.87	120.44
1	A	615	PRO	N-CA-C	5.45	118.85	111.22
1	B	139	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	395	GLU	CA-C-N	5.42	128.30	120.38
1	B	395	GLU	C-N-CA	5.42	128.30	120.38
1	A	237	ALA	CA-C-N	5.42	126.00	119.98
1	A	237	ALA	C-N-CA	5.42	126.00	119.98
1	A	239	CYS	CA-C-N	5.42	127.86	120.54
1	A	239	CYS	C-N-CA	5.42	127.86	120.54
1	A	56	THR	CA-CB-OG1	-5.41	101.49	109.60
1	B	309	ARG	CA-C-N	5.40	127.83	120.54
1	B	309	ARG	C-N-CA	5.40	127.83	120.54
1	A	582	GLU	CB-CG-CD	5.38	121.75	112.60
1	A	315	VAL	N-CA-C	5.36	116.50	109.58
1	B	390	VAL	N-CA-CB	5.33	117.03	110.64
1	A	355	LEU	N-CA-C	-5.33	105.55	111.36
1	A	404	ARG	N-CA-C	-5.30	105.42	111.14
1	B	368	MET	CA-C-N	5.29	127.80	120.29
1	B	368	MET	C-N-CA	5.29	127.80	120.29
1	A	383	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	593	ASN	N-CA-C	-5.18	103.64	111.56
1	A	617	MET	CA-C-N	5.16	125.67	120.00
1	A	617	MET	C-N-CA	5.16	125.67	120.00
1	B	348	LEU	CA-C-N	5.14	127.12	120.44
1	B	348	LEU	C-N-CA	5.14	127.12	120.44
1	A	248	GLN	CA-C-N	5.13	129.70	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	GLN	C-N-CA	5.13	129.70	122.46
1	A	155	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	794	ARG	CA-C-N	5.13	127.40	120.38
1	A	794	ARG	C-N-CA	5.13	127.40	120.38
1	A	309	ARG	CA-C-N	5.11	127.44	120.54
1	A	309	ARG	C-N-CA	5.11	127.44	120.54
1	B	182	GLU	CA-C-N	5.10	127.63	120.28
1	B	182	GLU	C-N-CA	5.10	127.63	120.28
1	B	700	SER	CA-C-N	5.08	127.34	120.38
1	B	700	SER	C-N-CA	5.08	127.34	120.38
1	B	739	MET	N-CA-C	5.07	116.90	109.24
1	B	35	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	282	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	507	LYS	CA-C-N	5.01	127.24	120.38
1	A	507	LYS	C-N-CA	5.01	127.24	120.38

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	ARG	Sidechain
1	A	420	ARG	Sidechain
1	B	108	ARG	Sidechain
1	B	379	ARG	Sidechain
1	B	455	ARG	Sidechain
1	B	457	ARG	Sidechain
1	B	479	ARG	Sidechain
1	B	500	ARG	Sidechain

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	6000	0	6069	106	0
1	B	6134	0	6176	123	0
2	A	60	0	80	13	0
2	B	18	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	25	0	0	0	0
3	B	20	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	76	0	0	2	0
5	B	64	0	0	0	0
All	All	12451	0	12373	225	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 9.

All (225) 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:183:ASP:OD1	1:A:201:LEU:HD21	1.68	0.93
1:B:463:LEU:HD21	1:B:475:ILE:HG22	1.55	0.87
1:A:39:LEU:C	1:A:40:PHE:CD1	2.53	0.87
1:B:479:ARG:HG2	1:B:498:ALA:CB	2.06	0.85
1:B:379:ARG:HG3	1:B:397:MET:CE	2.14	0.78
1:B:735:LEU:HD22	1:B:739:MET:HE2	1.64	0.78
1:B:31:TYR:CZ	1:B:108:ARG:HD3	2.19	0.77
1:A:39:LEU:C	1:A:40:PHE:HD1	1.94	0.75
1:B:479:ARG:CG	1:B:498:ALA:CB	2.66	0.74
1:B:479:ARG:HG2	1:B:498:ALA:HB1	1.70	0.73
1:B:31:TYR:CZ	1:B:108:ARG:CD	2.73	0.71
1:B:14:MET:HE2	1:B:41:TYR:HE2	1.56	0.71
1:B:443:ALA:HB1	1:B:513:VAL:HG13	1.75	0.68
1:B:93:CYS:SG	1:B:108:ARG:HG2	2.33	0.68
1:B:462:THR:O	1:B:462:THR:OG1	2.05	0.68
1:B:278:GLU:HG2	1:B:282:ASN:HA	1.76	0.66
1:B:31:TYR:OH	1:B:108:ARG:HD2	1.96	0.66
1:B:463:LEU:HD21	1:B:475:ILE:CG2	2.22	0.66
1:B:479:ARG:HG3	1:B:498:ALA:HB2	1.77	0.66
1:A:145:TYR:HB2	1:A:166:MET:HE1	1.78	0.65
1:A:56:THR:OG1	1:A:68:MET:HB3	1.96	0.65
1:B:479:ARG:NH2	1:B:497:ASN:O	2.29	0.64
1:B:730:PHE:HE2	1:B:767:ALA:HB3	1.62	0.64
1:A:60:ALA:HB2	1:A:66:ILE:HG13	1.78	0.64
1:B:479:ARG:CG	1:B:498:ALA:HB2	2.28	0.64
1:A:476:GLN:HG3	1:A:500:ARG:HG2	1.78	0.64
1:A:394:ARG:HH22	2:A:909:GOL:H12	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:MET:HE2	1:A:695:ILE:HG21	1.80	0.63
1:B:463:LEU:CD2	1:B:475:ILE:CG2	2.77	0.63
1:A:656:ARG:HH11	1:A:656:ARG:HG2	1.64	0.63
1:B:612:ILE:HD12	1:B:624:MET:HE3	1.81	0.63
1:A:190:ILE:HG13	1:A:190:ILE:O	1.99	0.62
1:B:463:LEU:CD2	1:B:475:ILE:HG22	2.28	0.62
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.82	0.62
1:B:93:CYS:SG	1:B:108:ARG:CG	2.88	0.62
1:A:190:ILE:HG13	1:A:196:LEU:HD21	1.83	0.61
1:A:394:ARG:HA	1:A:397:MET:HE2	1.82	0.61
1:A:394:ARG:HH12	2:A:909:GOL:H31	1.64	0.61
1:A:316:ARG:HH22	2:A:910:GOL:H12	1.67	0.60
1:A:681:LEU:HD22	1:A:714:ASN:HD22	1.67	0.59
1:B:477:ILE:HG13	1:B:501:TYR:CE2	2.37	0.59
1:B:463:LEU:HG	1:B:477:ILE:HG23	1.84	0.59
1:A:39:LEU:HD12	1:A:40:PHE:H	1.67	0.59
1:B:624:MET:HE1	1:B:726:ALA:H	1.68	0.59
1:A:766:ALA:H	2:A:903:GOL:H2	1.68	0.58
1:A:569:CYS:SG	2:A:902:GOL:H31	2.43	0.58
1:A:584:ARG:HD2	1:A:589:GLU:OE1	2.03	0.58
1:B:477:ILE:O	1:B:498:ALA:HB3	2.03	0.58
1:B:268:ILE:O	1:B:652:ARG:HG3	2.03	0.57
1:A:500:ARG:HH12	2:A:907:GOL:H2	1.68	0.57
1:B:579:ARG:HB2	1:B:646:GLU:HB2	1.86	0.57
1:B:605:PRO:O	1:B:608:ARG:HD3	2.05	0.57
1:A:40:PHE:CD1	1:A:40:PHE:N	2.73	0.57
1:B:14:MET:HE2	1:B:41:TYR:CE2	2.38	0.57
1:A:39:LEU:O	1:A:40:PHE:HD1	1.86	0.56
1:B:477:ILE:HG13	1:B:501:TYR:HE2	1.70	0.56
1:A:281:GLN:HE21	1:A:285:GLY:HA2	1.71	0.56
1:B:379:ARG:CG	1:B:397:MET:CE	2.83	0.56
1:A:151:SER:HB3	1:A:350:ARG:HG2	1.88	0.56
1:A:379:ARG:HH22	2:A:909:GOL:H11	1.71	0.56
1:B:31:TYR:CZ	1:B:108:ARG:HD2	2.41	0.55
1:A:603:LEU:HD13	1:A:722:LEU:HB3	1.88	0.55
1:B:10:HIS:HB3	1:B:14:MET:HB3	1.88	0.55
1:B:463:LEU:HG	1:B:477:ILE:HD13	1.87	0.55
1:B:474:TYR:CD1	1:B:500:ARG:HB2	2.41	0.55
1:A:163:ARG:HD2	1:A:186:GLU:OE1	2.07	0.54
1:A:505:GLU:HB2	5:A:1046:HOH:O	2.06	0.54
1:A:730:PHE:HE2	1:A:767:ALA:HB3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LYS:HG2	1:B:110:VAL:N	2.21	0.54
1:B:375:LEU:HD22	1:B:397:MET:HG2	1.90	0.54
1:A:34:GLY:O	1:A:36:PHE:CD2	2.61	0.54
1:B:477:ILE:HG22	1:B:481:GLN:HE21	1.73	0.54
1:A:603:LEU:HB3	1:A:722:LEU:HD22	1.90	0.53
1:A:193:ARG:HB3	1:A:196:LEU:HD13	1.90	0.53
1:B:692:MET:HE2	1:B:695:ILE:HG21	1.89	0.53
1:A:782:PRO:HA	2:A:906:GOL:H11	1.90	0.53
1:A:27:ILE:HG13	1:A:89:SER:HB2	1.91	0.53
1:B:479:ARG:HG2	1:B:498:ALA:CA	2.38	0.53
1:A:585:HIS:HD2	1:A:587:VAL:H	1.55	0.52
1:B:479:ARG:CG	1:B:498:ALA:HA	2.39	0.52
1:A:45:LYS:O	1:A:49:GLN:HB2	2.10	0.52
1:B:268:ILE:HB	1:B:652:ARG:HD2	1.92	0.52
1:B:157:LEU:HD13	1:B:233:GLY:HA3	1.90	0.52
1:A:628:ALA:HB2	1:A:691:LEU:HD11	1.92	0.52
1:B:736:PRO:HG2	1:B:744:ASN:HD22	1.75	0.51
1:A:186:GLU:C	1:A:188:SER:H	2.19	0.51
1:B:327:THR:HG21	1:B:555:LEU:HD13	1.93	0.51
1:B:562:ALA:HA	1:B:567:TYR:HB2	1.93	0.51
1:A:143:PHE:O	1:A:232:ARG:HD2	2.11	0.51
1:B:495:LEU:C	1:B:495:LEU:HD13	2.36	0.51
1:B:609:MET:HG3	1:B:723:THR:HB	1.92	0.51
1:B:628:ALA:HB2	1:B:691:LEU:HD11	1.91	0.51
1:B:137:TRP:HZ3	1:B:232:ARG:HG2	1.76	0.50
1:B:31:TYR:CE1	1:B:108:ARG:HD3	2.46	0.50
1:B:379:ARG:HG3	1:B:397:MET:HE3	1.90	0.50
1:B:623:TYR:O	1:B:626:GLN:HG2	2.12	0.50
1:B:477:ILE:CG1	1:B:501:TYR:HE2	2.24	0.50
1:B:727:THR:HG21	1:B:732:LEU:HD12	1.92	0.50
1:A:26:GLU:HG2	1:A:27:ILE:HD12	1.93	0.50
1:A:205:GLU:HB3	1:A:208:THR:HG22	1.94	0.50
1:B:500:ARG:HG3	1:B:500:ARG:O	2.11	0.50
1:A:420:ARG:O	1:A:521:LEU:HD21	2.12	0.50
1:A:579:ARG:HB2	1:A:646:GLU:HB2	1.92	0.50
1:B:14:MET:HE1	1:B:40:PHE:CD2	2.47	0.50
1:A:316:ARG:HH22	2:A:910:GOL:C1	2.25	0.49
1:A:387:SER:OG	1:A:389:PRO:HD2	2.12	0.49
1:A:746:HIS:HD2	1:A:765:GLY:O	1.95	0.49
1:B:179:LEU:HD12	1:B:197:ARG:HB2	1.92	0.49
1:B:328:ILE:HG23	1:B:559:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:HD11	1:B:93:CYS:HB2	1.95	0.49
1:A:418:LEU:HD23	1:A:419:VAL:H	1.78	0.49
1:B:498:ALA:O	1:B:499:GLU:HG3	2.12	0.49
1:A:585:HIS:CD2	1:A:588:VAL:H	2.30	0.49
1:A:585:HIS:CD2	1:A:588:VAL:HG23	2.47	0.49
1:B:178:LEU:HB3	1:B:196:LEU:HD23	1.94	0.48
1:A:453:ARG:HD2	5:A:1007:HOH:O	2.12	0.48
1:B:342:LEU:HD11	1:B:552:LEU:HD23	1.95	0.48
1:B:492:ARG:HD3	1:B:502:ILE:HG12	1.96	0.48
1:B:436:TRP:HB3	1:B:520:ALA:HB2	1.95	0.48
1:A:362:PRO:HD2	1:A:417:VAL:O	2.13	0.48
1:B:51:LEU:HD11	1:B:83:LEU:HD21	1.95	0.48
1:B:477:ILE:CD1	1:B:501:TYR:HE2	2.26	0.48
1:B:616:ASN:HB2	1:B:775:VAL:HG21	1.95	0.48
1:A:245:LYS:HG3	1:A:252:LEU:HD12	1.96	0.48
1:A:468:ASN:ND2	1:A:471:HIS:H	2.12	0.48
1:A:567:TYR:CE2	1:A:633:MET:HE1	2.49	0.48
1:B:630:ILE:HG12	1:B:641:PRO:HD2	1.96	0.48
1:A:31:TYR:CD1	1:A:40:PHE:HZ	2.32	0.47
1:A:46:ARG:O	1:A:49:GLN:N	2.46	0.47
1:A:396:LYS:HD3	1:A:548:ALA:HB2	1.97	0.47
1:B:155:PHE:CD2	1:B:258:ILE:HG12	2.50	0.47
1:B:227:VAL:HG21	1:B:258:ILE:CG2	2.44	0.47
1:B:479:ARG:HG2	1:B:498:ALA:HA	1.97	0.47
1:A:293:SER:HA	2:A:901:GOL:H2	1.97	0.47
1:A:138:GLN:HB2	1:A:184:PHE:CE1	2.50	0.47
1:A:624:MET:HE1	1:A:693:ASP:HB2	1.95	0.47
1:B:375:LEU:O	1:B:379:ARG:HG3	2.14	0.47
1:B:468:ASN:HB3	1:B:471:HIS:HB2	1.96	0.46
1:A:41:TYR:CG	1:A:41:TYR:O	2.69	0.46
1:A:694:GLU:OE1	1:B:698:GLY:HA2	2.15	0.46
1:B:379:ARG:CG	1:B:397:MET:HE2	2.44	0.46
1:B:264:GLN:H	1:B:264:GLN:HE21	1.63	0.46
1:B:160:PRO:HB3	1:B:165:THR:HG22	1.97	0.46
1:A:41:TYR:O	1:A:41:TYR:CD2	2.69	0.46
1:A:730:PHE:CE2	1:A:767:ALA:HB3	2.50	0.46
1:A:194:ARG:H	1:A:194:ARG:HD3	1.82	0.45
1:A:585:HIS:O	1:A:589:GLU:HG2	2.16	0.45
1:B:624:MET:HE2	1:B:724:LEU:C	2.41	0.45
1:A:632:LEU:HD23	1:A:632:LEU:C	2.41	0.45
1:B:463:LEU:HD22	1:B:475:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:HIS:HB3	1:B:588:VAL:HB	1.98	0.45
1:B:609:MET:HB3	1:B:742:VAL:HG22	1.99	0.45
1:A:322:LEU:O	1:A:326:GLN:HG3	2.16	0.45
1:A:60:ALA:CB	1:A:66:ILE:CG1	2.95	0.45
1:A:551:GLU:OE2	2:A:905:GOL:H32	2.17	0.45
1:B:493:GLN:CB	1:B:499:GLU:HG2	2.47	0.45
1:B:392:ALA:HB2	2:B:902:GOL:H31	1.99	0.45
1:B:477:ILE:HD11	1:B:501:TYR:HE2	1.82	0.45
1:B:657:VAL:HA	1:B:693:ASP:HB3	1.98	0.45
1:B:344:GLN:HB2	1:B:374:GLN:HG3	1.99	0.44
1:B:21:LYS:HE2	1:B:43:ASP:OD1	2.17	0.44
1:A:650:ILE:HA	1:A:687:TYR:O	2.18	0.44
1:B:430:ASN:HD22	1:B:433:LEU:HB2	1.82	0.44
1:B:447:LEU:HD23	1:B:450:LEU:HD13	1.99	0.44
1:A:119:ILE:HG21	1:A:124:LEU:HB2	2.00	0.44
1:B:479:ARG:CG	1:B:498:ALA:CA	2.95	0.44
1:B:479:ARG:HG3	1:B:498:ALA:CB	2.41	0.44
1:B:362:PRO:HB3	1:B:424:VAL:HG21	2.00	0.44
1:B:567:TYR:HB3	1:B:639:TYR:HB3	1.99	0.44
1:B:585:HIS:O	1:B:589:GLU:HG2	2.18	0.43
1:A:18:LEU:HD12	1:A:21:LYS:HB3	2.01	0.43
1:A:613:THR:HG23	1:A:767:ALA:H	1.83	0.43
1:A:47:ALA:O	1:A:51:LEU:HB2	2.18	0.43
1:B:450:LEU:HD11	1:B:506:LEU:HD13	1.99	0.43
1:A:715:LEU:HA	1:A:719:ILE:HB	1.99	0.43
1:A:24:HIS:HB2	1:A:27:ILE:HD13	2.01	0.43
1:A:148:LEU:HD11	1:A:255:ILE:HG12	2.00	0.43
1:B:156:ARG:HD3	1:B:259:THR:HB	2.01	0.43
1:B:206:ILE:H	1:B:206:ILE:HG13	1.49	0.43
1:A:33:MET:HE2	1:A:58:ARG:NH1	2.34	0.42
1:A:706:SER:HB3	1:B:789:ALA:O	2.19	0.42
1:B:493:GLN:HB3	1:B:499:GLU:HG2	2.01	0.42
1:A:89:SER:HB3	1:A:115:THR:HG22	2.01	0.42
1:B:393:LEU:HD13	1:B:552:LEU:HD12	2.01	0.42
1:A:186:GLU:C	1:A:188:SER:N	2.77	0.42
1:B:686:GLU:H	1:B:686:GLU:HG3	1.59	0.42
1:A:472:GLY:HA2	1:B:484:LEU:HD11	2.02	0.42
1:B:379:ARG:HG2	1:B:397:MET:HE2	2.01	0.42
1:A:84:VAL:HG21	1:A:114:VAL:HG12	2.01	0.42
1:A:580:ILE:HG12	1:A:645:VAL:HG22	2.00	0.42
1:A:624:MET:HB3	1:A:691:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:LEU:HD21	1:B:549:LEU:HD11	2.01	0.42
1:B:613:THR:O	1:B:746:HIS:HA	2.19	0.42
1:B:436:TRP:HA	1:B:436:TRP:CE3	2.55	0.42
1:B:450:LEU:HD21	1:B:506:LEU:HD13	2.02	0.42
1:B:479:ARG:HD3	1:B:498:ALA:HA	2.02	0.42
1:A:655:THR:HG22	1:A:691:LEU:HD12	2.02	0.41
1:A:60:ALA:CB	1:A:66:ILE:HG13	2.49	0.41
1:B:184:PHE:CE2	1:B:190:ILE:HD12	2.56	0.41
1:A:163:ARG:CD	1:A:186:GLU:OE1	2.68	0.41
1:A:157:LEU:HD13	1:A:233:GLY:HA3	2.01	0.41
1:B:119:ILE:HG21	1:B:124:LEU:HB3	2.02	0.41
1:B:225:PHE:HB3	1:B:258:ILE:O	2.20	0.41
1:B:460:LEU:HD22	1:B:477:ILE:HG21	2.01	0.41
1:A:623:TYR:CE1	1:A:762:VAL:HG21	2.55	0.41
1:A:163:ARG:HG3	1:A:186:GLU:OE1	2.21	0.41
1:A:579:ARG:O	1:A:645:VAL:HA	2.21	0.41
1:B:27:ILE:CG2	1:B:89:SER:HB2	2.50	0.41
1:A:157:LEU:O	1:A:260:MET:HA	2.20	0.41
1:A:46:ARG:HA	1:A:49:GLN:HB3	2.03	0.40
1:A:75:ALA:HB2	1:B:74:HIS:HD2	1.86	0.40
1:A:397:MET:HA	1:A:545:SER:HA	2.02	0.40
1:A:159:GLU:HG2	1:A:232:ARG:HB2	2.02	0.40
1:A:230:ALA:O	1:A:234:LEU:HG	2.21	0.40
1:B:608:ARG:HH12	1:B:740:GLU:CD	2.29	0.40
1:B:715:LEU:HA	1:B:719:ILE:HB	2.03	0.40
1:B:733:THR:HA	1:B:744:ASN:HD21	1.86	0.40
1:A:46:ARG:O	1:A:47:ALA:C	2.63	0.40
1:A:323:GLU:HB2	2:A:905:GOL:H11	2.03	0.40
1:A:486:PRO:HB2	1:A:488:ASN:OD1	2.22	0.40
1:A:609:MET:HA	1:A:723:THR:O	2.22	0.40
1:B:171:GLN:HE21	1:B:275:ARG:NH2	2.20	0.40
1:A:323:GLU:CB	2:A:905:GOL:H11	2.51	0.40
1:B:80:LEU:HD21	1:B:92:ILE:HD11	2.03	0.40
1:B:582:GLU:HB2	1:B:643:GLN:HB2	2.03	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	752/853 (88%)	715 (95%)	37 (5%)	0	100	100
1	B	772/853 (90%)	736 (95%)	36 (5%)	0	100	100
All	All	1524/1706 (89%)	1451 (95%)	73 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	635/710 (89%)	584 (92%)	51 (8%)	11	25
1	B	649/710 (91%)	590 (91%)	59 (9%)	9	19
All	All	1284/1420 (90%)	1174 (91%)	110 (9%)	10	22

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	TYR
1	A	18	LEU
1	A	21	LYS
1	A	26	GLU
1	A	29	LEU
1	A	33	MET
1	A	39	LEU
1	A	40	PHE

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Mol	Chain	Res	Type
1	A	50	LEU
1	A	57	LYS
1	A	64	GLU
1	A	66	ILE
1	A	68	MET
1	A	71	ILE
1	A	84	VAL
1	A	86	GLN
1	A	89	SER
1	A	119	ILE
1	A	150	ILE
1	A	164	GLU
1	A	182	GLU
1	A	187	MET
1	A	190	ILE
1	A	194	ARG
1	A	196	LEU
1	A	206	ILE
1	A	254	HIS
1	A	259	THR
1	A	260	MET
1	A	395	GLU
1	A	418	LEU
1	A	431	GLU
1	A	464	LYS
1	A	468	ASN
1	A	479	ARG
1	A	517	LYS
1	A	521	LEU
1	A	524	GLU
1	A	621	SER
1	A	636	ILE
1	A	656	ARG
1	A	668	SER
1	A	669	THR
1	A	675	THR
1	A	695	ILE
1	A	707	LEU
1	A	718	LYS
1	A	738	LYS
1	A	748	ASP
1	A	755	THR

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Mol	Chain	Res	Type
1	A	773	LEU
1	B	13	MET
1	B	20	LEU
1	B	24	HIS
1	B	26	GLU
1	B	56	THR
1	B	109	LYS
1	B	131	ASN
1	B	150	ILE
1	B	151	SER
1	B	154[A]	ARG
1	B	154[B]	ARG
1	B	163	ARG
1	B	183	ASP
1	B	190	ILE
1	B	201	LEU
1	B	206	ILE
1	B	229	ASN
1	B	239	CYS
1	B	257	SER
1	B	258	ILE
1	B	264	GLN
1	B	357	LEU
1	B	412	ILE
1	B	419	VAL
1	B	424	VAL
1	B	431	GLU
1	B	436	TRP
1	B	445	ASP
1	B	449	ARG
1	B	451	GLU
1	B	456	GLU
1	B	458	THR
1	B	460	LEU
1	B	462	THR
1	B	463	LEU
1	B	464	LYS
1	B	477	ILE
1	B	484	LEU
1	B	491	ARG
1	B	492	ARG
1	B	494	THR

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Mol	Chain	Res	Type
1	B	501	TYR
1	B	502	ILE
1	B	506	LEU
1	B	521	LEU
1	B	524	GLU
1	B	552	LEU
1	B	584	ARG
1	B	607	ARG
1	B	613	THR
1	B	617	MET
1	B	636	ILE
1	B	656	ARG
1	B	686	GLU
1	B	695	ILE
1	B	703	ASP
1	B	717	ASN
1	B	756	ILE
1	B	778	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	242	GLN
1	A	281	GLN
1	A	289	ASN
1	A	326	GLN
1	A	374	GLN
1	A	471	HIS
1	A	483	HIS
1	A	557	ASN
1	A	585	HIS
1	A	606	GLN
1	A	714	ASN
1	A	744	ASN
1	B	15	GLN
1	B	24	HIS
1	B	78	ASN
1	B	85	ASN
1	B	86	GLN
1	B	216	GLN
1	B	264	GLN

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Mol	Chain	Res	Type
1	B	276	ASN
1	B	282	ASN
1	B	289	ASN
1	B	370	HIS
1	B	430	ASN
1	B	476	GLN
1	B	481	GLN
1	B	566	ASN
1	B	683	ASN
1	B	744	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 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	GOL	B	903	-	5,5,5	0.13	0	5,5,5	0.11	0
3	SO4	A	915	-	4,4,4	0.28	0	6,6,6	0.09	0
2	GOL	B	901	-	5,5,5	0.08	0	5,5,5	0.13	0
4	ADP	B	908	-	28,29,29	0.52	0	43,45,45	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	910	-	5,5,5	0.15	0	5,5,5	0.56	0
2	GOL	A	904	-	5,5,5	0.09	0	5,5,5	0.28	0
2	GOL	A	901	-	5,5,5	0.10	0	5,5,5	0.28	0
2	GOL	A	906	-	5,5,5	0.09	0	5,5,5	0.25	0
3	SO4	A	911	-	4,4,4	0.32	0	6,6,6	0.16	0
2	GOL	A	905	-	5,5,5	0.13	0	5,5,5	0.48	0
3	SO4	A	913	-	4,4,4	0.23	0	6,6,6	0.10	0
2	GOL	B	902	-	5,5,5	0.17	0	5,5,5	0.33	0
2	GOL	A	908	-	5,5,5	0.10	0	5,5,5	0.19	0
3	SO4	B	904	-	4,4,4	0.15	0	6,6,6	0.47	0
3	SO4	B	907	-	4,4,4	0.23	0	6,6,6	0.17	0
3	SO4	B	906	-	4,4,4	0.25	0	6,6,6	0.15	0
2	GOL	A	902	-	5,5,5	0.21	0	5,5,5	0.41	0
3	SO4	B	905	-	4,4,4	0.19	0	6,6,6	0.32	0
3	SO4	A	912	-	4,4,4	0.28	0	6,6,6	0.27	0
2	GOL	A	907	-	5,5,5	0.14	0	5,5,5	0.24	0
2	GOL	A	903	-	5,5,5	0.11	0	5,5,5	0.24	0
3	SO4	A	914	-	4,4,4	0.31	0	6,6,6	0.17	0
2	GOL	A	909	-	5,5,5	0.11	0	5,5,5	0.33	0
4	ADP	A	916	-	28,29,29	0.46	0	43,45,45	0.83	1 (2%)

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
2	GOL	B	902	-	-	0/4/4/4	-
2	GOL	A	908	-	-	0/4/4/4	-
2	GOL	A	904	-	-	2/4/4/4	-
2	GOL	A	903	-	-	0/4/4/4	-
2	GOL	A	901	-	-	0/4/4/4	-
2	GOL	A	907	-	-	2/4/4/4	-
2	GOL	B	903	-	-	0/4/4/4	-
2	GOL	A	906	-	-	2/4/4/4	-
2	GOL	B	901	-	-	2/4/4/4	-
2	GOL	A	909	-	-	0/4/4/4	-
2	GOL	A	902	-	-	0/4/4/4	-
4	ADP	B	908	-	-	2/16/32/32	0/3/3/3
2	GOL	A	910	-	-	0/4/4/4	-
2	GOL	A	905	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	916	-	-	2/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	916	ADP	O2B-PB-O3A	3.15	115.19	104.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

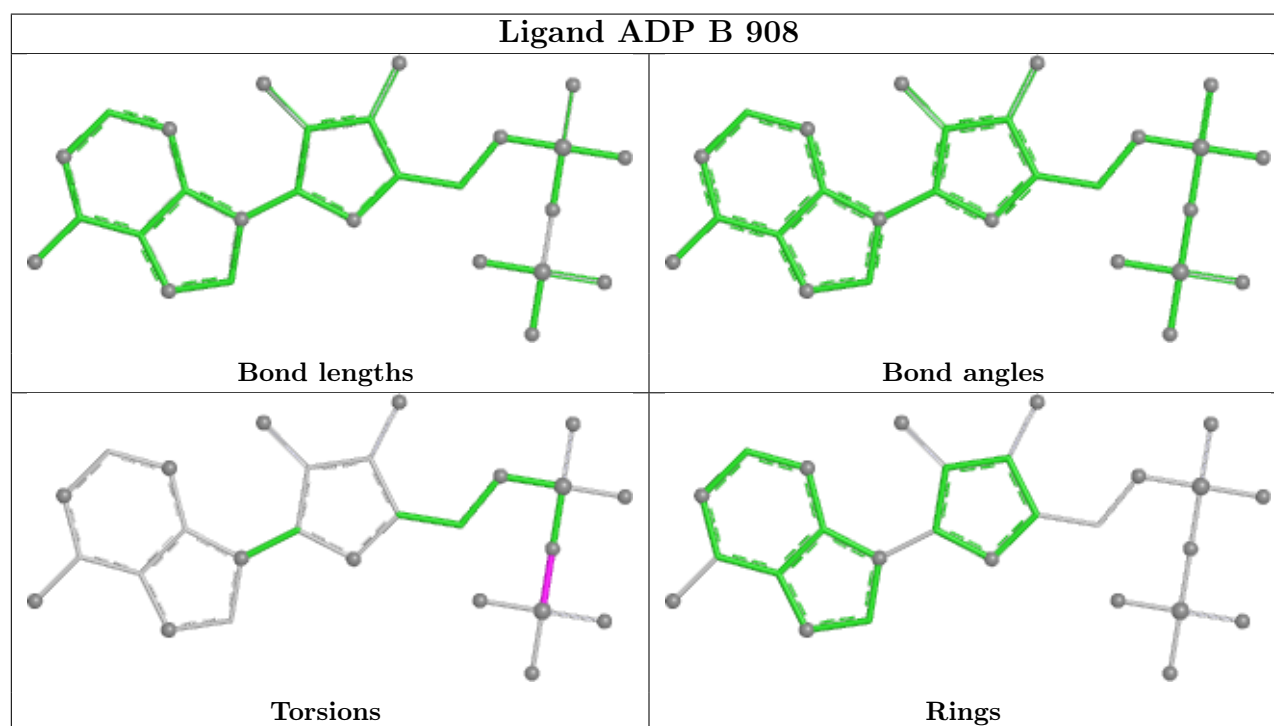
Mol	Chain	Res	Type	Atoms
4	B	908	ADP	PA-O3A-PB-O3B
2	A	904	GOL	O1-C1-C2-C3
2	A	905	GOL	O1-C1-C2-C3
2	A	906	GOL	C1-C2-C3-O3
2	A	907	GOL	C1-C2-C3-O3
2	B	901	GOL	C1-C2-C3-O3
2	A	904	GOL	O1-C1-C2-O2
2	A	905	GOL	O1-C1-C2-O2
2	A	906	GOL	O2-C2-C3-O3
4	A	916	ADP	PB-O3A-PA-O2A
2	A	907	GOL	O2-C2-C3-O3
2	B	901	GOL	O2-C2-C3-O3
4	B	908	ADP	PA-O3A-PB-O1B
4	A	916	ADP	O4'-C4'-C5'-O5'

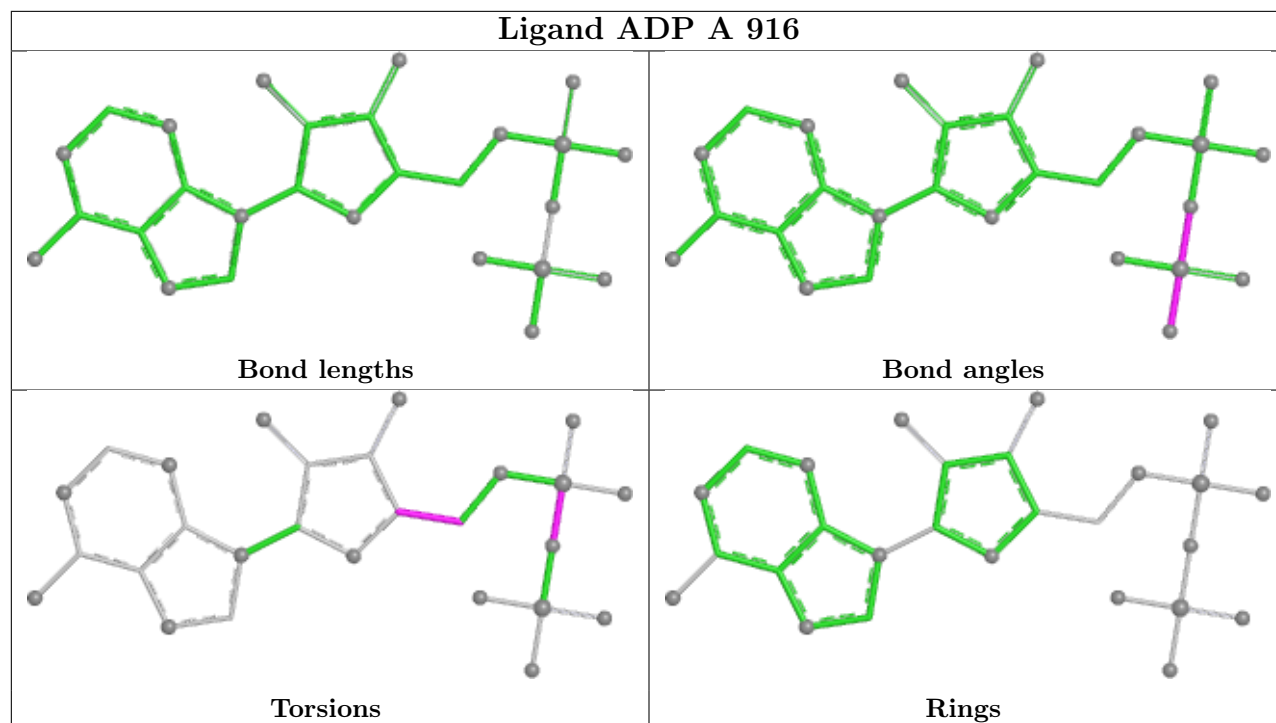
There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	910	GOL	2	0
2	A	901	GOL	1	0
2	A	906	GOL	1	0
2	A	905	GOL	3	0
2	B	902	GOL	1	0
2	A	902	GOL	1	0
2	A	907	GOL	1	0
2	A	903	GOL	1	0
2	A	909	GOL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	760/853 (89%)	0.58	119 (15%) 5 4	12, 45, 135, 158	0
1	B	777/853 (91%)	0.85	133 (17%) 4 3	14, 56, 130, 169	0
All	All	1537/1706 (90%)	0.72	252 (16%) 4 3	12, 51, 132, 169	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	480	GLY	6.8
1	B	473	TYR	6.2
1	B	484	LEU	6.0
1	B	495	LEU	5.7
1	A	66	ILE	5.6
1	A	29	LEU	5.5
1	A	67	PRO	5.5
1	A	50	LEU	5.2
1	A	79	TYR	5.1
1	B	465	VAL	5.0
1	A	14	MET	4.9
1	A	20	LEU	4.8
1	A	161	ALA	4.8
1	B	463	LEU	4.8
1	A	63	GLY	4.8
1	B	439	LEU	4.6
1	B	446	TYR	4.5
1	B	458	THR	4.5
1	B	106	VAL	4.5
1	A	65	PRO	4.4
1	B	521	LEU	4.4
1	A	31	TYR	4.4
1	A	18	LEU	4.3
1	B	192	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	73	TYR	4.3
1	B	483	HIS	4.2
1	B	799	ILE	4.2
1	A	17	TYR	4.1
1	A	12	PRO	4.1
1	B	105	PRO	4.0
1	B	464	LYS	4.0
1	A	71	ILE	4.0
1	B	517	LYS	4.0
1	A	41	TYR	4.0
1	A	36	PHE	4.0
1	B	452	VAL	4.0
1	A	93	CYS	4.0
1	B	201	LEU	4.0
1	A	47	ALA	4.0
1	B	658	GLY	4.0
1	A	34	GLY	3.9
1	B	461	ASP	3.9
1	A	202	TRP	3.9
1	B	460	LEU	3.9
1	A	53	ILE	3.8
1	A	80	LEU	3.8
1	B	485	ALA	3.8
1	B	487	ILE	3.7
1	B	478	SER	3.7
1	B	440	ALA	3.7
1	A	43	ASP	3.7
1	A	62	ALA	3.7
1	A	111	VAL	3.7
1	A	799	ILE	3.6
1	B	426	ALA	3.6
1	A	28	LEU	3.6
1	A	75	ALA	3.6
1	A	185	ALA	3.6
1	A	30	PHE	3.6
1	B	471	HIS	3.6
1	A	56	THR	3.6
1	B	424	VAL	3.6
1	B	438	ALA	3.4
1	A	27	ILE	3.4
1	B	489	TYR	3.4
1	B	511	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	15	GLN	3.4
1	B	514	LEU	3.4
1	B	479	ARG	3.4
1	A	13	MET	3.4
1	B	209	ALA	3.4
1	B	475	ILE	3.4
1	B	202	TRP	3.4
1	B	509	TYR	3.4
1	A	110	VAL	3.4
1	B	436	TRP	3.3
1	A	33	MET	3.3
1	B	447	LEU	3.3
1	B	519	LYS	3.3
1	A	55	LEU	3.3
1	B	756	ILE	3.3
1	B	443	ALA	3.3
1	A	54	SER	3.2
1	B	477	ILE	3.2
1	A	78	ASN	3.2
1	B	457	ARG	3.2
1	B	500	ARG	3.2
1	A	755	THR	3.2
1	A	92	ILE	3.2
1	A	72	PRO	3.2
1	A	69	ALA	3.1
1	A	184	PHE	3.1
1	A	208	THR	3.1
1	A	70	GLY	3.1
1	B	455	ARG	3.1
1	B	50	LEU	3.0
1	B	474	TYR	3.0
1	B	412	ILE	3.0
1	A	418	LEU	3.0
1	B	501	TYR	3.0
1	B	450	LEU	2.9
1	B	504	PRO	2.9
1	A	142	GLY	2.9
1	B	423	GLY	2.9
1	B	482	SER	2.9
1	B	755	THR	2.9
1	B	141	LYS	2.9
1	A	76	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	45	LYS	2.9
1	B	466	GLY	2.9
1	A	139	ASP	2.8
1	B	486	PRO	2.8
1	A	215	LEU	2.8
1	A	223	VAL	2.8
1	A	438	ALA	2.8
1	B	410	ALA	2.8
1	A	51	LEU	2.8
1	B	104	GLY	2.8
1	B	459	GLY	2.8
1	B	444	THR	2.8
1	A	197	ARG	2.8
1	B	437	ARG	2.8
1	B	672	VAL	2.7
1	B	37	TYR	2.7
1	B	425	ILE	2.7
1	B	497	ASN	2.7
1	B	798	SER	2.7
1	B	499	GLU	2.7
1	A	40	PHE	2.7
1	B	419	VAL	2.7
1	B	516	SER	2.7
1	B	754	ASP	2.7
1	B	503	ILE	2.7
1	B	430	ASN	2.7
1	B	184	PHE	2.7
1	B	86	GLN	2.6
1	B	418	LEU	2.6
1	A	59	GLY	2.6
1	A	64	GLU	2.6
1	A	44	ALA	2.6
1	A	60	ALA	2.6
1	B	417	VAL	2.6
1	B	462	THR	2.6
1	B	467	PHE	2.6
1	B	429	TYR	2.6
1	A	140	SER	2.6
1	B	470	VAL	2.6
1	A	180	TYR	2.6
1	B	449	ARG	2.6
1	B	453	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	753	GLY	2.6
1	B	469	ALA	2.6
1	B	750	LEU	2.6
1	A	85	ASN	2.6
1	A	189	LEU	2.5
1	A	24	HIS	2.5
1	B	107	GLU	2.5
1	B	498	ALA	2.5
1	A	198	ARG	2.5
1	B	163	ARG	2.5
1	B	451	GLU	2.5
1	A	444	THR	2.5
1	B	515	THR	2.5
1	A	196	LEU	2.5
1	A	420	ARG	2.5
1	A	74	HIS	2.5
1	A	39	LEU	2.4
1	A	222	LEU	2.4
1	B	506	LEU	2.4
1	A	16	GLN	2.4
1	A	168	ALA	2.4
1	B	749	ALA	2.4
1	B	117	GLY	2.4
1	A	82	LYS	2.4
1	A	206	ILE	2.4
1	A	61	SER	2.4
1	A	52	ASP	2.4
1	B	522	ALA	2.4
1	A	750	LEU	2.4
1	B	196	LEU	2.4
1	B	502	ILE	2.4
1	A	516	SER	2.4
1	A	668	SER	2.4
1	B	416	PRO	2.4
1	A	19	ARG	2.4
1	A	22	ALA	2.4
1	A	471	HIS	2.3
1	B	212	GLN	2.3
1	A	522	ALA	2.3
1	B	520	ALA	2.3
1	A	37	TYR	2.3
1	A	165	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	68	MET	2.3
1	A	112	ARG	2.3
1	A	138	GLN	2.3
1	B	87	GLY	2.3
1	B	496	LYS	2.3
1	B	518	GLY	2.3
1	B	513	VAL	2.3
1	A	38	GLU	2.3
1	A	58	ARG	2.3
1	A	496	LYS	2.2
1	A	497	ASN	2.2
1	A	220	ARG	2.2
1	A	35	ASP	2.2
1	B	434	ASP	2.2
1	B	44	ALA	2.2
1	B	454	GLU	2.2
1	B	524	GLU	2.2
1	B	488	ASN	2.2
1	A	49	GLN	2.2
1	A	467	PHE	2.2
1	B	490	MET	2.2
1	A	164	GLU	2.2
1	B	194	ARG	2.2
1	A	57	LYS	2.2
1	A	518	GLY	2.2
1	A	515	THR	2.2
1	A	32	ARG	2.2
1	A	514	LEU	2.2
1	B	187	MET	2.2
1	A	90	VAL	2.2
1	B	140	SER	2.2
1	B	435	GLU	2.1
1	B	448	GLU	2.1
1	A	46	ARG	2.1
1	B	12	PRO	2.1
1	A	86	GLN	2.1
1	B	593	ASN	2.1
1	B	139	ASP	2.1
1	A	250	THR	2.1
1	B	494	THR	2.1
1	A	25	PRO	2.1
1	A	204	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	517	LYS	2.1
1	A	201	LEU	2.1
1	B	527	LEU	2.1
1	A	756	ILE	2.1
1	B	203	GLU	2.0
1	B	220	ARG	2.0
1	A	109	LYS	2.0
1	B	669	THR	2.0
1	A	187	MET	2.0
1	B	415	PRO	2.0
1	B	283	LEU	2.0
1	A	190	ILE	2.0
1	B	84	VAL	2.0
1	B	532	PHE	2.0
1	A	42	ASP	2.0
1	B	52	ASP	2.0
1	B	181	ALA	2.0
1	B	46	ARG	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(Å ²)	Q<0.9
2	GOL	A	910	6/6	0.73	0.18	50,52,53,54	0
2	GOL	A	906	6/6	0.78	0.15	55,56,57,59	0
2	GOL	B	903	6/6	0.78	0.15	61,63,63,64	0
2	GOL	A	907	6/6	0.81	0.12	41,43,46,47	0
3	SO4	B	905	5/5	0.81	0.24	78,81,82,85	0

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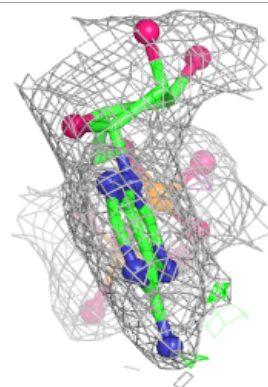
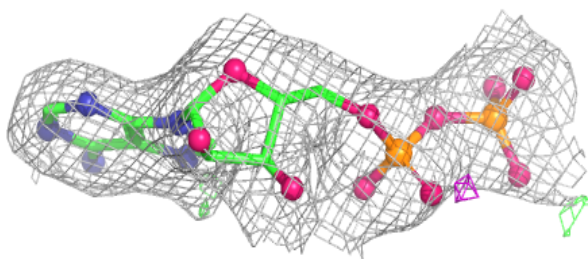
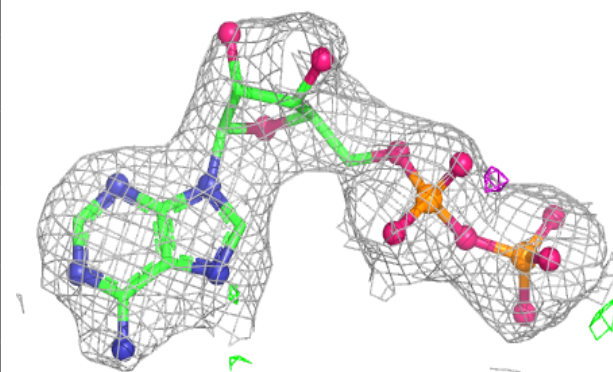
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	906	5/5	0.82	0.13	108,108,108,109	0
3	SO4	A	913	5/5	0.84	0.12	98,98,98,99	0
3	SO4	A	914	5/5	0.84	0.16	114,114,115,115	0
2	GOL	A	903	6/6	0.86	0.15	49,52,55,56	0
2	GOL	A	908	6/6	0.86	0.13	64,67,67,68	0
2	GOL	B	902	6/6	0.87	0.23	46,55,56,57	0
2	GOL	A	901	6/6	0.87	0.19	49,53,55,55	0
2	GOL	A	904	6/6	0.88	0.15	51,53,57,59	0
3	SO4	A	911	5/5	0.88	0.18	89,89,90,92	0
2	GOL	A	902	6/6	0.88	0.14	34,35,37,38	0
2	GOL	A	909	6/6	0.90	0.09	41,42,44,45	0
2	GOL	B	901	6/6	0.91	0.11	31,34,36,36	0
3	SO4	A	915	5/5	0.92	0.14	106,106,107,107	0
2	GOL	A	905	6/6	0.93	0.10	27,33,37,38	0
3	SO4	B	907	5/5	0.93	0.12	91,93,94,94	0
4	ADP	A	916	27/27	0.93	0.10	49,57,64,68	0
4	ADP	B	908	27/27	0.95	0.08	48,51,53,54	0
3	SO4	B	904	5/5	0.97	0.07	37,37,38,41	0
3	SO4	A	912	5/5	0.98	0.10	34,36,37,40	0

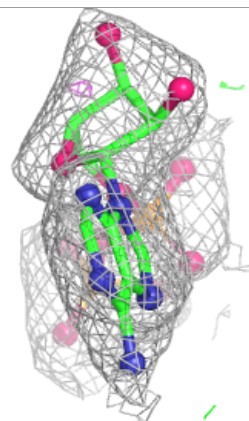
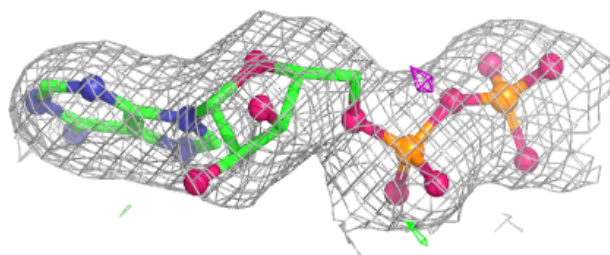
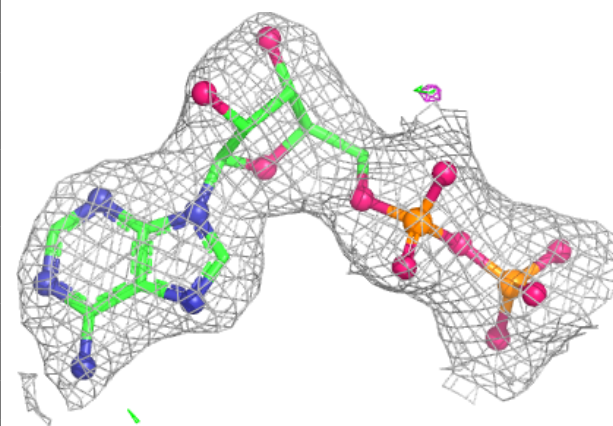
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 916:

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

**Electron density around ADP B 908:**

$2mF_o - DF_c$ (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.