



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:02 PM UTC

PDB ID : 6JT7 / pdb_00006jt7
Title : Crystal structure of 452-453_deletion mutant of FGAM Synthetase
Authors : Sharma, N.; Ahalawat, N.; Sandhu, P.; Mondal, J.; Anand, R.
Deposited on : 2019-04-10
Resolution : 1.86 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

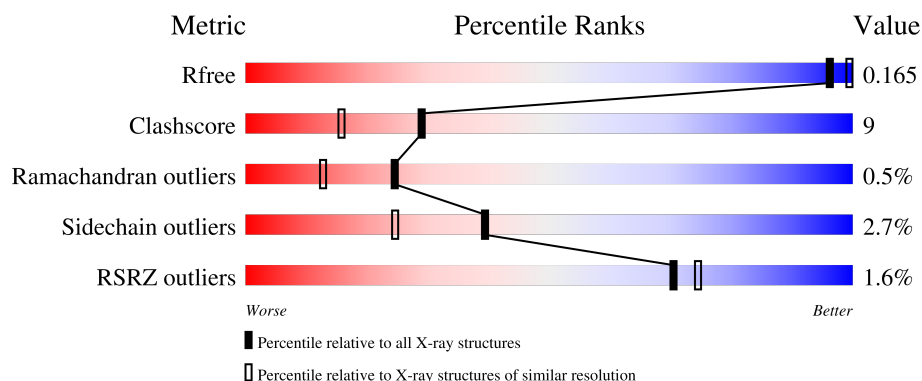
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

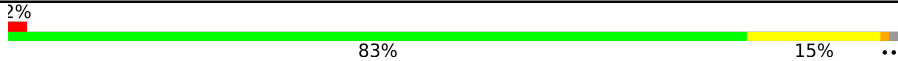
The reported resolution of this entry is 1.86 Å.

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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	1301	

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
2	EDO	A	1503	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	1506	-	-	X	-
2	EDO	A	1518	-	-	X	-
2	EDO	A	1530	-	-	X	-
2	EDO	A	1594	-	-	X	-
5	SO4	A	1539	-	X	-	-
7	GOL	A	1559	-	X	X	-
7	GOL	A	1562	-	-	X	-
7	GOL	A	1579	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11716 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 Phosphoribosylformylglycinamide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1282	Total	C	N	O	S	0	53	0
			10153	6399	1793	1909	52			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A0A0D6F9Y3
A	-6	LEU	-	expression tag	UNP A0A0D6F9Y3
A	-5	VAL	-	expression tag	UNP A0A0D6F9Y3
A	-4	PRO	-	expression tag	UNP A0A0D6F9Y3
A	-3	ARG	-	expression tag	UNP A0A0D6F9Y3
A	-2	GLY	-	expression tag	UNP A0A0D6F9Y3
A	-1	SER	-	expression tag	UNP A0A0D6F9Y3
A	0	HIS	-	expression tag	UNP A0A0D6F9Y3
A	?	-	ALA	deletion	UNP A0A0D6F9Y3
A	?	-	ALA	deletion	UNP A0A0D6F9Y3

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	1
			8	4	4		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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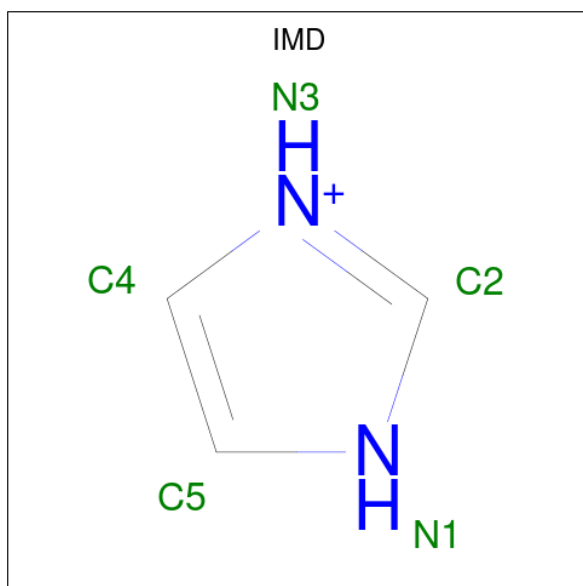
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	1
			8	4	4		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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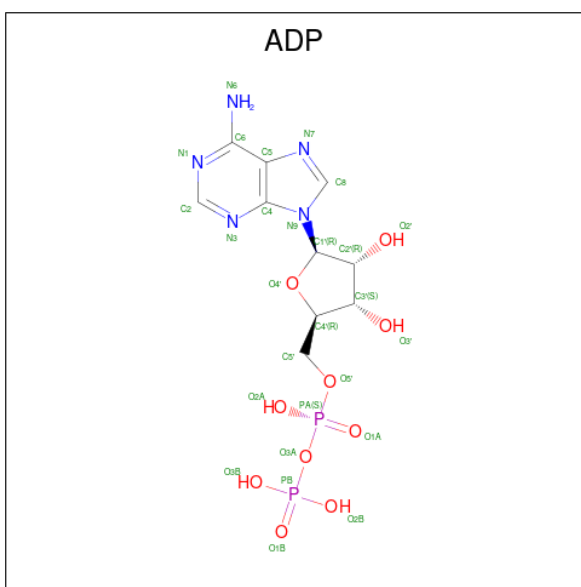
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



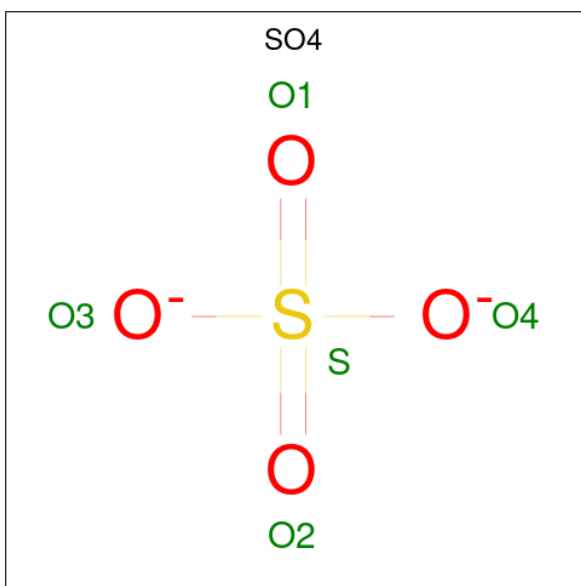
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		

- 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	0	0
			27	10	5	10	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Mg 3 3	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Cl 2 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1083	Total O 1083 1083	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: Phosphoribosylformylglycinamide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	146.27Å 146.27Å 140.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.88 – 1.86 47.88 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.88-1.86) 100.0 (47.88-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.123 , 0.156 0.137 , 0.165	Depositor DCC
R_{free} test set	7237 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11716	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: ADP, IMD, MG, SO4, CL, EDO, CYG, 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	1.40	35/10495 (0.3%)	1.16	18/14242 (0.1%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	TYR	N-CA	7.46	1.55	1.46
1	A	432	VAL	CA-CB	7.07	1.61	1.54
1	A	318	ASP	C-O	-7.04	1.16	1.24
1	A	1023	PHE	CA-C	-6.63	1.44	1.52
1	A	6	ARG	C-O	-6.54	1.15	1.23
1	A	48	ASN	N-CA	6.41	1.54	1.45
1	A	512	MET	N-CA	-6.38	1.41	1.46
1	A	392	TYR	C-O	-6.34	1.16	1.24
1	A	915	ASP	CA-C	6.27	1.60	1.52
1	A	971	GLN	CA-C	6.25	1.60	1.52
1	A	639	ARG	C-O	-6.21	1.17	1.24
1	A	635	ASP	C-O	-6.15	1.16	1.24
1	A	572	ALA	CA-C	6.14	1.59	1.52
1	A	1048	GLN	CA-CB	-5.97	1.44	1.53
1	A	993	GLN	CD-OE1	5.90	1.34	1.23
1	A	966	ILE	CA-C	5.78	1.60	1.52
1	A	847	TYR	N-CA	5.57	1.52	1.46
1	A	674	GLN	CD-OE1	5.57	1.34	1.23
1	A	776	LYS	C-O	5.55	1.30	1.23
1	A	113	TYR	N-CA	5.54	1.53	1.46
1	A	200	ASN	CA-C	5.50	1.59	1.53
1	A	1104	GLU	C-O	-5.47	1.17	1.24
1	A	480	ARG	C-O	-5.43	1.17	1.24
1	A	1091	CYS	CA-CB	5.39	1.62	1.53
1	A	223	ASN	CA-C	5.37	1.60	1.52
1	A	50	SER	CA-C	5.36	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1148	ILE	N-CA	-5.35	1.41	1.46
1	A	440	GLY	C-O	-5.34	1.18	1.24
1	A	561	PRO	CA-C	5.31	1.59	1.52
1	A	969	ASN	C-O	5.28	1.29	1.24
1	A	1119	GLU	C-O	-5.25	1.18	1.24
1	A	1221	ARG	C-O	-5.21	1.17	1.23
1	A	777	ASP	C-O	-5.11	1.17	1.23
1	A	795	THR	C-O	-5.10	1.17	1.24
1	A	70	PRO	CA-CB	-5.08	1.46	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	THR	CA-C-N	-7.82	112.61	120.98
1	A	609	THR	C-N-CA	-7.82	112.61	120.98
1	A	1079[A]	ARG	N-CA-C	-7.33	104.33	113.28
1	A	1079[B]	ARG	N-CA-C	-7.33	104.33	113.28
1	A	440	GLY	N-CA-C	5.81	119.08	110.60
1	A	1050	VAL	CA-C-O	-5.75	115.83	121.58
1	A	216	HIS	N-CA-C	5.35	116.80	110.97
1	A	511	ALA	N-CA-C	5.30	117.05	111.28
1	A	1079[A]	ARG	CA-C-N	-5.25	114.81	122.58
1	A	1079[A]	ARG	C-N-CA	-5.25	114.81	122.58
1	A	1079[B]	ARG	CA-C-N	-5.25	114.81	122.58
1	A	1079[B]	ARG	C-N-CA	-5.25	114.81	122.58
1	A	154	GLN	CA-C-N	-5.18	114.23	119.83
1	A	154	GLN	C-N-CA	-5.18	114.23	119.83
1	A	1104	GLU	N-CA-C	5.17	116.72	111.14
1	A	156	ALA	CA-C-N	-5.13	115.44	120.52
1	A	156	ALA	C-N-CA	-5.13	115.44	120.52
1	A	313	GLY	N-CA-C	5.13	118.88	112.73

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	10153	0	10063	162	0
2	A	180	0	270	57	0
3	A	5	0	5	0	0
4	A	27	0	12	0	0
5	A	95	0	0	1	0
6	A	3	0	0	0	0
7	A	168	0	224	21	0
8	A	2	0	0	0	0
9	A	1083	0	0	36	0
All	All	11716	0	10574	184	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 (184) 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:1045[B]:LEU:CD1	1:A:1088[B]:LEU:HD11	1.52	1.36
1:A:274:ASP:HB2	2:A:1503:EDO:C1	1.65	1.27
2:A:1528:EDO:H11	9:A:2367:HOH:O	1.37	1.24
1:A:950:ASP:CB	2:A:1518:EDO:H12	1.67	1.23
1:A:274:ASP:CB	2:A:1503:EDO:H11	1.69	1.20
1:A:994:ARG:HH12	2:A:1521:EDO:H12	1.10	1.13
1:A:950:ASP:HB2	2:A:1518:EDO:C1	1.78	1.12
1:A:1045[B]:LEU:HD11	1:A:1088[B]:LEU:CD1	1.80	1.12
1:A:251:TYR:H	2:A:1529:EDO:H12	1.07	1.08
1:A:510[A]:ASN:ND2	1:A:514[A]:GLU:OE1	1.90	1.04
1:A:1:MET:HE2	9:A:2429:HOH:O	1.61	1.00
1:A:1055:GLU:HB2	9:A:1720:HOH:O	1.65	0.95
1:A:6:ARG:HB3	9:A:1960:HOH:O	1.68	0.92
1:A:1045[B]:LEU:CD1	1:A:1088[B]:LEU:CD1	2.45	0.86
1:A:936:ARG:HH22	2:A:1504[A]:EDO:H12	1.40	0.86
1:A:251:TYR:N	2:A:1529:EDO:H12	1.91	0.85
2:A:1503:EDO:H12	9:A:1601:HOH:O	1.76	0.84
1:A:1045[B]:LEU:HD11	1:A:1088[B]:LEU:HD11	0.86	0.84
1:A:270:ARG:HH21	2:A:1530:EDO:H22	1.42	0.83
1:A:994:ARG:NH1	2:A:1521:EDO:H12	1.93	0.83
1:A:820:SER:H	1:A:930:GLN:HE22	1.25	0.81
1:A:238:PHE:CE2	1:A:242:LYS:HE2	2.17	0.79
1:A:713:ARG:HH12	7:A:1562:GOL:H32	1.46	0.79
1:A:69[A]:THR:HG21	9:A:1916:HOH:O	1.84	0.77
1:A:624:ASP:HB2	2:A:1506:EDO:H11	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:ASN:HD21	1:A:958:ALA:H	1.29	0.77
1:A:175:ASN:HD21	1:A:182:LEU:H	1.31	0.75
1:A:950:ASP:HB2	2:A:1518:EDO:H12	0.82	0.75
2:A:1503:EDO:C1	9:A:1601:HOH:O	2.35	0.75
1:A:1045[B]:LEU:CG	1:A:1088[B]:LEU:HD11	2.17	0.75
1:A:276:ASN:HB2	9:A:1926:HOH:O	1.89	0.71
1:A:270:ARG:NH2	2:A:1530:EDO:H22	2.05	0.71
1:A:767[B]:GLN:HE22	7:A:1558:GOL:H12	1.56	0.70
1:A:96:HIS:HE1	1:A:103:VAL:O	1.74	0.69
7:A:1562:GOL:H2	9:A:1613:HOH:O	1.91	0.69
1:A:443:ALA:HB3	9:A:1756:HOH:O	1.93	0.68
1:A:1045[B]:LEU:CG	1:A:1088[B]:LEU:CD1	2.72	0.67
7:A:1579:GOL:H12	9:A:2423:HOH:O	1.94	0.67
1:A:11[B]:LEU:HD13	1:A:16:ILE:HD13	1.76	0.67
1:A:680:CYS:SG	1:A:726[A]:THR:HG21	2.35	0.66
1:A:1113:ASN:HD22	1:A:1116:VAL:H	1.44	0.65
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.78	0.65
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.80	0.65
1:A:80:ARG:HB3	1:A:138[B]:THR:HG22	1.77	0.65
1:A:936:ARG:NH2	2:A:1504[A]:EDO:H12	2.11	0.64
1:A:274:ASP:OD1	2:A:1503:EDO:H21	1.97	0.64
1:A:0:HIS:HB3	9:A:2522:HOH:O	1.98	0.64
1:A:1045[B]:LEU:HG	1:A:1088[B]:LEU:CD1	2.27	0.64
1:A:80:ARG:HA	1:A:138[B]:THR:HG23	1.80	0.64
1:A:922:ASN:HD22	1:A:924:GLU:H	1.46	0.63
2:A:1501:EDO:H12	2:A:1513:EDO:O1	1.99	0.62
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.64	0.62
1:A:471:GLN:HE21	1:A:472:ARG:H	1.45	0.62
1:A:499:PHE:CD2	1:A:515[B]:LEU:HD12	2.35	0.62
1:A:1045[B]:LEU:HG	1:A:1088[B]:LEU:HD12	1.81	0.62
1:A:1275:GLU:H	2:A:1510:EDO:C2	2.12	0.62
1:A:545:ASN:HD22	1:A:547:SER:H	1.48	0.61
1:A:283:HIS:NE2	2:A:1503:EDO:H22	2.15	0.61
1:A:510[A]:ASN:ND2	1:A:514[A]:GLU:CD	2.58	0.61
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.82	0.60
1:A:274:ASP:HB2	2:A:1503:EDO:H11	0.75	0.60
1:A:849:GLN:HB3	2:A:1506:EDO:H22	1.82	0.60
1:A:329[A]:LYS:NZ	1:A:419:ASN:HD21	2.00	0.60
1:A:787:GLU:HB2	1:A:792:ARG:HG3	1.83	0.60
1:A:296:HIS:HD2	1:A:307:GLY:O	1.84	0.60
1:A:1268:VAL:HA	7:A:1563:GOL:H2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051[A]:ASN:OD1	1:A:1052[A]:SER:OG	2.16	0.59
1:A:137:GLU:OE2	2:A:1594:EDO:H11	2.03	0.59
7:A:1559:GOL:H32	2:A:1594:EDO:C1	2.33	0.59
1:A:270:ARG:HH21	2:A:1530:EDO:C2	2.12	0.58
1:A:830:ASP:O	1:A:951[B]:CYS:HB2	2.01	0.58
1:A:767[B]:GLN:HE21	7:A:1577:GOL:C3	2.16	0.58
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.86	0.58
1:A:609:THR:HB	1:A:610:PRO:CD	2.34	0.57
1:A:851:GLY:H	2:A:1506:EDO:H12	1.68	0.57
1:A:1183:GLN:HG3	9:A:2640:HOH:O	2.03	0.57
1:A:274:ASP:OD1	2:A:1503:EDO:C2	2.52	0.57
1:A:1251:ASN:ND2	1:A:1253:ARG:H	2.02	0.57
1:A:1104:GLU:OE1	1:A:1108[A]:LYS:HE3	2.04	0.57
1:A:1251:ASN:HD22	1:A:1253:ARG:H	1.52	0.56
1:A:782:LYS:NZ	1:A:793:GLU:OE1	2.38	0.56
1:A:6:ARG:CB	9:A:1960:HOH:O	2.39	0.56
1:A:443:ALA:HB2	9:A:1651:HOH:O	2.05	0.56
1:A:968:ALA:HB1	2:A:1527:EDO:H11	1.87	0.56
1:A:1275:GLU:H	2:A:1510:EDO:H21	1.71	0.56
1:A:11[B]:LEU:CD1	1:A:16:ILE:CD1	2.84	0.55
1:A:346:GLU:HB2	9:A:1972:HOH:O	2.06	0.55
7:A:1562:GOL:C1	9:A:1613:HOH:O	2.53	0.55
1:A:327:LYS:HD3	2:A:1530:EDO:H21	1.88	0.55
1:A:1052[B]:SER:OG	1:A:1055:GLU:OE2	2.20	0.55
1:A:936:ARG:HH22	2:A:1504[A]:EDO:C1	2.15	0.55
1:A:270:ARG:HE	2:A:1530:EDO:H22	1.71	0.55
1:A:58:LEU:HD23	1:A:1108[A]:LYS:HD3	1.88	0.54
1:A:573:PRO:HA	2:A:1523:EDO:H12	1.89	0.54
1:A:585:HIS:HE1	1:A:599:ASP:OD1	1.91	0.54
7:A:1559:GOL:C3	2:A:1594:EDO:H12	2.38	0.54
1:A:746:HIS:HD2	1:A:782:LYS:NZ	2.06	0.53
1:A:61:TYR:C	7:A:1573:GOL:H31	2.34	0.53
1:A:354:GLY:O	1:A:408:HIS:HE1	1.92	0.53
1:A:168:ARG:NH1	1:A:188:ASP:OD1	2.34	0.53
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.07	0.53
7:A:1559:GOL:H32	2:A:1594:EDO:C2	2.39	0.53
1:A:787:GLU:CB	1:A:792:ARG:HG3	2.38	0.53
1:A:1128:GLN:HB2	9:A:1629:HOH:O	2.09	0.52
1:A:11[B]:LEU:HG	1:A:35:ALA:HB3	1.92	0.52
1:A:80:ARG:HB3	1:A:138[B]:THR:CG2	2.40	0.52
1:A:1076[B]:LEU:C	1:A:1077[B]:GLY:O	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.17	0.52
1:A:499:PHE:CD2	1:A:515[B]:LEU:CD1	2.93	0.52
1:A:950:ASP:CA	2:A:1518:EDO:H12	2.36	0.51
1:A:358:ARG:HD3	5:A:1550:SO4:O2	2.11	0.51
1:A:11[B]:LEU:HD13	1:A:16:ILE:CD1	2.41	0.51
1:A:851:GLY:H	2:A:1506:EDO:C1	2.24	0.50
1:A:11[B]:LEU:HB2	1:A:16:ILE:HD11	1.93	0.50
7:A:1562:GOL:C2	9:A:1613:HOH:O	2.52	0.50
2:A:1519:EDO:C2	9:A:1990:HOH:O	2.59	0.50
1:A:22:ARG:HD3	1:A:130:GLU:OE1	2.11	0.50
7:A:1559:GOL:H32	2:A:1594:EDO:H22	1.95	0.49
1:A:216:HIS:HD2	9:A:1637:HOH:O	1.94	0.49
1:A:403:GLU:OE2	1:A:746:HIS:HE1	1.96	0.49
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.59	0.49
1:A:969:ASN:ND2	9:A:1633:HOH:O	2.45	0.49
1:A:338:SER:OG	1:A:408:HIS:HD2	1.95	0.49
1:A:786:GLN:OE1	1:A:791:GLN:HG2	2.14	0.48
2:A:1521:EDO:H11	9:A:2568:HOH:O	2.13	0.48
1:A:651:PHE:H	1:A:989:THR:HG1	1.60	0.48
1:A:723:ILE:O	1:A:726[A]:THR:HG23	2.14	0.47
2:A:1593:EDO:H21	9:A:2388:HOH:O	2.14	0.47
1:A:315:GLU:OE2	1:A:319:GLU:OE2	2.31	0.47
1:A:298:HIS:HE1	1:A:469:SER:OG	1.97	0.47
1:A:950:ASP:H	2:A:1518:EDO:C2	2.28	0.47
1:A:1006:HIS:HD2	9:A:1997:HOH:O	1.97	0.47
7:A:1578:GOL:C1	9:A:1640:HOH:O	2.62	0.47
1:A:501[B]:HIS:HE1	1:A:518:ASP:OD2	1.98	0.46
1:A:275:HIS:HD2	9:A:2613:HOH:O	1.97	0.46
1:A:782:LYS:NZ	7:A:1565:GOL:O3	2.49	0.46
1:A:120:THR:H	1:A:123:GLN:HE21	1.63	0.46
1:A:238:PHE:CZ	1:A:242:LYS:HE2	2.51	0.46
1:A:270:ARG:NE	2:A:1530:EDO:H22	2.30	0.46
1:A:443:ALA:CB	9:A:1651:HOH:O	2.62	0.45
1:A:11[B]:LEU:CD1	1:A:16:ILE:HD13	2.45	0.45
1:A:1183:GLN:HE22	1:A:1285:ARG:HH21	1.65	0.45
7:A:1559:GOL:O2	2:A:1594:EDO:H21	2.16	0.45
1:A:445:ASN:C	1:A:445:ASN:HD22	2.25	0.45
1:A:851:GLY:H	2:A:1506:EDO:C2	2.30	0.45
1:A:1113:ASN:ND2	1:A:1116:VAL:H	2.14	0.45
1:A:11[B]:LEU:CD1	1:A:16:ILE:HD11	2.47	0.44
1:A:317:ARG:HH22	1:A:548:GLN:NE2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:GLY:N	2:A:1506:EDO:H12	2.32	0.44
1:A:293:VAL:HB	1:A:739:ASN:HD21	1.83	0.44
2:A:1593:EDO:C2	9:A:2388:HOH:O	2.65	0.44
1:A:238:PHE:CE2	1:A:242:LYS:CE	2.95	0.43
1:A:620:LYS:CE	9:A:2425:HOH:O	2.65	0.43
2:A:1593:EDO:H11	9:A:2388:HOH:O	2.17	0.43
1:A:11[B]:LEU:HD12	1:A:16:ILE:HD11	2.01	0.43
1:A:1051[B]:ASN:HD21	1:A:1093:GLY:HA2	1.82	0.43
1:A:1164:ARG:HD3	9:A:1981:HOH:O	2.17	0.43
1:A:634:ALA:HB3	2:A:1508:EDO:H22	2.01	0.43
1:A:862:GLN:NE2	2:A:1518:EDO:H21	2.34	0.43
1:A:282:PHE:CD2	7:A:1580:GOL:H2	2.54	0.43
1:A:585:HIS:CE1	1:A:599:ASP:OD1	2.72	0.43
7:A:1578:GOL:H11	9:A:1640:HOH:O	2.19	0.43
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.54	0.42
1:A:1019[A]:VAL:HG12	1:A:1021:LEU:HG	2.01	0.42
1:A:211[B]:GLN:NE2	1:A:506:GLY:HA2	2.34	0.42
1:A:573:PRO:CA	2:A:1523:EDO:H12	2.49	0.42
1:A:448:LEU:HD21	1:A:541:GLU:HA	2.01	0.42
1:A:574:TYR:H	2:A:1523:EDO:C1	2.33	0.42
1:A:175:ASN:ND2	1:A:182:LEU:H	2.06	0.42
1:A:1183:GLN:NE2	9:A:1652:HOH:O	2.53	0.42
1:A:950:ASP:CB	2:A:1518:EDO:C1	2.61	0.41
1:A:680:CYS:SG	1:A:726[A]:THR:CG2	3.07	0.41
1:A:270:ARG:CZ	2:A:1530:EDO:H22	2.49	0.41
7:A:1558:GOL:C3	9:A:1983:HOH:O	2.69	0.41
7:A:1558:GOL:H31	9:A:1983:HOH:O	2.20	0.41
1:A:1136:ASN:HA	1:A:1139:GLN:OE1	2.21	0.41
1:A:270:ARG:HE	2:A:1530:EDO:H12	1.85	0.41
1:A:936:ARG:HH22	2:A:1504[B]:EDO:H22	1.85	0.41
1:A:1050:VAL:HG13	1:A:1092:GLY:O	2.20	0.41
1:A:116:ALA:C	1:A:117:SER:O	2.64	0.40
1:A:861:ALA:HA	7:A:1577:GOL:C1	2.51	0.40
1:A:1051[B]:ASN:ND2	1:A:1093:GLY:HA2	2.37	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	1330/1301 (102%)	1289 (97%)	33 (2%)	8 (1%)	21	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1077[A]	GLY
1	A	1077[B]	GLY
1	A	117	SER
1	A	886	SER
1	A	1078[A]	GLY
1	A	1078[B]	GLY
1	A	609	THR
1	A	622	LYS

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	1074/1040 (103%)	1041 (97%)	33 (3%)	35	20

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	18	LYS
1	A	27	ASN

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Mol	Chain	Res	Type
1	A	69[A]	THR
1	A	69[B]	THR
1	A	104	ASP
1	A	119	LEU
1	A	122	GLU
1	A	154	GLN
1	A	169[A]	GLN
1	A	169[B]	GLN
1	A	176	LEU
1	A	184	GLU
1	A	206	LEU
1	A	218	ARG
1	A	228[A]	ILE
1	A	228[B]	ILE
1	A	296	HIS
1	A	346	GLU
1	A	358	ARG
1	A	429	GLU
1	A	442[A]	PRO
1	A	442[B]	PRO
1	A	448	LEU
1	A	471	GLN
1	A	609	THR
1	A	792	ARG
1	A	1144	LEU
1	A	1190[A]	MET
1	A	1190[B]	MET
1	A	1194	VAL
1	A	1195	SER
1	A	1251	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	39	HIS
1	A	68	HIS
1	A	96	HIS
1	A	123	GLN
1	A	126	GLN
1	A	175	ASN
1	A	191	GLN

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Mol	Chain	Res	Type
1	A	275	HIS
1	A	284	GLN
1	A	296	HIS
1	A	298	HIS
1	A	339	ASN
1	A	408	HIS
1	A	419	ASN
1	A	445	ASN
1	A	471	GLN
1	A	545	ASN
1	A	548	GLN
1	A	559	GLN
1	A	585	HIS
1	A	592	HIS
1	A	739	ASN
1	A	746	HIS
1	A	786	GLN
1	A	791	GLN
1	A	824	ASN
1	A	836	ASN
1	A	862	GLN
1	A	883	HIS
1	A	922	ASN
1	A	930	GLN
1	A	969	ASN
1	A	993	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1026	ASN
1	A	1084	ASN
1	A	1113	ASN
1	A	1183	GLN
1	A	1189	GLN
1	A	1251	ASN
1	A	1260	HIS
1	A	1276	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CYG	A	1135	1	12,14,15	3.96	5 (41%)	10,17,19	3.96	6 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CYG	A	1135	1	-	2/14/16/18	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	CYG	CD1-SG	-8.88	1.55	1.76
1	A	1135	CYG	OE2-CD1	-7.14	1.09	1.21
1	A	1135	CYG	CG1-CD1	5.90	1.56	1.50
1	A	1135	CYG	CB-SG	3.14	1.88	1.81
1	A	1135	CYG	CB-CA	-2.54	1.46	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1135	CYG	OE2-CD1-SG	-6.46	114.47	122.68
1	A	1135	CYG	CB1-CG1-CD1	-6.03	98.96	112.27
1	A	1135	CYG	CG1-CD1-SG	5.93	120.46	113.40
1	A	1135	CYG	CB-SG-CD1	5.17	107.86	100.76
1	A	1135	CYG	CB-CA-C	2.83	118.50	110.80
1	A	1135	CYG	CB1-CA1-N1	2.17	115.79	110.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1135	CYG	N-CA-CB-SG
1	A	1135	CYG	N1-CA1-CB1-CG1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 99 ligands modelled in this entry, 5 are monoatomic - leaving 94 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	EDO	A	1589	-	3,3,3	0.54	0	2,2,2	0.26	0
2	EDO	A	1595	-	3,3,3	0.58	0	2,2,2	1.53	0
7	GOL	A	1580	-	5,5,5	1.06	0	5,5,5	1.39	1 (20%)
7	GOL	A	1565	-	5,5,5	1.02	0	5,5,5	2.09	1 (20%)
2	EDO	A	1526	-	3,3,3	0.24	0	2,2,2	0.52	0
2	EDO	A	1585	-	3,3,3	0.24	0	2,2,2	0.95	0
7	GOL	A	1577	-	5,5,5	0.31	0	5,5,5	0.83	0
7	GOL	A	1559	-	5,5,5	0.81	0	5,5,5	2.34	2 (40%)
2	EDO	A	1583	-	3,3,3	0.50	0	2,2,2	0.39	0
2	EDO	A	1530	-	3,3,3	0.63	0	2,2,2	0.78	0
5	SO4	A	1551	-	4,4,4	0.91	0	6,6,6	0.91	0
2	EDO	A	1510	-	3,3,3	0.48	0	2,2,2	0.60	0
2	EDO	A	1504[A]	-	3,3,3	0.18	0	2,2,2	0.55	0
7	GOL	A	1563	-	5,5,5	0.99	0	5,5,5	1.63	1 (20%)
5	SO4	A	1544	-	4,4,4	0.47	0	6,6,6	0.89	0
5	SO4	A	1535	-	4,4,4	1.05	0	6,6,6	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	1512	-	3,3,3	0.31	0	2,2,2	0.63	0
2	EDO	A	1519	-	3,3,3	0.28	0	2,2,2	0.18	0
2	EDO	A	1503	-	3,3,3	0.25	0	2,2,2	0.21	0
7	GOL	A	1560	-	5,5,5	0.73	0	5,5,5	0.48	0
2	EDO	A	1524[A]	-	3,3,3	0.36	0	2,2,2	0.40	0
5	SO4	A	1538	-	4,4,4	0.79	0	6,6,6	0.40	0
7	GOL	A	1572	-	5,5,5	0.39	0	5,5,5	1.01	1 (20%)
2	EDO	A	1529	-	3,3,3	0.63	0	2,2,2	0.46	0
7	GOL	A	1575	-	5,5,5	0.65	0	5,5,5	0.60	0
7	GOL	A	1569	-	5,5,5	0.20	0	5,5,5	0.50	0
2	EDO	A	1521	-	3,3,3	0.29	0	2,2,2	0.47	0
2	EDO	A	1517	-	3,3,3	0.32	0	2,2,2	0.09	0
7	GOL	A	1564	-	5,5,5	1.58	1 (20%)	5,5,5	1.24	1 (20%)
7	GOL	A	1579	-	5,5,5	2.00	3 (60%)	5,5,5	3.09	4 (80%)
4	ADP	A	1532	6	28,29,29	1.47	5 (17%)	43,45,45	1.35	8 (18%)
2	EDO	A	1588	-	3,3,3	0.32	0	2,2,2	0.66	0
2	EDO	A	1518	-	3,3,3	0.36	0	2,2,2	0.42	0
2	EDO	A	1586	-	3,3,3	0.57	0	2,2,2	0.88	0
5	SO4	A	1550	-	4,4,4	0.82	0	6,6,6	1.21	1 (16%)
2	EDO	A	1525	-	3,3,3	0.36	0	2,2,2	0.30	0
2	EDO	A	1505	-	3,3,3	0.36	0	2,2,2	0.71	0
7	GOL	A	1573	-	5,5,5	0.87	0	5,5,5	1.00	0
5	SO4	A	1533	-	4,4,4	0.23	0	6,6,6	1.70	3 (50%)
5	SO4	A	1539	-	4,4,4	1.89	1 (25%)	6,6,6	2.85	3 (50%)
5	SO4	A	1547	-	4,4,4	0.86	0	6,6,6	0.68	0
2	EDO	A	1593	-	3,3,3	0.43	0	2,2,2	0.54	0
7	GOL	A	1574	-	5,5,5	0.63	0	5,5,5	0.59	0
2	EDO	A	1528	-	3,3,3	0.25	0	2,2,2	0.42	0
5	SO4	A	1536	-	4,4,4	0.46	0	6,6,6	1.22	1 (16%)
7	GOL	A	1566	-	5,5,5	1.19	1 (20%)	5,5,5	1.07	0
2	EDO	A	1523	-	3,3,3	0.53	0	2,2,2	0.43	0
2	EDO	A	1507	-	3,3,3	0.49	0	2,2,2	0.52	0
7	GOL	A	1570	-	5,5,5	0.37	0	5,5,5	1.10	0
7	GOL	A	1582	-	5,5,5	0.36	0	5,5,5	1.03	0
7	GOL	A	1578	-	5,5,5	0.94	0	5,5,5	1.36	0
2	EDO	A	1591	-	3,3,3	0.65	0	2,2,2	0.31	0
2	EDO	A	1594	-	3,3,3	0.44	0	2,2,2	0.87	0
2	EDO	A	1513	-	3,3,3	0.39	0	2,2,2	0.85	0
2	EDO	A	1592	-	3,3,3	0.52	0	2,2,2	0.59	0
2	EDO	A	1587	-	3,3,3	0.65	0	2,2,2	0.54	0
7	GOL	A	1568	-	5,5,5	0.21	0	5,5,5	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	1541	-	4,4,4	0.79	0	6,6,6	1.09	1 (16%)
7	GOL	A	1557	-	5,5,5	1.21	0	5,5,5	1.54	1 (20%)
7	GOL	A	1567	-	5,5,5	0.72	0	5,5,5	1.37	1 (20%)
2	EDO	A	1501	-	3,3,3	0.69	0	2,2,2	1.36	0
2	EDO	A	1520	-	3,3,3	0.51	0	2,2,2	0.56	0
3	IMD	A	1531	-	5,5,5	0.69	0	5,5,5	0.28	0
5	SO4	A	1546	-	4,4,4	0.73	0	6,6,6	0.94	0
2	EDO	A	1511	-	3,3,3	0.27	0	2,2,2	0.18	0
2	EDO	A	1506	-	3,3,3	0.42	0	2,2,2	0.54	0
7	GOL	A	1562	-	5,5,5	0.90	0	5,5,5	1.41	0
5	SO4	A	1543	-	4,4,4	0.50	0	6,6,6	1.89	2 (33%)
2	EDO	A	1522	-	3,3,3	0.19	0	2,2,2	0.88	0
5	SO4	A	1534	-	4,4,4	0.48	0	6,6,6	0.70	0
5	SO4	A	1545	-	4,4,4	0.38	0	6,6,6	0.68	0
7	GOL	A	1571	-	5,5,5	0.52	0	5,5,5	0.91	0
2	EDO	A	1590	-	3,3,3	0.41	0	2,2,2	0.32	0
2	EDO	A	1508	-	3,3,3	0.42	0	2,2,2	0.24	0
7	GOL	A	1558	-	5,5,5	1.08	0	5,5,5	1.31	1 (20%)
5	SO4	A	1540	-	4,4,4	0.51	0	6,6,6	0.44	0
5	SO4	A	1537	-	4,4,4	1.08	0	6,6,6	0.45	0
2	EDO	A	1584	-	3,3,3	0.72	0	2,2,2	0.24	0
5	SO4	A	1542	-	4,4,4	0.86	0	6,6,6	0.53	0
2	EDO	A	1504[B]	-	3,3,3	0.42	0	2,2,2	0.57	0
5	SO4	A	1549	-	4,4,4	0.41	0	6,6,6	0.72	0
7	GOL	A	1581	-	5,5,5	0.47	0	5,5,5	0.87	0
7	GOL	A	1556	-	5,5,5	0.59	0	5,5,5	1.20	0
7	GOL	A	1555	-	5,5,5	0.87	0	5,5,5	0.72	0
2	EDO	A	1516	-	3,3,3	0.40	0	2,2,2	0.04	0
2	EDO	A	1527	-	3,3,3	0.20	0	2,2,2	0.30	0
2	EDO	A	1502	-	3,3,3	0.66	0	2,2,2	0.45	0
2	EDO	A	1509	-	3,3,3	0.19	0	2,2,2	0.53	0
2	EDO	A	1515	-	3,3,3	0.14	0	2,2,2	0.65	0
5	SO4	A	1548	-	4,4,4	0.58	0	6,6,6	0.56	0
7	GOL	A	1561	-	5,5,5	0.83	0	5,5,5	0.47	0
7	GOL	A	1576	-	5,5,5	0.56	0	5,5,5	0.49	0
2	EDO	A	1514	-	3,3,3	0.46	0	2,2,2	0.57	0
2	EDO	A	1524[B]	-	3,3,3	0.46	0	2,2,2	0.67	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
2	EDO	A	1589	-	-	1/1/1/1	-
2	EDO	A	1506	-	-	0/1/1/1	-
2	EDO	A	1595	-	-	0/1/1/1	-
7	GOL	A	1562	-	-	4/4/4/4	-
2	EDO	A	1522	-	-	0/1/1/1	-
7	GOL	A	1566	-	-	4/4/4/4	-
7	GOL	A	1571	-	-	1/4/4/4	-
7	GOL	A	1580	-	-	3/4/4/4	-
2	EDO	A	1590	-	-	0/1/1/1	-
7	GOL	A	1575	-	-	2/4/4/4	-
7	GOL	A	1569	-	-	1/4/4/4	-
2	EDO	A	1521	-	-	1/1/1/1	-
2	EDO	A	1508	-	-	1/1/1/1	-
2	EDO	A	1517	-	-	1/1/1/1	-
2	EDO	A	1523	-	-	1/1/1/1	-
7	GOL	A	1564	-	-	1/4/4/4	-
7	GOL	A	1565	-	-	2/4/4/4	-
7	GOL	A	1558	-	-	0/4/4/4	-
7	GOL	A	1579	-	-	2/4/4/4	-
2	EDO	A	1526	-	-	1/1/1/1	-
2	EDO	A	1507	-	-	0/1/1/1	-
7	GOL	A	1570	-	-	4/4/4/4	-
7	GOL	A	1582	-	-	2/4/4/4	-
2	EDO	A	1585	-	-	1/1/1/1	-
4	ADP	A	1532	6	-	2/16/32/32	0/3/3/3
7	GOL	A	1577	-	-	2/4/4/4	-
7	GOL	A	1578	-	-	2/4/4/4	-
2	EDO	A	1584	-	-	0/1/1/1	-
2	EDO	A	1583	-	-	1/1/1/1	-
2	EDO	A	1530	-	-	1/1/1/1	-
2	EDO	A	1591	-	-	1/1/1/1	-
7	GOL	A	1559	-	-	4/4/4/4	-
2	EDO	A	1510	-	-	0/1/1/1	-
2	EDO	A	1504[A]	-	-	1/1/1/1	-
2	EDO	A	1594	-	-	0/1/1/1	-
2	EDO	A	1588	-	-	1/1/1/1	-
2	EDO	A	1518	-	-	1/1/1/1	-
2	EDO	A	1586	-	-	0/1/1/1	-
2	EDO	A	1504[B]	-	-	1/1/1/1	-
2	EDO	A	1513	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	1525	-	-	0/1/1/1	-
2	EDO	A	1592	-	-	1/1/1/1	-
2	EDO	A	1587	-	-	1/1/1/1	-
7	GOL	A	1581	-	-	2/4/4/4	-
7	GOL	A	1563	-	-	0/4/4/4	-
7	GOL	A	1556	-	-	2/4/4/4	-
7	GOL	A	1555	-	-	0/4/4/4	-
2	EDO	A	1505	-	-	0/1/1/1	-
7	GOL	A	1557	-	-	1/4/4/4	-
2	EDO	A	1516	-	-	1/1/1/1	-
7	GOL	A	1567	-	-	2/4/4/4	-
7	GOL	A	1568	-	-	0/4/4/4	-
2	EDO	A	1501	-	-	1/1/1/1	-
2	EDO	A	1512	-	-	1/1/1/1	-
7	GOL	A	1573	-	-	2/4/4/4	-
2	EDO	A	1519	-	-	1/1/1/1	-
2	EDO	A	1527	-	-	1/1/1/1	-
2	EDO	A	1520	-	-	0/1/1/1	-
2	EDO	A	1502	-	-	1/1/1/1	-
2	EDO	A	1503	-	-	0/1/1/1	-
2	EDO	A	1509	-	-	1/1/1/1	-
2	EDO	A	1515	-	-	1/1/1/1	-
2	EDO	A	1593	-	-	1/1/1/1	-
3	IMD	A	1531	-	-	-	0/1/1/1
7	GOL	A	1574	-	-	2/4/4/4	-
2	EDO	A	1528	-	-	0/1/1/1	-
7	GOL	A	1560	-	-	1/4/4/4	-
7	GOL	A	1561	-	-	0/4/4/4	-
2	EDO	A	1524[A]	-	-	1/1/1/1	-
7	GOL	A	1572	-	-	4/4/4/4	-
7	GOL	A	1576	-	-	2/4/4/4	-
2	EDO	A	1514	-	-	0/1/1/1	-
2	EDO	A	1529	-	-	0/1/1/1	-
2	EDO	A	1511	-	-	1/1/1/1	-
2	EDO	A	1524[B]	-	-	1/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1539	SO4	O2-S	3.66	1.66	1.44
4	A	1532	ADP	C5-C4	3.65	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1532	ADP	C4-N9	-3.58	1.30	1.37
7	A	1579	GOL	O1-C1	3.21	1.55	1.42
4	A	1532	ADP	C5-N7	-3.05	1.33	1.39
7	A	1564	GOL	O1-C1	2.96	1.54	1.42
4	A	1532	ADP	PA-O3A	2.47	1.62	1.59
4	A	1532	ADP	O3'-C3'	2.22	1.48	1.43
7	A	1579	GOL	C3-C2	-2.15	1.43	1.51
7	A	1579	GOL	C1-C2	2.04	1.59	1.51
7	A	1566	GOL	O2-C2	-2.00	1.37	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1579	GOL	O2-C2-C3	-4.91	88.84	109.18
5	A	1539	SO4	O3-S-O2	4.77	134.49	109.56
7	A	1559	GOL	O2-C2-C1	4.05	125.94	109.18
7	A	1565	GOL	O1-C1-C2	4.00	128.38	110.38
5	A	1539	SO4	O4-S-O3	-3.61	88.65	108.54
7	A	1579	GOL	O1-C1-C2	3.40	125.68	110.38
4	A	1532	ADP	C5-C4-N3	-3.27	122.22	126.72
5	A	1539	SO4	O4-S-O1	3.04	125.45	109.56
7	A	1559	GOL	O3-C3-C2	-2.94	97.13	110.38
4	A	1532	ADP	N3-C4-N9	2.91	132.12	127.17
5	A	1543	SO4	O4-S-O1	2.88	124.61	109.56
7	A	1579	GOL	O2-C2-C1	2.77	120.63	109.18
4	A	1532	ADP	C4-N9-C8	2.75	108.63	105.74
4	A	1532	ADP	C4-C5-N7	-2.74	107.45	110.58
4	A	1532	ADP	O2A-PA-O1A	2.67	124.88	112.44
5	A	1543	SO4	O3-S-O2	2.60	123.16	109.56
4	A	1532	ADP	C5-N7-C8	2.56	107.48	103.45
5	A	1533	SO4	O3-S-O2	-2.52	96.40	109.56
7	A	1564	GOL	C3-C2-C1	2.50	120.95	111.80
5	A	1536	SO4	O4-S-O1	-2.42	96.88	109.56
7	A	1580	GOL	O2-C2-C3	2.42	119.22	109.18
5	A	1533	SO4	O4-S-O1	2.33	121.74	109.56
7	A	1558	GOL	O2-C2-C1	2.29	118.67	109.18
7	A	1557	GOL	O2-C2-C1	2.28	118.63	109.18
5	A	1541	SO4	O4-S-O1	-2.27	97.67	109.56
4	A	1532	ADP	N9-C8-N7	-2.23	110.77	113.94
5	A	1550	SO4	O4-S-O2	2.23	121.19	109.56
5	A	1533	SO4	O4-S-O3	-2.16	96.61	108.54
7	A	1563	GOL	O1-C1-C2	-2.14	100.74	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1572	GOL	O3-C3-C2	-2.13	100.77	110.38
7	A	1579	GOL	C3-C2-C1	2.12	119.57	111.80
7	A	1567	GOL	O2-C2-C3	2.05	117.66	109.18
4	A	1532	ADP	O4'-C1'-N9	2.01	111.96	108.09

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1532	ADP	PA-O3A-PB-O3B
7	A	1559	GOL	O1-C1-C2-O2
7	A	1559	GOL	O1-C1-C2-C3
7	A	1559	GOL	C1-C2-C3-O3
7	A	1559	GOL	O2-C2-C3-O3
7	A	1562	GOL	C1-C2-C3-O3
7	A	1566	GOL	C1-C2-C3-O3
7	A	1566	GOL	O2-C2-C3-O3
7	A	1567	GOL	C1-C2-C3-O3
7	A	1570	GOL	O1-C1-C2-C3
7	A	1572	GOL	O1-C1-C2-O2
7	A	1572	GOL	O1-C1-C2-C3
7	A	1573	GOL	C1-C2-C3-O3
7	A	1574	GOL	C1-C2-C3-O3
7	A	1574	GOL	O2-C2-C3-O3
7	A	1575	GOL	C1-C2-C3-O3
7	A	1576	GOL	O1-C1-C2-C3
7	A	1577	GOL	O1-C1-C2-C3
7	A	1579	GOL	O1-C1-C2-C3
7	A	1580	GOL	O1-C1-C2-C3
7	A	1582	GOL	O1-C1-C2-C3
7	A	1580	GOL	O1-C1-C2-O2
7	A	1582	GOL	O1-C1-C2-O2
7	A	1556	GOL	C1-C2-C3-O3
7	A	1557	GOL	O1-C1-C2-C3
7	A	1562	GOL	O1-C1-C2-C3
7	A	1565	GOL	C1-C2-C3-O3
7	A	1566	GOL	O1-C1-C2-C3
7	A	1570	GOL	C1-C2-C3-O3
7	A	1572	GOL	C1-C2-C3-O3
7	A	1578	GOL	O1-C1-C2-C3
7	A	1562	GOL	O2-C2-C3-O3
7	A	1565	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	A	1566	GOL	O1-C1-C2-O2
7	A	1575	GOL	O2-C2-C3-O3
7	A	1576	GOL	O1-C1-C2-O2
7	A	1577	GOL	O1-C1-C2-O2
7	A	1579	GOL	O1-C1-C2-O2
2	A	1501	EDO	O1-C1-C2-O2
2	A	1513	EDO	O1-C1-C2-O2
2	A	1527	EDO	O1-C1-C2-O2
2	A	1583	EDO	O1-C1-C2-O2
2	A	1585	EDO	O1-C1-C2-O2
2	A	1591	EDO	O1-C1-C2-O2
7	A	1556	GOL	O2-C2-C3-O3
7	A	1567	GOL	O2-C2-C3-O3
7	A	1570	GOL	O1-C1-C2-O2
7	A	1573	GOL	O2-C2-C3-O3
2	A	1502	EDO	O1-C1-C2-O2
2	A	1519	EDO	O1-C1-C2-O2
2	A	1523	EDO	O1-C1-C2-O2
2	A	1587	EDO	O1-C1-C2-O2
2	A	1588	EDO	O1-C1-C2-O2
2	A	1592	EDO	O1-C1-C2-O2
4	A	1532	ADP	PA-O3A-PB-O1B
7	A	1581	GOL	C1-C2-C3-O3
2	A	1518	EDO	O1-C1-C2-O2
2	A	1526	EDO	O1-C1-C2-O2
7	A	1570	GOL	O2-C2-C3-O3
2	A	1517	EDO	O1-C1-C2-O2
2	A	1512	EDO	O1-C1-C2-O2
7	A	1562	GOL	O1-C1-C2-O2
7	A	1572	GOL	O2-C2-C3-O3
7	A	1578	GOL	O1-C1-C2-O2
2	A	1504[B]	EDO	O1-C1-C2-O2
2	A	1515	EDO	O1-C1-C2-O2
7	A	1580	GOL	O2-C2-C3-O3
7	A	1569	GOL	O1-C1-C2-C3
2	A	1504[A]	EDO	O1-C1-C2-O2
2	A	1511	EDO	O1-C1-C2-O2
2	A	1516	EDO	O1-C1-C2-O2
2	A	1524[B]	EDO	O1-C1-C2-O2
2	A	1589	EDO	O1-C1-C2-O2
7	A	1581	GOL	O2-C2-C3-O3
2	A	1509	EDO	O1-C1-C2-O2

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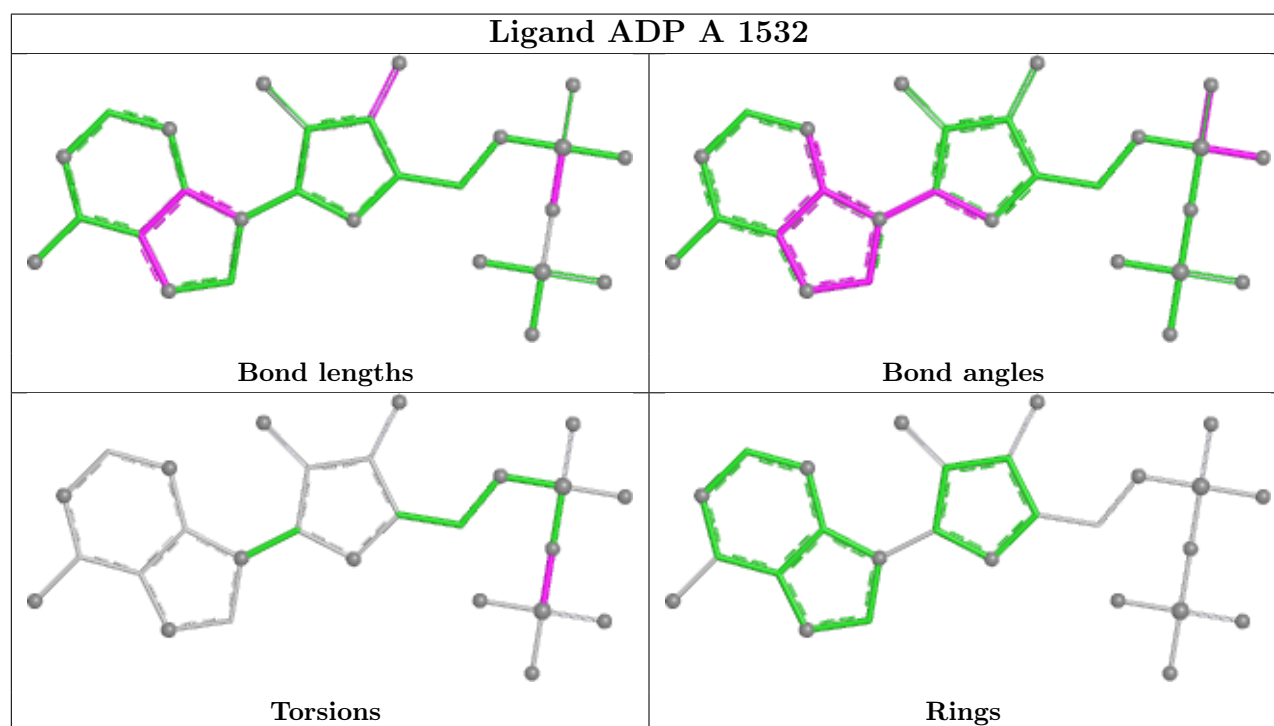
Mol	Chain	Res	Type	Atoms
2	A	1593	EDO	O1-C1-C2-O2
7	A	1560	GOL	O1-C1-C2-C3
7	A	1564	GOL	C1-C2-C3-O3
2	A	1508	EDO	O1-C1-C2-O2
2	A	1524[A]	EDO	O1-C1-C2-O2
2	A	1530	EDO	O1-C1-C2-O2
7	A	1571	GOL	O1-C1-C2-C3
2	A	1521	EDO	O1-C1-C2-O2

There are no ring outliers.

29 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1580	GOL	1	0
7	A	1565	GOL	1	0
7	A	1577	GOL	2	0
7	A	1559	GOL	5	0
2	A	1530	EDO	8	0
2	A	1510	EDO	2	0
2	A	1504[A]	EDO	3	0
7	A	1563	GOL	1	0
2	A	1519	EDO	1	0
2	A	1503	EDO	8	0
2	A	1529	EDO	2	0
2	A	1521	EDO	3	0
7	A	1579	GOL	1	0
2	A	1518	EDO	7	0
5	A	1550	SO4	1	0
7	A	1573	GOL	1	0
2	A	1593	EDO	3	0
2	A	1528	EDO	1	0
2	A	1523	EDO	3	0
7	A	1578	GOL	2	0
2	A	1594	EDO	6	0
2	A	1513	EDO	1	0
2	A	1501	EDO	1	0
2	A	1506	EDO	6	0
7	A	1562	GOL	4	0
2	A	1508	EDO	1	0
7	A	1558	GOL	3	0
2	A	1504[B]	EDO	1	0
2	A	1527	EDO	1	0

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



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	1281/1301 (98%)	-0.48	20 (1%) 70 74	8, 18, 42, 94	53 (4%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	609	THR	5.6
1	A	-2	GLY	4.5
1	A	610	PRO	4.3
1	A	607	GLY	3.1
1	A	-1	SER	3.0
1	A	1	MET	2.8
1	A	217[A]	CYS	2.6
1	A	622	LYS	2.6
1	A	31	HIS	2.6
1	A	216	HIS	2.5
1	A	121	ALA	2.4
1	A	788	GLY	2.4
1	A	152	HIS	2.3
1	A	442[A]	PRO	2.2
1	A	623	GLY	2.1
1	A	0	HIS	2.1
1	A	465	LEU	2.1
1	A	117	SER	2.1
1	A	119	LEU	2.0
1	A	358	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CYG	A	1135	15/16	0.97	0.08	13,23,28,29	2

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
2	EDO	A	1511	4/4	0.67	0.28	49,58,62,62	0
2	EDO	A	1529	4/4	0.67	0.23	34,39,48,51	0
2	EDO	A	1527	4/4	0.71	0.20	45,47,49,50	0
2	EDO	A	1521	4/4	0.71	0.19	55,58,58,59	0
2	EDO	A	1517	4/4	0.73	0.17	53,54,55,56	0
2	EDO	A	1509	4/4	0.73	0.20	50,54,55,58	0
2	EDO	A	1594	4/4	0.74	0.27	47,65,69,76	0
2	EDO	A	1519	4/4	0.75	0.22	59,63,64,65	0
2	EDO	A	1589	4/4	0.76	0.19	62,63,67,69	0
2	EDO	A	1515	4/4	0.77	0.23	47,55,59,63	0
2	EDO	A	1587	4/4	0.77	0.18	54,59,62,63	0
2	EDO	A	1513	4/4	0.78	0.22	45,50,55,65	0
2	EDO	A	1510	4/4	0.78	0.22	38,50,53,58	0
7	GOL	A	1566	6/6	0.78	0.18	35,38,40,45	0
7	GOL	A	1581	6/6	0.78	0.16	45,58,66,76	0
2	EDO	A	1522	4/4	0.80	0.17	33,40,48,52	0
7	GOL	A	1575	6/6	0.80	0.18	57,63,66,69	0
7	GOL	A	1580	6/6	0.80	0.18	34,45,61,61	0
2	EDO	A	1516	4/4	0.80	0.19	41,51,57,58	0
7	GOL	A	1565	6/6	0.81	0.19	46,59,64,77	0
2	EDO	A	1592	4/4	0.81	0.18	43,53,54,55	0
7	GOL	A	1572	6/6	0.81	0.16	40,55,57,59	0
2	EDO	A	1514	4/4	0.82	0.18	33,46,52,54	0
2	EDO	A	1528	4/4	0.82	0.22	66,68,68,72	0
2	EDO	A	1520	4/4	0.82	0.17	53,54,56,56	0
7	GOL	A	1577	6/6	0.82	0.17	43,56,59,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	1578	6/6	0.82	0.17	36,59,61,65	0
2	EDO	A	1583	4/4	0.82	0.15	45,59,61,69	0
2	EDO	A	1584	4/4	0.82	0.21	38,61,66,67	0
2	EDO	A	1524[B]	4/4	0.83	0.16	32,51,55,68	4
2	EDO	A	1526	4/4	0.83	0.15	50,51,60,60	0
2	EDO	A	1586	4/4	0.83	0.16	44,55,60,61	0
2	EDO	A	1512	4/4	0.83	0.21	42,53,59,67	0
2	EDO	A	1501	4/4	0.83	0.17	28,35,40,58	0
2	EDO	A	1524[A]	4/4	0.83	0.16	24,36,39,46	4
2	EDO	A	1530	4/4	0.83	0.17	27,31,35,42	0
5	SO4	A	1549	5/5	0.83	0.11	55,56,78,82	0
7	GOL	A	1582	6/6	0.83	0.18	57,63,67,70	0
7	GOL	A	1571	6/6	0.84	0.15	47,50,52,57	0
5	SO4	A	1545	5/5	0.84	0.18	31,34,53,54	0
2	EDO	A	1585	4/4	0.84	0.16	54,54,56,57	0
7	GOL	A	1569	6/6	0.84	0.18	54,57,61,66	0
2	EDO	A	1590	4/4	0.85	0.16	55,60,62,64	0
7	GOL	A	1568	6/6	0.85	0.13	33,45,52,53	0
2	EDO	A	1505	4/4	0.85	0.17	48,55,57,60	0
7	GOL	A	1570	6/6	0.85	0.18	56,59,67,68	0
7	GOL	A	1567	6/6	0.86	0.14	40,41,51,52	0
2	EDO	A	1504[B]	4/4	0.86	0.14	26,29,29,34	4
3	IMD	A	1531	5/5	0.86	0.14	49,50,55,58	0
2	EDO	A	1504[A]	4/4	0.86	0.14	28,30,32,34	4
5	SO4	A	1551	5/5	0.87	0.11	51,52,61,69	0
7	GOL	A	1562	6/6	0.87	0.12	33,40,45,46	0
2	EDO	A	1502	4/4	0.87	0.16	40,46,47,56	0
2	EDO	A	1503	4/4	0.87	0.29	37,44,46,48	0
2	EDO	A	1595	4/4	0.87	0.13	36,42,44,46	0
7	GOL	A	1573	6/6	0.87	0.13	47,52,57,61	0
2	EDO	A	1591	4/4	0.88	0.13	36,42,49,50	0
2	EDO	A	1588	4/4	0.88	0.14	57,59,59,60	0
5	SO4	A	1544	5/5	0.89	0.18	33,40,49,62	0
2	EDO	A	1593	4/4	0.89	0.13	33,47,48,50	0
2	EDO	A	1506	4/4	0.89	0.20	30,32,35,52	0
5	SO4	A	1539	5/5	0.89	0.12	27,28,47,53	0
2	EDO	A	1508	4/4	0.90	0.12	35,42,46,46	0
2	EDO	A	1523	4/4	0.90	0.17	30,39,50,59	0
7	GOL	A	1579	6/6	0.90	0.13	27,32,41,44	0
7	GOL	A	1558	6/6	0.90	0.14	26,39,45,49	0
7	GOL	A	1559	6/6	0.90	0.11	29,30,39,42	0
5	SO4	A	1548	5/5	0.90	0.08	58,63,71,74	0

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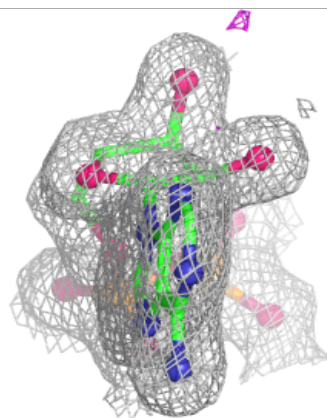
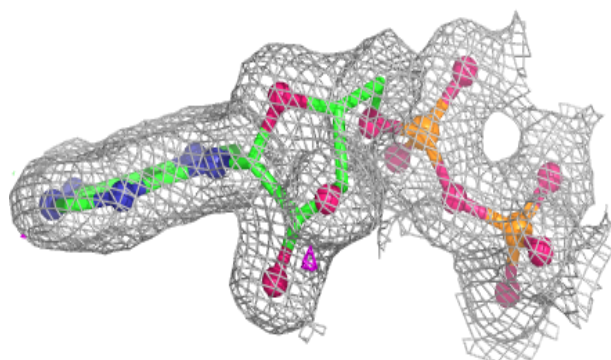
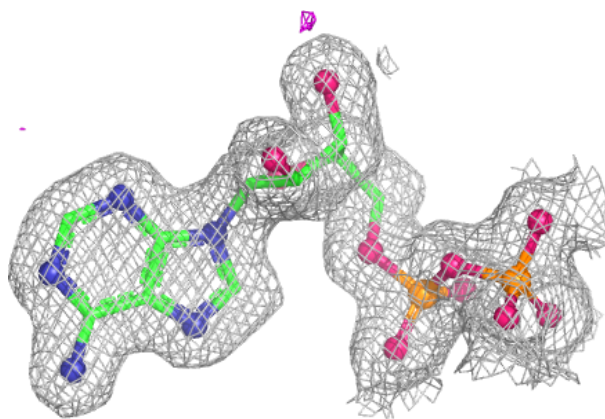
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	1574	6/6	0.91	0.13	22,43,44,64	0
7	GOL	A	1560	6/6	0.91	0.10	25,30,31,33	0
2	EDO	A	1507	4/4	0.91	0.12	31,31,37,38	0
7	GOL	A	1564	6/6	0.91	0.14	26,33,40,41	0
7	GOL	A	1563	6/6	0.92	0.12	28,38,41,46	0
7	GOL	A	1576	6/6	0.92	0.13	33,52,61,64	0
2	EDO	A	1525	4/4	0.92	0.13	39,40,51,57	0
2	EDO	A	1518	4/4	0.92	0.11	37,43,44,49	0
5	SO4	A	1542	5/5	0.93	0.14	41,45,49,54	0
5	SO4	A	1537	5/5	0.93	0.14	34,35,37,54	0
8	CL	A	1596	1/1	0.93	0.10	47,47,47,47	0
5	SO4	A	1543	5/5	0.94	0.12	31,40,50,51	0
5	SO4	A	1546	5/5	0.94	0.12	36,46,49,57	0
5	SO4	A	1536	5/5	0.94	0.14	37,37,44,50	0
8	CL	A	1597	1/1	0.94	0.11	55,55,55,55	0
5	SO4	A	1540	5/5	0.95	0.07	42,45,53,56	0
7	GOL	A	1561	6/6	0.95	0.10	23,29,31,32	0
7	GOL	A	1556	6/6	0.95	0.08	16,21,25,30	0
5	SO4	A	1541	5/5	0.95	0.07	44,46,55,56	0
5	SO4	A	1538	5/5	0.95	0.13	37,37,38,38	0
5	SO4	A	1550	5/5	0.96	0.10	36,38,43,45	0
7	GOL	A	1557	6/6	0.97	0.08	21,24,34,41	0
7	GOL	A	1555	6/6	0.97	0.06	20,22,23,26	0
5	SO4	A	1535	5/5	0.98	0.09	19,26,30,30	0
5	SO4	A	1547	5/5	0.98	0.12	32,33,35,38	0
5	SO4	A	1534	5/5	0.99	0.08	25,31,36,36	0
4	ADP	A	1532	27/27	0.99	0.03	11,12,13,13	0
5	SO4	A	1533	5/5	0.99	0.05	24,27,31,34	0
6	MG	A	1552	1/1	0.99	0.03	12,12,12,12	0
6	MG	A	1553	1/1	0.99	0.01	13,13,13,13	0
6	MG	A	1554	1/1	0.99	0.02	13,13,13,13	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 1532:

$2mF_o-DF_c$ (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.