



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:18 PM UTC

PDB ID : 1T3T / pdb_00001t3t
Title : Structure of Formylglycinamide synthetase
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Deposited on : 2004-04-27
Resolution : 1.90 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

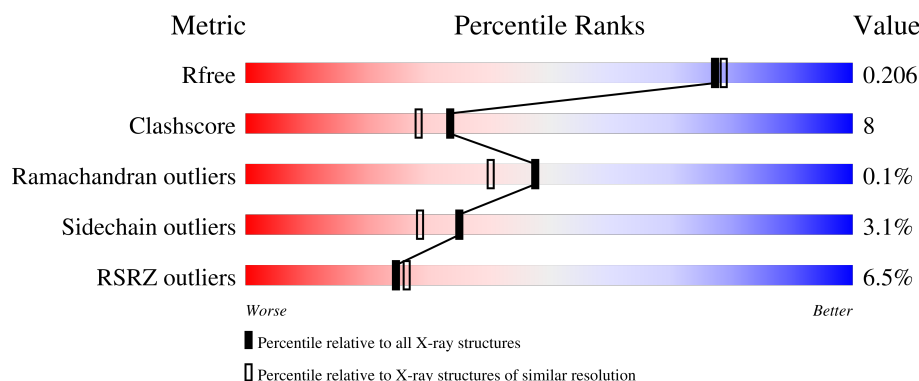
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	1303	6% 80% 17% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11024 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	1284	Total	C	N	O	S	0	0	0
			9885	6204	1761	1872	48			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	cloning artifact	UNP P74881
A	-6	LEU	-	cloning artifact	UNP P74881
A	-5	VAL	-	cloning artifact	UNP P74881
A	-4	PRO	-	cloning artifact	UNP P74881
A	-3	ARG	-	cloning artifact	UNP P74881
A	-2	GLY	-	cloning artifact	UNP P74881
A	-1	SER	-	cloning artifact	UNP P74881
A	0	HIS	-	cloning artifact	UNP P74881
A	1135	CYG	CYS	modified residue	UNP P74881

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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



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

- 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		

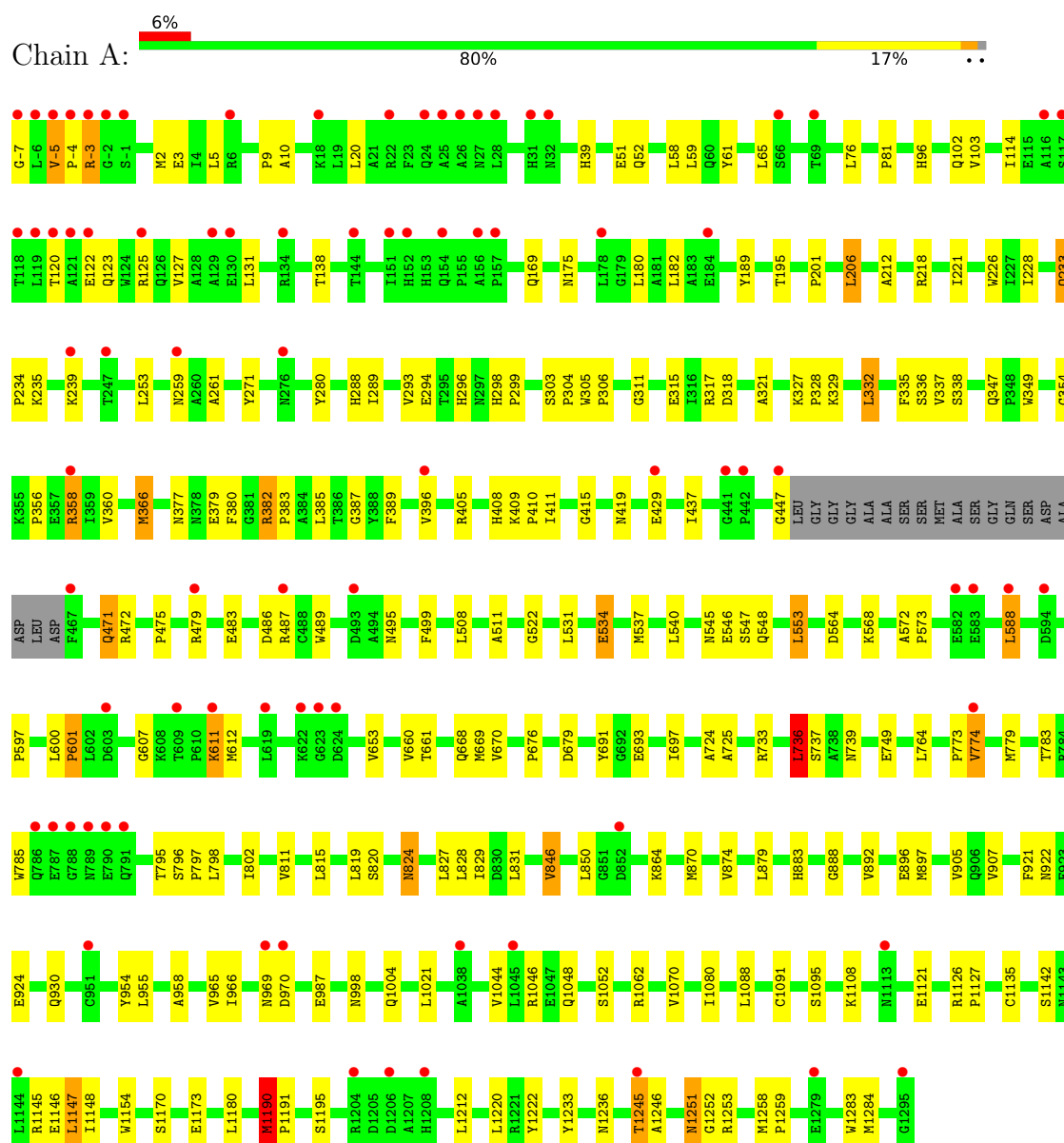
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1079	Total	O	0	0
			1079	1079		

3 Residue-property plots [i](#)

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	145.81Å 145.81Å 141.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.73 – 1.90 47.73 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.4 (47.73-1.90) 95.4 (47.73-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.206 0.188 , 0.206	Depositor DCC
R_{free} test set	10822 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11024	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: CYG, SO4, ADP, MG

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	0.41	2/10082 (0.0%)	0.92	41/13686 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	MET	SD-CE	-9.97	1.54	1.79
1	A	1190	MET	SD-CE	-7.60	1.60	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	GLU	CA-C-N	8.49	129.31	119.47
1	A	534	GLU	C-N-CA	8.49	129.31	119.47
1	A	303	SER	CA-C-N	7.34	126.88	119.24
1	A	303	SER	C-N-CA	7.34	126.88	119.24
1	A	409	LYS	N-CA-C	-7.31	95.39	108.47
1	A	779	MET	N-CA-C	7.30	121.04	112.72
1	A	724	ALA	N-CA-C	6.56	120.15	111.75
1	A	764	LEU	N-CA-C	6.47	118.02	110.97
1	A	1236	ASN	N-CA-C	-6.05	96.72	108.59
1	A	385	LEU	N-CA-C	5.99	121.50	113.72
1	A	233	GLN	CA-C-N	5.97	125.68	119.05
1	A	233	GLN	C-N-CA	5.97	125.68	119.05
1	A	670	VAL	N-CA-C	5.91	116.99	108.48
1	A	797	PRO	N-CA-C	-5.89	102.58	111.41
1	A	653	VAL	N-CA-C	5.71	117.10	111.67
1	A	347	GLN	CA-C-N	5.70	125.82	119.32
1	A	347	GLN	C-N-CA	5.70	125.82	119.32
1	A	736	LEU	N-CA-C	5.66	118.94	109.95
1	A	289	ILE	N-CA-C	5.57	115.96	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	GLY	N-CA-C	-5.52	105.81	112.49
1	A	1091	CYS	N-CA-C	5.50	117.62	110.53
1	A	691	TYR	N-CA-C	-5.48	103.29	110.53
1	A	798	LEU	N-CA-C	-5.45	101.98	110.10
1	A	511	ALA	N-CA-C	5.42	116.87	111.07
1	A	601	PRO	N-CA-C	-5.41	102.70	111.19
1	A	522	GLY	N-CA-C	-5.40	105.36	112.81
1	A	998	ASN	CA-C-N	5.39	125.47	119.32
1	A	998	ASN	C-N-CA	5.39	125.47	119.32
1	A	987	GLU	N-CA-C	5.32	117.82	111.71
1	A	10	ALA	N-CA-C	5.31	119.81	113.23
1	A	1126	ARG	CA-C-N	5.28	125.09	119.28
1	A	1126	ARG	C-N-CA	5.28	125.09	119.28
1	A	1127	PRO	N-CA-C	5.20	120.67	113.65
1	A	921	PHE	N-CA-C	5.19	120.25	113.30
1	A	965	VAL	N-CA-C	5.18	115.36	108.11
1	A	737	SER	N-CA-C	-5.14	100.80	109.07
1	A	195	THR	N-CA-C	-5.10	105.80	111.36
1	A	824	ASN	N-CA-C	5.07	116.70	109.14
1	A	495	ASN	CA-C-N	5.05	124.67	119.56
1	A	495	ASN	C-N-CA	5.05	124.67	119.56
1	A	1148	ILE	N-CA-C	5.01	113.44	107.73

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	9885	0	9662	150	0
2	A	3	0	0	0	0
3	A	30	0	0	0	0
4	A	27	0	12	1	0
5	A	1079	0	0	24	0
All	All	11024	0	9674	150	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 8.

All (150) 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:335:PHE:HB3	1:A:366:MET:HE1	1.40	1.03
1:A:175:ASN:HD21	1:A:182:LEU:H	1.16	0.93
1:A:1190:MET:H	1:A:1190:MET:HE2	1.34	0.92
1:A:366:MET:HE3	1:A:389:PHE:CE1	2.04	0.92
1:A:820:SER:H	1:A:930:GLN:HE22	1.16	0.91
1:A:824:ASN:HD21	1:A:958:ALA:H	1.15	0.88
1:A:1190:MET:HE2	1:A:1190:MET:N	1.96	0.79
1:A:358:ARG:HD3	1:A:358:ARG:H	1.55	0.71
1:A:396:VAL:CG1	1:A:850:LEU:HD22	2.22	0.70
1:A:733:ARG:HB3	5:A:2810:HOH:O	1.90	0.70
1:A:305:TRP:HB3	1:A:306:PRO:HD3	1.73	0.69
1:A:396:VAL:HG11	1:A:850:LEU:HD22	1.74	0.69
1:A:545:ASN:HD22	1:A:547:SER:H	1.40	0.69
1:A:922:ASN:HD22	1:A:924:GLU:H	1.41	0.68
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.59	0.67
1:A:321:ALA:HB3	5:A:2828:HOH:O	1.93	0.67
1:A:1251:ASN:ND2	1:A:1253:ARG:H	1.92	0.67
1:A:471:GLN:HE21	1:A:472:ARG:H	1.41	0.67
1:A:366:MET:HE3	1:A:389:PHE:HE1	1.53	0.67
1:A:437:ILE:HB	1:A:553:LEU:HD12	1.78	0.66
1:A:1052:SER:HB3	5:A:2537:HOH:O	1.94	0.66
1:A:534:GLU:HG3	1:A:537:MET:HG3	1.78	0.65
1:A:669:MET:SD	1:A:676:PRO:HG3	2.36	0.65
1:A:5:LEU:HD22	1:A:59:LEU:HD12	1.77	0.65
1:A:175:ASN:ND2	1:A:182:LEU:H	1.94	0.64
1:A:796:SER:O	5:A:2760:HOH:O	2.15	0.64
1:A:1190:MET:HE3	1:A:1283:TRP:CZ2	2.34	0.63
1:A:76:LEU:HD23	5:A:2982:HOH:O	1.98	0.63
1:A:337:VAL:HG13	1:A:366:MET:HE2	1.82	0.62
1:A:114:ILE:HD11	1:A:131:LEU:HD11	1.82	0.62
1:A:487:ARG:NH2	5:A:2846:HOH:O	2.33	0.61
1:A:-5:VAL:HG12	5:A:2587:HOH:O	2.01	0.61
1:A:317:ARG:HH22	1:A:548:GLN:NE2	1.99	0.60
1:A:356:PRO:HG3	1:A:785:TRP:HB3	1.83	0.60
1:A:1251:ASN:C	1:A:1251:ASN:HD22	2.08	0.60
1:A:1222:TYR:OH	1:A:1245:THR:HG21	2.01	0.60
1:A:358:ARG:HD3	1:A:358:ARG:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.50	0.59
1:A:827:LEU:HD23	1:A:954:TYR:HA	1.83	0.59
1:A:221:ILE:HD13	1:A:612:MET:SD	2.43	0.58
1:A:228:ILE:HD13	1:A:233:GLN:HG3	1.86	0.58
1:A:259:ASN:HB2	5:A:2299:HOH:O	2.03	0.58
1:A:366:MET:HE3	1:A:389:PHE:CD1	2.38	0.58
1:A:337:VAL:CG1	1:A:366:MET:HE2	2.33	0.58
1:A:1146:GLU:HG3	1:A:1147:LEU:HD13	1.85	0.58
1:A:52:GLN:NE2	5:A:2964:HOH:O	2.37	0.57
1:A:354:GLY:O	1:A:408:HIS:HE1	1.86	0.57
1:A:259:ASN:ND2	5:A:2828:HOH:O	2.38	0.56
1:A:261:ALA:HB2	1:A:774:VAL:HG13	1.87	0.56
1:A:96:HIS:HE1	1:A:103:VAL:O	1.89	0.56
1:A:336:SER:HB2	1:A:411:ILE:HB	1.88	0.56
1:A:1245:THR:HG22	1:A:1258:MET:HB2	1.88	0.56
1:A:1044:VAL:HG12	5:A:3079:HOH:O	2.05	0.55
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.04	0.55
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.90	0.54
1:A:1070:VAL:HG22	1:A:1080:ILE:HD13	1.88	0.54
1:A:380:PHE:O	1:A:479:ARG:HD3	2.07	0.54
1:A:358:ARG:H	1:A:358:ARG:CD	2.15	0.53
1:A:379:GLU:HB3	1:A:475:PRO:HB2	1.90	0.53
1:A:405:ARG:NH2	5:A:2760:HOH:O	2.41	0.53
1:A:-3:ARG:HG3	1:A:2:MET:HB2	1.91	0.53
1:A:377:ASN:OD1	1:A:382:ARG:HD2	2.08	0.53
1:A:1251:ASN:HD22	1:A:1253:ARG:H	1.56	0.52
1:A:120:THR:HG23	1:A:123:GLN:HE21	1.74	0.51
1:A:332:LEU:HG	1:A:697:ILE:HD11	1.93	0.51
1:A:905:VAL:HG13	1:A:907:VAL:HG13	1.91	0.51
1:A:668:GLN:HG2	4:A:2005:ADP:H1'	1.92	0.51
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.95	0.50
1:A:201:PRO:HB2	1:A:206:LEU:HD13	1.94	0.50
1:A:315:GLU:HG2	5:A:2833:HOH:O	2.12	0.49
1:A:58:LEU:HD23	1:A:1108:LYS:HD3	1.95	0.49
1:A:356:PRO:HG2	1:A:783:THR:CG2	2.43	0.49
1:A:1190:MET:HE3	1:A:1283:TRP:HZ2	1.76	0.49
1:A:888:GLY:HA3	1:A:892:VAL:HG21	1.95	0.49
1:A:483:GLU:O	1:A:487:ARG:HG2	2.13	0.48
1:A:531:LEU:HD12	5:A:2814:HOH:O	2.13	0.48
1:A:1021:LEU:HD13	5:A:2907:HOH:O	2.12	0.48
1:A:-7:GLY:O	1:A:3:GLU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:GLU:CD	5:A:2760:HOH:O	2.55	0.48
1:A:829:ILE:HB	5:A:3018:HOH:O	2.13	0.48
1:A:486:ASP:HA	1:A:489:TRP:NE1	2.29	0.48
1:A:337:VAL:CG2	1:A:366:MET:HE2	2.44	0.47
1:A:564:ASP:O	1:A:568:LYS:HG2	2.15	0.47
1:A:969:ASN:CG	1:A:970:ASP:H	2.21	0.47
1:A:1220:LEU:HB2	1:A:1246:ALA:HB3	1.97	0.47
1:A:1251:ASN:HD22	1:A:1252:GLY:N	2.13	0.47
1:A:337:VAL:HG22	1:A:366:MET:HE2	1.96	0.47
1:A:226:TRP:HB3	1:A:228:ILE:CD1	2.45	0.46
1:A:122:GLU:HG2	1:A:125:ARG:NH1	2.30	0.46
1:A:819:LEU:HG	1:A:897:MET:HB3	1.98	0.46
1:A:1190:MET:HE2	1:A:1190:MET:O	2.16	0.46
1:A:-5:VAL:HG13	1:A:-4:PRO:HD2	1.97	0.46
1:A:114:ILE:HD13	1:A:127:VAL:HG11	1.98	0.46
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.99	0.46
1:A:828:LEU:HB2	1:A:955:LEU:HD11	1.97	0.45
1:A:51:GLU:CD	1:A:102:GLN:HE22	2.24	0.45
1:A:293:VAL:HB	1:A:739:ASN:HD21	1.82	0.45
1:A:1212:LEU:HD22	5:A:2531:HOH:O	2.17	0.45
1:A:298:HIS:HB3	1:A:299:PRO:HD3	1.99	0.45
1:A:1170:SER:O	1:A:1191:PRO:HA	2.17	0.45
1:A:736:LEU:HG	1:A:802:ILE:HG23	1.99	0.45
1:A:499:PHE:HA	5:A:2968:HOH:O	2.17	0.45
1:A:545:ASN:ND2	1:A:547:SER:H	2.13	0.44
1:A:1245:THR:HG22	1:A:1259:PRO:HD3	2.00	0.44
1:A:1145:ARG:HD3	1:A:1154:TRP:HB2	1.99	0.44
1:A:20:LEU:HD11	5:A:2906:HOH:O	2.17	0.44
1:A:1190:MET:N	1:A:1190:MET:CE	2.76	0.44
1:A:212:ALA:HB2	5:A:2535:HOH:O	2.17	0.44
1:A:437:ILE:HB	1:A:553:LEU:CD1	2.46	0.44
1:A:588:LEU:O	1:A:597:PRO:HD2	2.18	0.43
1:A:9:PRO:HB2	1:A:65:LEU:HB2	2.00	0.43
1:A:81:PRO:HD3	1:A:138:THR:HG21	1.99	0.43
1:A:338:SER:OG	1:A:408:HIS:HD2	2.02	0.43
1:A:387:GLY:HA2	1:A:697:ILE:HD12	2.01	0.43
1:A:1142:SER:O	1:A:1145:ARG:HG3	2.19	0.43
1:A:1222:TYR:CZ	1:A:1245:THR:HG21	2.53	0.43
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.54	0.43
1:A:189:TYR:OH	1:A:607:GLY:HA3	2.18	0.42
1:A:233:GLN:HA	1:A:234:PRO:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:LEU:O	1:A:773:PRO:HD2	2.18	0.42
1:A:123:GLN:O	1:A:127:VAL:HG23	2.19	0.42
1:A:228:ILE:HD13	1:A:233:GLN:CG	2.49	0.42
1:A:1048:GLN:O	1:A:1095:SER:HA	2.19	0.42
1:A:1121:GLU:HB2	1:A:1147:LEU:HG	2.02	0.42
1:A:349:TRP:CZ3	1:A:846:VAL:HG22	2.55	0.42
1:A:1062:ARG:HB3	1:A:1284:MET:CE	2.50	0.42
1:A:611:LYS:HB2	1:A:611:LYS:NZ	2.35	0.41
1:A:1062:ARG:HB3	1:A:1284:MET:HE1	2.00	0.41
1:A:304:PRO:HG3	1:A:360:VAL:HG21	2.02	0.41
1:A:318:ASP:HA	5:A:2828:HOH:O	2.20	0.41
1:A:815:LEU:HD13	1:A:879:LEU:HD12	2.02	0.41
1:A:1046:ARG:HB3	5:A:3079:HOH:O	2.18	0.41
1:A:1251:ASN:ND2	1:A:1251:ASN:C	2.77	0.41
1:A:540:LEU:C	1:A:540:LEU:HD23	2.46	0.41
1:A:486:ASP:HA	1:A:489:TRP:CD1	2.55	0.41
1:A:235:LYS:HD3	1:A:239:LYS:HG3	2.03	0.41
1:A:572:ALA:HA	1:A:573:PRO:HD3	1.94	0.41
1:A:383:PRO:HD3	1:A:660:VAL:HG13	2.03	0.41
1:A:487:ARG:HA	1:A:487:ARG:HD3	1.81	0.41
1:A:175:ASN:ND2	1:A:180:LEU:HB2	2.32	0.40
1:A:288:HIS:O	1:A:419:ASN:HA	2.21	0.40
1:A:329:LYS:HE2	1:A:693:GLU:OE1	2.21	0.40
1:A:405:ARG:HA	1:A:795:THR:O	2.21	0.40
1:A:447:GLY:CA	1:A:546:GLU:H	2.34	0.40
1:A:725:ALA:HB1	1:A:815:LEU:HB2	2.03	0.40
1:A:332:LEU:HD22	1:A:415:GLY:CA	2.51	0.40
1:A:870:MET:O	1:A:874:VAL:HG23	2.20	0.40
1:A:327:LYS:HA	1:A:328:PRO:HD3	1.94	0.40
1:A:600:LEU:HA	1:A:601:PRO:HD3	1.96	0.40
1:A:966:ILE:HG13	5:A:3046:HOH:O	2.21	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	1279/1303 (98%)	1239 (97%)	39 (3%)	1 (0%)	48 40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	661	THR

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	1026/1040 (99%)	994 (97%)	32 (3%)	35 29

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	VAL
1	A	-3	ARG
1	A	169	GLN
1	A	206	LEU
1	A	218	ARG
1	A	253	LEU
1	A	294	GLU
1	A	296	HIS
1	A	332	LEU
1	A	358	ARG
1	A	382	ARG
1	A	410	PRO
1	A	429	GLU
1	A	471	GLN
1	A	508	LEU
1	A	553	LEU
1	A	588	LEU
1	A	611	LYS

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Mol	Chain	Res	Type
1	A	736	LEU
1	A	774	VAL
1	A	811	VAL
1	A	831	LEU
1	A	846	VAL
1	A	864	LYS
1	A	1088	LEU
1	A	1147	LEU
1	A	1173	GLU
1	A	1180	LEU
1	A	1190	MET
1	A	1195	SER
1	A	1245	THR
1	A	1251	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	39	HIS
1	A	52	GLN
1	A	68	HIS
1	A	96	HIS
1	A	123	GLN
1	A	175	ASN
1	A	191	GLN
1	A	211	GLN
1	A	216	HIS
1	A	219	HIS
1	A	243	ASN
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	592	HIS
1	A	596	GLN
1	A	739	ASN

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Mol	Chain	Res	Type
1	A	746	HIS
1	A	824	ASN
1	A	835	HIS
1	A	862	GLN
1	A	883	HIS
1	A	906	GLN
1	A	922	ASN
1	A	930	GLN
1	A	957	GLN
1	A	993	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1018	ASN
1	A	1026	ASN
1	A	1143	ASN
1	A	1189	GLN
1	A	1251	ASN
1	A	1260	HIS
1	A	1293	GLN

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	1.05	1 (8%)	10,17,19	3.62	4 (40%)

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	-	4/14/16/18	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	CYG	O1-C1	3.02	1.31	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1135	CYG	OE2-CD1-CG1	-6.93	115.99	123.98
1	A	1135	CYG	CG1-CD1-SG	6.33	120.95	113.40
1	A	1135	CYG	CB-SG-CD1	-5.43	93.30	100.76
1	A	1135	CYG	O2-C1-O1	-3.10	117.04	124.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1135	CYG	C-CA-CB-SG
1	A	1135	CYG	N-CA-CB-SG
1	A	1135	CYG	OE2-CD1-SG-CB
1	A	1135	CYG	CG1-CD1-SG-CB

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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	$\# Z > 2$
3	SO4	A	2010	-	4,4,4	0.42	0	6,6,6	0.17	0
3	SO4	A	2009	-	4,4,4	0.39	0	6,6,6	0.12	0
3	SO4	A	2002	-	4,4,4	0.41	0	6,6,6	0.15	0
3	SO4	A	2001	-	4,4,4	0.39	0	6,6,6	0.12	0
3	SO4	A	2012	-	4,4,4	0.41	0	6,6,6	0.17	0
4	ADP	A	2005	2	28,29,29	0.96	2 (7%)	43,45,45	1.31	4 (9%)
3	SO4	A	2011	-	4,4,4	0.39	0	6,6,6	0.12	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
4	ADP	A	2005	2	-	0/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2005	ADP	PA-O3A	2.36	1.62	1.59
4	A	2005	ADP	C4-N9	2.12	1.42	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2005	ADP	C2-N1-C6	4.04	125.36	118.73
4	A	2005	ADP	N3-C2-N1	-3.07	123.94	128.58
4	A	2005	ADP	C5-C4-N3	2.99	130.84	126.72
4	A	2005	ADP	O2B-PB-O3A	2.10	111.67	104.64

There are no chirality outliers.

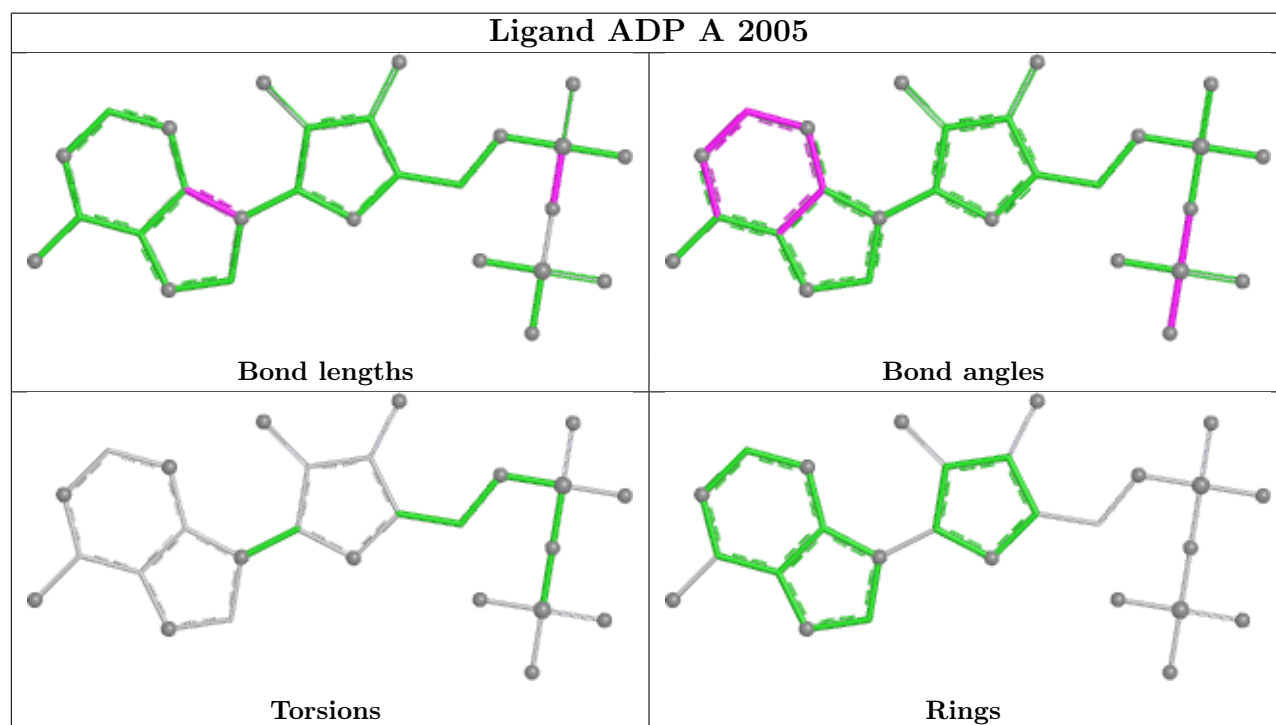
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2005	ADP	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

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	1283/1303 (98%)	0.25	84 (6%)	25 26	10, 20, 40, 67	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	GLY	7.0
1	A	118	THR	6.0
1	A	116	ALA	4.6
1	A	121	ALA	4.6
1	A	-1	SER	4.2
1	A	117	SER	4.2
1	A	6	ARG	4.1
1	A	25	ALA	4.1
1	A	791	GLN	4.1
1	A	31	HIS	4.0
1	A	119	LEU	3.8
1	A	467	PHE	3.8
1	A	152	HIS	3.7
1	A	259	ASN	3.6
1	A	789	ASN	3.6
1	A	790	GLU	3.6
1	A	1204	ARG	3.5
1	A	-7	GLY	3.4
1	A	125	ARG	3.4
1	A	611	LYS	3.4
1	A	358	ARG	3.3
1	A	969	ASN	3.3
1	A	24	GLN	3.2
1	A	788	GLY	3.2
1	A	69	THR	3.1
1	A	594	ASP	3.0
1	A	429	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	624	ASP	3.0
1	A	151	ILE	3.0
1	A	144	THR	3.0
1	A	623	GLY	2.9
1	A	787	GLU	2.9
1	A	1113	ASN	2.9
1	A	120	THR	2.8
1	A	26	ALA	2.8
1	A	-3	ARG	2.8
1	A	-4	PRO	2.8
1	A	276	ASN	2.7
1	A	774	VAL	2.7
1	A	66	SER	2.7
1	A	622	LYS	2.7
1	A	1208	HIS	2.7
1	A	1206	ASP	2.6
1	A	786	GLN	2.6
1	A	247	THR	2.6
1	A	129	ALA	2.6
1	A	154	GLN	2.5
1	A	-2	GLY	2.5
1	A	603	ASP	2.5
1	A	1295	GLY	2.4
1	A	583	GLU	2.4
1	A	28	LEU	2.4
1	A	588	LEU	2.4
1	A	619	LEU	2.4
1	A	970	ASP	2.4
1	A	22	ARG	2.4
1	A	122	GLU	2.4
1	A	32	ASN	2.4
1	A	442	PRO	2.3
1	A	852	ASP	2.3
1	A	184	GLU	2.3
1	A	-5	VAL	2.3
1	A	609	THR	2.3
1	A	27	ASN	2.3
1	A	156	ALA	2.2
1	A	582	GLU	2.2
1	A	1045	LEU	2.2
1	A	239	LYS	2.2
1	A	1279	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	-6	LEU	2.2
1	A	441	GLY	2.2
1	A	178	LEU	2.1
1	A	487	ARG	2.1
1	A	130	GLU	2.1
1	A	396	VAL	2.1
1	A	18	LYS	2.1
1	A	951	CYS	2.1
1	A	134	ARG	2.1
1	A	1245	THR	2.1
1	A	1144	LEU	2.1
1	A	1038	ALA	2.1
1	A	157	PRO	2.0
1	A	493	ASP	2.0
1	A	479	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(Å ²)	Q<0.9
1	CYG	A	1135	15/16	0.98	0.06	13,15,16,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

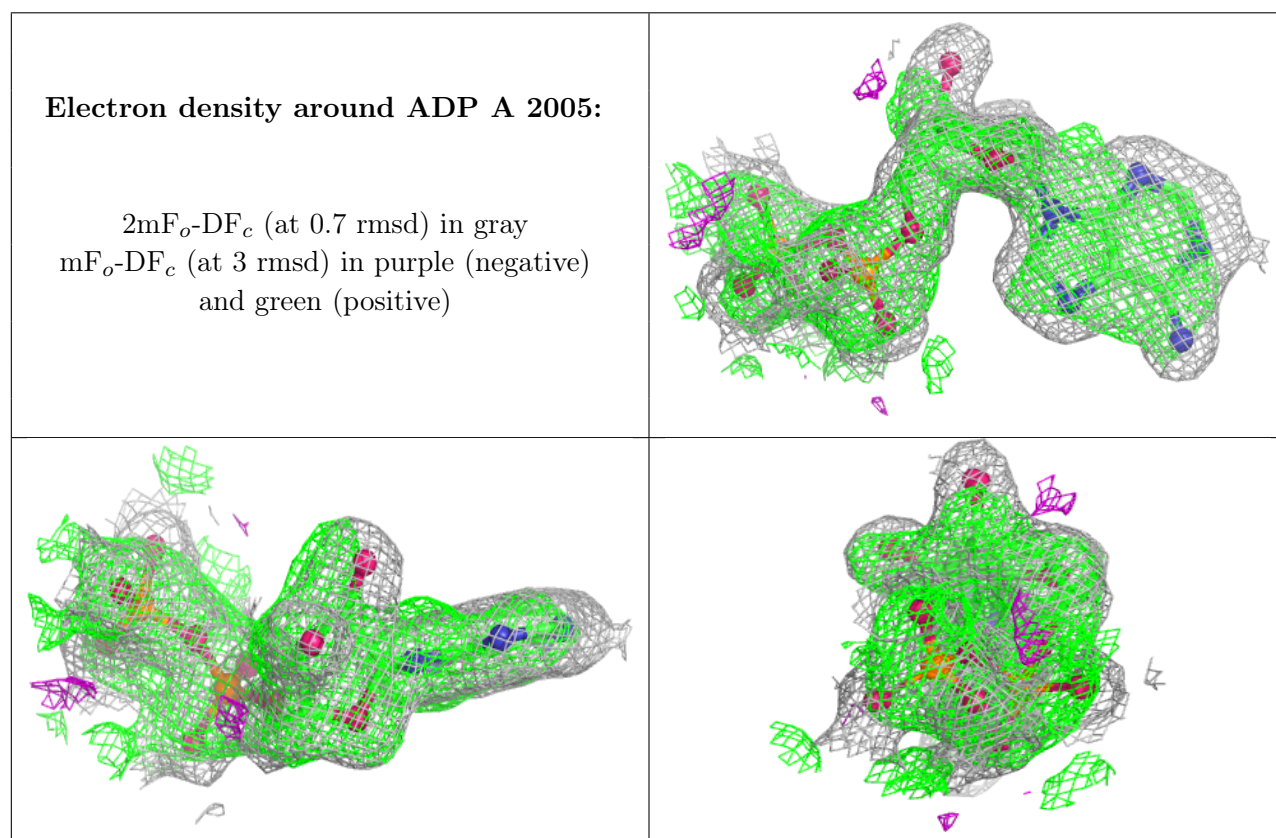
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	2001	5/5	0.92	0.14	41,41,43,44	0
3	SO4	A	2009	5/5	0.94	0.12	38,39,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	2011	5/5	0.95	0.13	41,42,43,43	0
4	ADP	A	2005	27/27	0.95	0.11	1,1,3,3	27
3	SO4	A	2002	5/5	0.96	0.08	23,25,27,27	0
3	SO4	A	2010	5/5	0.96	0.09	27,29,31,31	0
2	MG	A	2006	1/1	0.98	0.05	15,15,15,15	0
2	MG	A	2007	1/1	0.98	0.07	21,21,21,21	0
3	SO4	A	2012	5/5	0.98	0.07	32,32,33,33	0
2	MG	A	2008	1/1	0.98	0.10	19,19,19,19	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.