



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:11 AM GMT

PDB ID : 3OBK
Title : Crystal structure of delta-aminolevulinic acid dehydratase (porphobilinogen synthase) from toxoplasma gondii ME49 in complex with the reaction product porphobilinogen
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2010-08-06
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

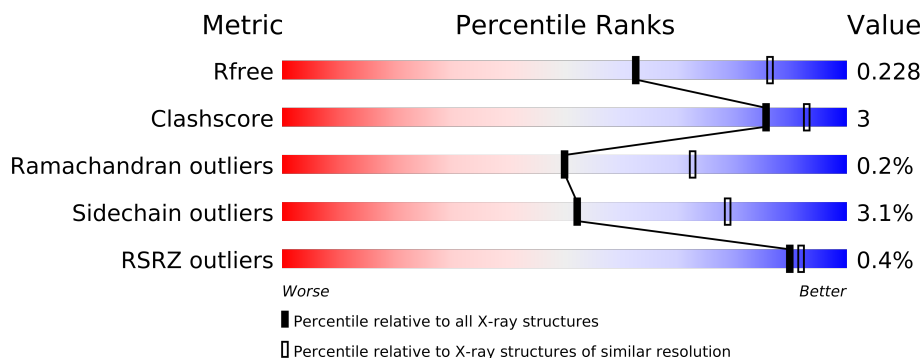
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	356	
1	B	356	
1	C	356	
1	D	356	
1	E	356	
1	F	356	
1	G	356	
1	H	356	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	F	365	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	PBG	D	360	-	X
5	EDO	A	380	-	X
5	EDO	A	385	-	X
5	EDO	B	370	-	X
5	EDO	C	370	-	X
5	EDO	D	370	-	X
5	EDO	E	375	-	X
5	EDO	E	390	-	X
5	EDO	G	375	-	X
5	EDO	G	385	-	X
5	EDO	G	390	-	X
5	EDO	H	385	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22298 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Delta-aminolevulinic acid dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2696	1694	457	522	23			
1	B	352	Total	C	N	O	S	0	0	0
			2676	1681	455	517	23			
1	C	352	Total	C	N	O	S	0	0	0
			2677	1680	454	522	21			
1	D	352	Total	C	N	O	S	0	0	0
			2674	1681	452	518	23			
1	E	352	Total	C	N	O	S	0	0	0
			2705	1699	457	526	23			
1	F	352	Total	C	N	O	S	0	1	0
			2692	1691	457	521	23			
1	G	352	Total	C	N	O	S	0	0	0
			2688	1686	455	524	23			
1	H	352	Total	C	N	O	S	0	0	0
			2676	1683	452	518	23			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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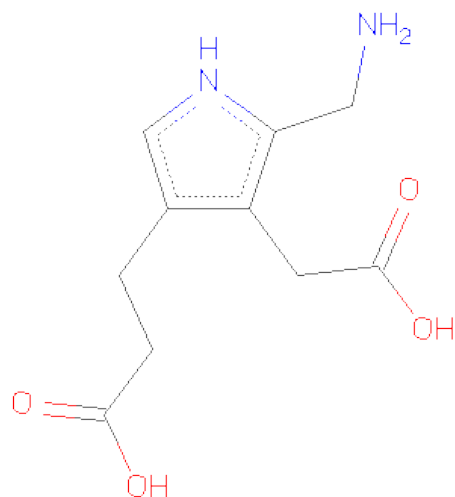
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

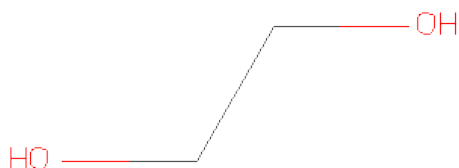
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total 3	Cl 3	0	0
3	D	2	Total 2	Cl 2	0	0
3	E	2	Total 2	Cl 2	0	0
3	H	1	Total 1	Cl 1	0	0
3	B	2	Total 2	Cl 2	0	0
3	C	2	Total 2	Cl 2	0	0
3	A	2	Total 2	Cl 2	0	0
3	F	2	Total 2	Cl 2	0	0

- Molecule 4 is 3-[5-(AMINOMETHYL)-4-(CARBOXYMETHYL)-1H-PYRROL-3-YL]PROPANOICACID (three-letter code: PBG) (formula: C₁₀H₁₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	10	2	4		
4	B	1	Total	C	N	O	0	0
			16	10	2	4		
4	C	1	Total	C	N	O	0	0
			16	10	2	4		
4	D	1	Total	C	N	O	0	0
			16	10	2	4		
4	E	1	Total	C	N	O	0	0
			16	10	2	4		
4	F	1	Total	C	N	O	0	0
			16	10	2	4		
4	G	1	Total	C	N	O	0	0
			16	10	2	4		
4	H	1	Total	C	N	O	0	0
			16	10	2	4		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	101	Total O 101 101	0	0
6	B	69	Total O 69 69	0	0
6	C	81	Total O 81 81	0	0
6	D	78	Total O 78 78	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	76	Total 76	O 76	0	0
6	F	59	Total 59	O 59	0	0
6	G	58	Total 58	O 58	0	0
6	H	64	Total 64	O 64	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

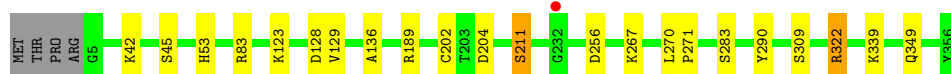
- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain A: 



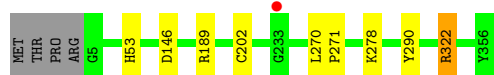
- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain B: 



- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain C: 



- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain D: 



- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain E: 

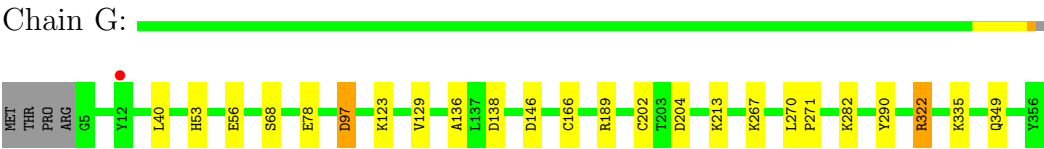


- Molecule 1: Delta-aminolevulinic acid dehydratase

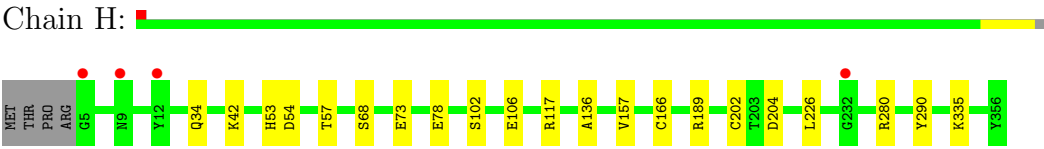
Chain F: 



● Molecule 1: Delta-aminolevulinic acid dehydratase



● Molecule 1: Delta-aminolevulinic acid dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	177.11Å 187.17Å 95.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 2.50 48.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.93-2.50) 98.3 (48.55-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.232 0.179 , 0.228	Depositor DCC
R_{free} test set	5439 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 3.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 108860 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22298	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 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PBG, EDO, CL

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	0.71	0/2748	0.79	5/3716 (0.1%)
1	B	0.71	0/2728	0.75	2/3691 (0.1%)
1	C	0.67	0/2729	0.74	1/3696 (0.0%)
1	D	0.67	1/2726 (0.0%)	0.75	1/3690 (0.0%)
1	E	0.70	0/2757	0.78	3/3727 (0.1%)
1	F	0.66	0/2747	0.74	1/3717 (0.0%)
1	G	0.66	0/2740	0.75	1/3706 (0.0%)
1	H	0.68	0/2728	0.76	0/3693
All	All	0.68	1/21903 (0.0%)	0.76	14/29636 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	304	GLU	CG-CD	5.24	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	27	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	E	322	ARG	CG-CD-NE	-6.32	98.54	111.80
1	A	322	ARG	CG-CD-NE	-6.23	98.71	111.80
1	B	322	ARG	CG-CD-NE	-5.82	99.57	111.80
1	E	69	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	117	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	G	322	ARG	CG-CD-NE	-5.70	99.84	111.80
1	F	322	ARG	CG-CD-NE	-5.63	99.98	111.80
1	B	322	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	256	ASP	CB-CG-OD1	5.16	122.94	118.30
1	D	27	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	117	ARG	NE-CZ-NH1	-5.08	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	322	ARG	CG-CD-NE	-5.05	101.19	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2696	0	0	5	0
1	B	2676	0	0	7	0
1	C	2677	0	0	2	0
1	D	2674	0	0	8	0
1	E	2705	0	0	8	0
1	F	2692	0	0	11	0
1	G	2688	0	0	11	0
1	H	2676	0	0	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
4	A	16	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	12	1	0
4	C	16	0	12	0	0
4	D	16	0	12	2	0
4	E	16	0	12	2	0
4	F	16	0	12	3	0
4	G	16	0	12	3	0
4	H	16	0	12	0	0
5	A	12	0	18	1	0
5	B	8	0	12	1	0
5	C	8	0	12	0	0
5	D	8	0	12	1	0
5	E	8	0	12	0	0
5	F	12	0	18	1	0
5	G	12	0	18	1	0
5	H	8	0	12	1	0
6	A	101	0	0	1	0
6	B	69	0	0	1	0
6	C	81	0	0	1	0
6	D	78	0	0	3	0
6	E	76	0	0	2	0
6	F	59	0	0	2	0
6	G	58	0	0	2	0
6	H	64	0	0	2	0
All	All	22298	0	210	58	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:202:CYS:SG	6:A:430:HOH:O	2.15	1.05
1:G:202:CYS:SG	6:G:402:HOH:O	2.23	0.95
1:F:166:CYS:SG	6:F:401:HOH:O	2.23	0.95
1:D:202:CYS:SG	6:D:404:HOH:O	2.27	0.93
1:F:202:CYS:SG	6:F:404:HOH:O	2.24	0.93
1:E:202:CYS:SG	6:E:408:HOH:O	2.31	0.88
1:H:166:CYS:SG	6:H:391:HOH:O	2.31	0.87
1:E:166:CYS:SG	6:E:409:HOH:O	2.34	0.82
1:C:202:CYS:SG	6:C:418:HOH:O	2.37	0.81
1:B:202:CYS:SG	6:B:401:HOH:O	2.39	0.78
1:G:166:CYS:SG	6:G:403:HOH:O	2.42	0.77
1:H:202:CYS:SG	6:H:390:HOH:O	2.50	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:166:CYS:SG	6:D:407:HOH:O	2.50	0.69
1:F:97:ASP:CB	1:F:99:GLU:OE2	2.43	0.67
1:G:123:LYS:NZ	1:G:129:VAL:O	2.28	0.66
1:D:267:LYS:NZ	4:D:360:PBG:C4A	2.62	0.63
1:B:267:LYS:NZ	4:B:360:PBG:C4A	2.63	0.61
1:F:78:GLU:OE2	1:F:335:LYS:NZ	2.32	0.61
1:G:68:SER:N	5:G:385:EDO:HO1	1.99	0.61
1:D:40:LEU:N	5:D:370:EDO:HO1	2.02	0.57
1:B:123:LYS:NZ	1:B:129:VAL:O	2.38	0.56
1:F:267:LYS:NZ	4:F:360:PBG:C4A	2.69	0.56
1:G:78:GLU:OE2	1:G:335:LYS:NZ	2.39	0.55
1:H:78:GLU:OE2	1:H:335:LYS:NZ	2.40	0.54
1:B:211:SER:OG	1:B:256:ASP:OD2	2.26	0.54
1:E:78:GLU:OE2	1:E:335:LYS:NZ	2.42	0.53
1:G:267:LYS:NZ	4:G:360:PBG:C4A	2.72	0.52
1:G:270:LEU:N	1:G:271:PRO:CD	2.73	0.52
1:A:138:ASP:OD2	4:A:360:PBG:HHA1	2.10	0.51
1:F:126:PHE:O	1:F:129:VAL:CG1	2.59	0.51
1:F:183:SER:OG	4:F:360:PBG:N1	2.41	0.49
1:G:138:ASP:OD2	4:G:360:PBG:HHA1	2.13	0.49
1:D:183:SER:OG	4:D:360:PBG:N1	2.47	0.48
1:E:138:ASP:OD2	4:E:360:PBG:HHA1	2.14	0.47
1:F:222:PHE:CD2	4:F:360:PBG:H8A2	2.50	0.47
1:A:68:SER:N	5:A:385:EDO:HO2	2.12	0.46
1:F:123:LYS:NZ	1:F:129:VAL:O	2.47	0.46
1:H:54:ASP:OD1	1:H:117:ARG:NH2	2.49	0.46
1:F:42:LYS:NZ	1:F:44:SER:OG	2.49	0.45
1:B:270:LEU:N	1:B:271:PRO:CD	2.80	0.45
1:E:267:LYS:NZ	4:E:360:PBG:C4A	2.80	0.45
1:E:310:GLU:OE1	1:E:333:TYR:OH	2.36	0.44
1:A:42:LYS:NZ	1:A:45:SER:OG	2.51	0.43
1:A:138:ASP:N	1:A:139:PRO:CD	2.82	0.43
5:B:370:EDO:HO2	1:E:40:LEU:N	2.17	0.43
1:D:88:LYS:NZ	1:H:34:GLN:OE1	2.52	0.43
1:D:69:ARG:NE	1:D:225:ALA:O	2.52	0.42
1:G:213:LYS:NZ	4:G:360:PBG:H12	2.16	0.42
1:G:97:ASP:N	1:G:97:ASP:OD1	2.51	0.42
1:E:42:LYS:NZ	1:E:45:SER:OG	2.53	0.41
1:C:270:LEU:N	1:C:271:PRO:CD	2.83	0.41
1:D:30:ARG:NH2	6:D:394:HOH:O	2.54	0.41
1:B:42:LYS:NZ	1:B:45:SER:OG	2.53	0.41
1:F:270:LEU:N	1:F:271:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:102:SER:OG	1:H:106:GLU:OE1	2.38	0.41
5:F:370:EDO:HO2	1:G:40:LEU:N	2.19	0.41
1:B:83:ARG:NH1	1:B:128:ASP:OD2	2.54	0.40
1:H:68:SER:N	5:H:385:EDO:HO2	2.19	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	350/356 (98%)	340 (97%)	9 (3%)	1 (0%)	50	73
1	B	350/356 (98%)	337 (96%)	12 (3%)	1 (0%)	50	73
1	C	350/356 (98%)	340 (97%)	10 (3%)	0	100	100
1	D	350/356 (98%)	336 (96%)	13 (4%)	1 (0%)	50	73
1	E	350/356 (98%)	339 (97%)	10 (3%)	1 (0%)	50	73
1	F	351/356 (99%)	340 (97%)	10 (3%)	1 (0%)	50	73
1	G	350/356 (98%)	335 (96%)	14 (4%)	1 (0%)	50	73
1	H	350/356 (98%)	338 (97%)	11 (3%)	1 (0%)	50	73
All	All	2801/2848 (98%)	2705 (97%)	89 (3%)	7 (0%)	50	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ALA
1	G	136	ALA
1	H	136	ALA
1	B	136	ALA
1	E	136	ALA
1	F	136	ALA
1	D	136	ALA

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	287/299 (96%)	277 (96%)	10 (4%)	48	74
1	B	280/299 (94%)	270 (96%)	10 (4%)	47	73
1	C	281/299 (94%)	275 (98%)	6 (2%)	66	88
1	D	281/299 (94%)	273 (97%)	8 (3%)	56	82
1	E	289/299 (97%)	281 (97%)	8 (3%)	56	82
1	F	284/299 (95%)	276 (97%)	8 (3%)	56	82
1	G	284/299 (95%)	274 (96%)	10 (4%)	48	74
1	H	282/299 (94%)	272 (96%)	10 (4%)	48	74
All	All	2268/2392 (95%)	2198 (97%)	70 (3%)	52	79

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	53	HIS
1	A	88	LYS
1	A	189	ARG
1	A	204	ASP
1	A	208	LEU
1	A	280	ARG
1	A	282	LYS
1	A	290	TYR
1	A	348	THR
1	B	53	HIS
1	B	189	ARG
1	B	204	ASP
1	B	211	SER
1	B	283	SER
1	B	290	TYR
1	B	309	SER
1	B	322	ARG
1	B	339	LYS
1	B	349	GLN
1	C	53	HIS

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Mol	Chain	Res	Type
1	C	146	ASP
1	C	189	ARG
1	C	278	LYS
1	C	290	TYR
1	C	322	ARG
1	D	53	HIS
1	D	92	LEU
1	D	128	ASP
1	D	189	ARG
1	D	226	LEU
1	D	290	TYR
1	D	322	ARG
1	D	348	THR
1	E	53	HIS
1	E	129	VAL
1	E	189	ARG
1	E	280	ARG
1	E	290	TYR
1	E	299	LEU
1	E	315	LEU
1	E	349	GLN
1	F	28	LYS
1	F	30	ARG
1	F	53	HIS
1	F	99	GLU
1	F	189	ARG
1	F	280	ARG
1	F	290	TYR
1	F	349	GLN
1	G	53	HIS
1	G	56	GLU
1	G	97	ASP
1	G	146	ASP
1	G	189	ARG
1	G	204	ASP
1	G	282	LYS
1	G	290	TYR
1	G	322	ARG
1	G	349	GLN
1	H	42	LYS
1	H	53	HIS
1	H	57	THR

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Mol	Chain	Res	Type
1	H	73	GLU
1	H	157	VAL
1	H	189	ARG
1	H	204	ASP
1	H	226	LEU
1	H	280	ARG
1	H	290	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 51 ligands modelled in this entry, 24 are monoatomic - leaving 27 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	$\# Z > 2$
4	PBG	A	360	-	16,16,16	1.15	0	20,21,21	1.80	5 (25%)
5	EDO	A	375	-	3,3,3	0.63	0	2,2,2	0.23	0
5	EDO	A	380	-	3,3,3	0.59	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	385	-	3,3,3	0.77	0	2,2,2	0.18	0
4	PBG	B	360	-	16,16,16	1.13	1 (6%)	20,21,21	1.85	5 (25%)
5	EDO	B	370	-	3,3,3	0.49	0	2,2,2	0.51	0
5	EDO	B	375	-	3,3,3	0.25	0	2,2,2	0.28	0
4	PBG	C	360	-	16,16,16	1.11	2 (12%)	20,21,21	1.70	5 (25%)
5	EDO	C	370	-	3,3,3	0.46	0	2,2,2	0.48	0
5	EDO	C	375	-	3,3,3	0.49	0	2,2,2	0.41	0
4	PBG	D	360	-	16,16,16	1.01	1 (6%)	20,21,21	1.86	6 (30%)
5	EDO	D	370	-	3,3,3	0.76	0	2,2,2	0.25	0
5	EDO	D	375	-	3,3,3	0.47	0	2,2,2	0.19	0
4	PBG	E	360	-	16,16,16	1.13	2 (12%)	20,21,21	1.97	6 (30%)
5	EDO	E	375	-	3,3,3	0.48	0	2,2,2	0.12	0
5	EDO	E	390	-	3,3,3	0.81	0	2,2,2	0.19	0
4	PBG	F	360	-	16,16,16	0.95	0	20,21,21	2.00	5 (25%)
5	EDO	F	370	-	3,3,3	0.40	0	2,2,2	0.49	0
5	EDO	F	375	-	3,3,3	0.54	0	2,2,2	0.35	0
5	EDO	F	385	-	3,3,3	0.69	0	2,2,2	0.10	0
4	PBG	G	360	-	16,16,16	1.10	1 (6%)	20,21,21	1.79	4 (20%)
5	EDO	G	375	-	3,3,3	0.48	0	2,2,2	0.27	0
5	EDO	G	385	-	3,3,3	0.59	0	2,2,2	0.15	0
5	EDO	G	390	-	3,3,3	0.86	0	2,2,2	0.14	0
4	PBG	H	360	-	16,16,16	1.25	2 (12%)	20,21,21	1.67	5 (25%)
5	EDO	H	375	-	3,3,3	0.53	0	2,2,2	0.30	0
5	EDO	H	385	-	3,3,3	0.44	0	2,2,2	0.50	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	PBG	A	360	-	-	0/9/11/11	0/1/1/1
5	EDO	A	375	-	-	0/1/1/1	0/0/0/0
5	EDO	A	380	-	-	0/1/1/1	0/0/0/0
5	EDO	A	385	-	-	0/1/1/1	0/0/0/0
4	PBG	B	360	-	-	0/9/11/11	0/1/1/1
5	EDO	B	370	-	-	0/1/1/1	0/0/0/0
5	EDO	B	375	-	-	0/1/1/1	0/0/0/0
4	PBG	C	360	-	-	0/9/11/11	0/1/1/1
5	EDO	C	370	-	-	0/1/1/1	0/0/0/0
5	EDO	C	375	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PBG	D	360	-	-	0/9/11/11	0/1/1/1
5	EDO	D	370	-	-	0/1/1/1	0/0/0/0
5	EDO	D	375	-	-	0/1/1/1	0/0/0/0
4	PBG	E	360	-	-	0/9/11/11	0/1/1/1
5	EDO	E	375	-	-	0/1/1/1	0/0/0/0
5	EDO	E	390	-	-	0/1/1/1	0/0/0/0
4	PBG	F	360	-	-	0/9/11/11	0/1/1/1
5	EDO	F	370	-	-	0/1/1/1	0/0/0/0
5	EDO	F	375	-	-	0/1/1/1	0/0/0/0
5	EDO	F	385	-	-	0/1/1/1	0/0/0/0
4	PBG	G	360	-	-	0/9/11/11	0/1/1/1
5	EDO	G	375	-	-	0/1/1/1	0/0/0/0
5	EDO	G	385	-	-	0/1/1/1	0/0/0/0
5	EDO	G	390	-	-	0/1/1/1	0/0/0/0
4	PBG	H	360	-	-	0/9/11/11	0/1/1/1
5	EDO	H	375	-	-	0/1/1/1	0/0/0/0
5	EDO	H	385	-	-	0/1/1/1	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	360	PBG	C4A-NA	-2.47	1.33	1.36
4	G	360	PBG	C4A-NA	-2.46	1.33	1.36
4	C	360	PBG	C4A-NA	-2.39	1.33	1.36
4	H	360	PBG	C1A-C2A	2.30	1.41	1.37
4	E	360	PBG	C1A-C2A	2.25	1.41	1.37
4	H	360	PBG	C4A-NA	-2.18	1.33	1.36
4	E	360	PBG	C4A-NA	-2.17	1.33	1.36
4	D	360	PBG	C4A-NA	-2.14	1.34	1.36
4	C	360	PBG	C1A-NA	-2.06	1.33	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	360	PBG	C2A-C1A-NA	4.52	109.37	105.77
4	G	360	PBG	C2A-C5A-C6A	4.41	121.88	113.95
4	E	360	PBG	C2A-C5A-C6A	4.32	121.70	113.95
4	D	360	PBG	C2A-C5A-C6A	4.24	121.57	113.95
4	A	360	PBG	C2A-C1A-NA	4.22	109.13	105.77
4	F	360	PBG	C2A-C5A-C6A	4.05	121.22	113.95
4	C	360	PBG	C2A-C1A-NA	3.97	108.93	105.77
4	G	360	PBG	C2A-C1A-NA	3.97	108.93	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	360	PBG	C2A-C1A-NA	3.94	108.91	105.77
4	F	360	PBG	C8A-C7A-C3A	3.85	121.31	112.24
4	B	360	PBG	C2A-C5A-C6A	3.72	120.63	113.95
4	D	360	PBG	C2A-C1A-NA	3.42	108.49	105.77
4	H	360	PBG	C2A-C5A-C6A	3.36	119.98	113.95
4	E	360	PBG	C2A-C1A-NA	3.33	108.42	105.77
4	H	360	PBG	C2A-C1A-NA	3.19	108.31	105.77
4	C	360	PBG	C2A-C5A-C6A	3.14	119.58	113.95
4	E	360	PBG	C8A-C7A-C3A	2.85	118.96	112.24
4	B	360	PBG	O2A-C6A-C5A	2.73	120.66	113.80
4	A	360	PBG	O4A-C9A-C8A	2.66	123.61	114.22
4	D	360	PBG	C4A-NA-C1A	2.63	110.17	108.59
4	A	360	PBG	O1A-C6A-C5A	-2.61	116.78	123.19
4	H	360	PBG	C4A-NA-C1A	2.58	110.14	108.59
4	E	360	PBG	O4A-C9A-C8A	2.52	123.13	114.22
4	B	360	PBG	C4A-NA-C1A	2.52	110.10	108.59
4	A	360	PBG	O2A-C6A-C5A	2.50	120.07	113.80
4	B	360	PBG	C7A-C3A-C4A	-2.49	123.86	128.12
4	D	360	PBG	C8A-C7A-C3A	2.48	118.09	112.24
4	A	360	PBG	O4A-C9A-O3A	-2.39	117.21	123.30
4	F	360	PBG	O2A-C6A-C5A	2.37	119.76	113.80
4	C	360	PBG	C8A-C7A-C3A	2.37	117.82	112.24
4	E	360	PBG	C4A-NA-C1A	2.34	109.99	108.59
4	E	360	PBG	O2A-C6A-C5A	2.33	119.64	113.80
4	H	360	PBG	C8A-C7A-C3A	2.32	117.70	112.24
4	G	360	PBG	C8A-C7A-C3A	2.27	117.59	112.24
4	G	360	PBG	C7A-C3A-C4A	-2.24	124.28	128.12
4	C	360	PBG	O1A-C6A-C5A	-2.23	117.71	123.19
4	D	360	PBG	O4A-C9A-C8A	2.19	121.96	114.22
4	C	360	PBG	O2A-C6A-C5A	2.18	119.26	113.80
4	F	360	PBG	CHA-C1A-C2A	-2.12	125.96	129.51
4	H	360	PBG	O2A-C6A-C5A	2.10	119.06	113.80
4	D	360	PBG	O4A-C9A-O3A	-2.05	118.07	123.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	352/356 (98%)	-0.59	2 (0%) 86 88	9, 17, 33, 60	0
1	B	352/356 (98%)	-0.38	1 (0%) 91 93	9, 22, 39, 47	0
1	C	352/356 (98%)	-0.50	1 (0%) 91 93	8, 20, 40, 52	0
1	D	352/356 (98%)	-0.42	1 (0%) 91 93	10, 23, 41, 46	0
1	E	352/356 (98%)	-0.49	1 (0%) 91 93	9, 22, 43, 52	0
1	F	352/356 (98%)	-0.46	0 100 100	10, 23, 44, 53	0
1	G	352/356 (98%)	-0.42	1 (0%) 91 93	10, 23, 46, 57	0
1	H	352/356 (98%)	-0.43	4 (1%) 77 79	10, 24, 44, 58	0
All	All	2816/2848 (98%)	-0.46	11 (0%) 90 92	8, 22, 43, 60	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	12	TYR	4.1
1	C	233	GLY	3.1
1	B	232	GLY	3.0
1	D	232	GLY	2.9
1	G	12	TYR	2.9
1	H	12	TYR	2.9
1	H	232	GLY	2.7
1	H	9	ASN	2.7
1	H	5	GLY	2.3
1	A	6	PRO	2.2
1	A	13	GLY	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	H	385	4/4	0.21	7.04	34,35,38,41	0
5	EDO	C	370	4/4	0.21	6.39	30,31,31,32	0
5	EDO	G	390	4/4	0.13	4.40	29,29,30,31	0
5	EDO	E	375	4/4	0.19	4.29	19,21,21,24	0
5	EDO	E	390	4/4	0.13	4.20	31,32,32,34	0
2	MG	F	365	1/1	0.16	3.76	35,35,35,35	0
5	EDO	B	370	4/4	0.17	3.69	26,26,27,27	0
5	EDO	G	375	4/4	0.15	3.37	23,23,24,24	0
5	EDO	A	380	4/4	0.24	3.26	54,55,55,55	0
5	EDO	G	385	4/4	0.19	2.88	32,32,32,32	0
4	PBG	D	360	16/16	0.17	2.62	26,32,35,36	0
5	EDO	A	385	4/4	0.13	2.51	15,18,20,22	0
5	EDO	D	370	4/4	0.14	2.07	30,33,33,34	0
5	EDO	B	375	4/4	0.15	1.79	13,14,15,16	0
4	PBG	E	360	16/16	0.13	1.77	20,26,32,34	0
4	PBG	A	360	16/16	0.12	1.76	9,18,21,22	0
5	EDO	F	370	4/4	0.13	1.72	20,22,23,24	0
4	PBG	C	360	16/16	0.13	1.70	20,24,28,28	0
5	EDO	F	385	4/4	0.12	1.47	28,32,32,34	0
4	PBG	G	360	16/16	0.13	1.06	19,29,32,34	0
5	EDO	C	375	4/4	0.14	1.03	11,12,14,14	0
5	EDO	D	375	4/4	0.12	0.97	11,12,12,13	0
5	EDO	F	375	4/4	0.14	0.86	17,18,19,19	0
5	EDO	A	375	4/4	0.12	0.69	14,15,16,16	0
3	CL	G	357	1/1	0.11	0.42	52,52,52,52	0
3	CL	G	400	1/1	0.09	0.35	43,43,43,43	0
3	CL	G	395	1/1	0.17	0.35	54,54,54,54	0
5	EDO	H	375	4/4	0.12	0.34	17,19,19,19	0
4	PBG	B	360	16/16	0.13	0.29	20,33,36,36	0
3	CL	F	397	1/1	0.16	0.23	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	H	400	1/1	0.10	0.13	55,55,55,55	0
4	PBG	F	360	16/16	0.12	0.13	14,27,32,32	0
3	CL	C	395	1/1	0.12	0.07	62,62,62,62	0
3	CL	D	405	1/1	0.12	-0.01	40,40,40,40	0
4	PBG	H	360	16/16	0.11	-0.02	19,27,31,32	0
3	CL	A	405	1/1	0.11	-0.17	47,47,47,47	0
3	CL	F	400	1/1	0.13	-0.35	50,50,50,50	0
3	CL	B	405	1/1	0.11	-0.36	39,39,39,39	0
3	CL	C	400	1/1	0.11	-0.51	59,59,59,59	0
3	CL	E	395	1/1	0.08	-1.04	52,52,52,52	0
3	CL	E	400	1/1	0.10	-1.84	57,57,57,57	0
2	MG	G	365	1/1	0.07	-2.07	34,34,34,34	0
2	MG	E	365	1/1	0.08	-2.14	31,31,31,31	0
2	MG	D	365	1/1	0.07	-2.37	32,32,32,32	0
2	MG	C	365	1/1	0.07	-2.52	17,17,17,17	0
3	CL	A	400	1/1	0.06	-3.79	49,49,49,49	0
2	MG	B	365	1/1	0.04	-3.81	20,20,20,20	0
3	CL	D	400	1/1	0.09	-4.16	50,50,50,50	0
2	MG	A	365	1/1	0.04	-4.20	16,16,16,16	0
2	MG	H	365	1/1	0.05	-4.50	21,21,21,21	0
3	CL	B	400	1/1	0.08	-5.75	50,50,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.