



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:20 AM UTC

PDB ID : 3OBK / pdb_00003obk
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 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

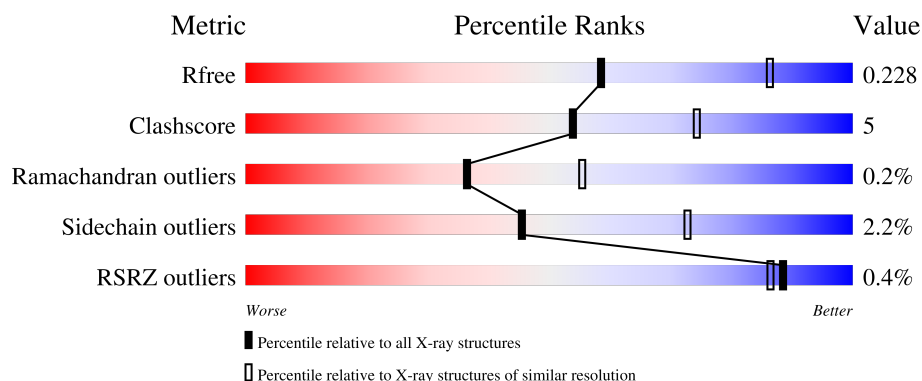
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	356	% 89% 9% .
1	B	356	86% 12% ..
1	C	356	% 88% 11% .
1	D	356	85% 14% .
1	E	356	83% 15% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	356	 83% 15% ..
1	G	356	 84% 13% ..
1	H	356	 89% 9% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22298 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 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 (CCD ID: MG) (formula: Mg).

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

Continued on next page...

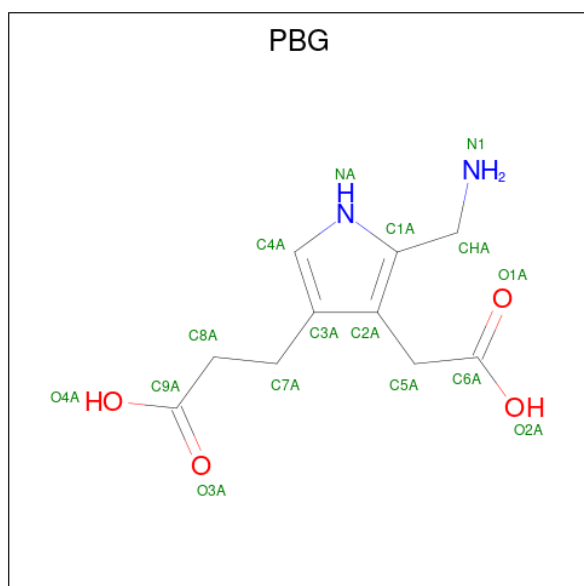
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Mg 1	0	0
2	H	1	Total 1	Mg 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

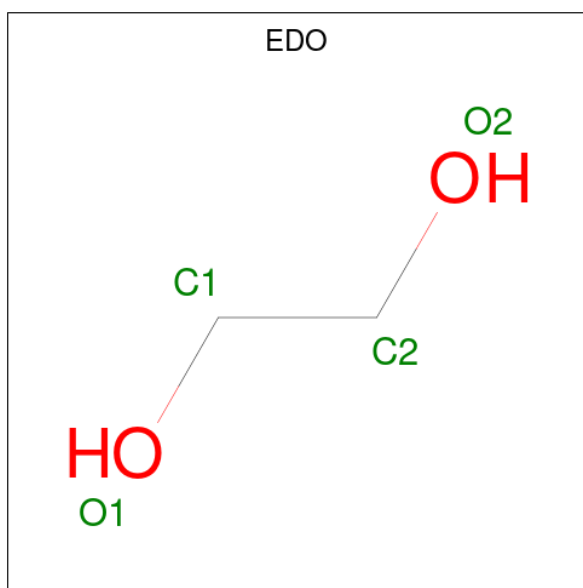
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Cl 2	0	0
3	B	2	Total 2	Cl 2	0	0
3	C	2	Total 2	Cl 2	0	0
3	D	2	Total 2	Cl 2	0	0
3	E	2	Total 2	Cl 2	0	0
3	F	2	Total 2	Cl 2	0	0
3	G	3	Total 3	Cl 3	0	0
3	H	1	Total 1	Cl 1	0	0

- Molecule 4 is 3-[5-(AMINOMETHYL)-4-(CARBOXYMETHYL)-1H-PYRROL-3-YL]PROPANOIC ACID (CCD ID: 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 (CCD ID: 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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

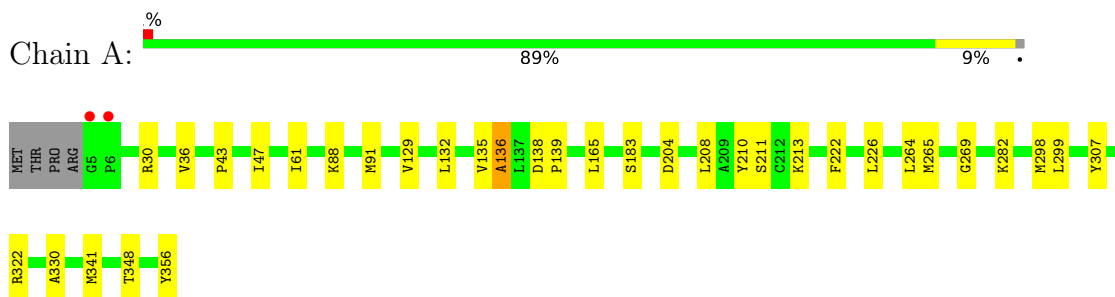
Continued from previous page...

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

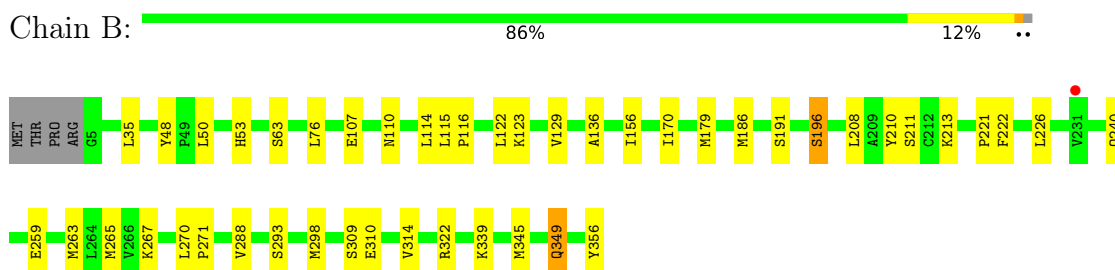
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

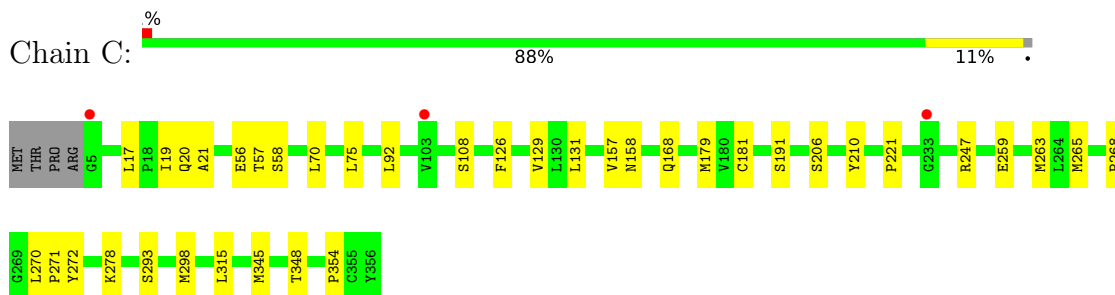
- Molecule 1: Delta-aminolevulinic acid dehydratase



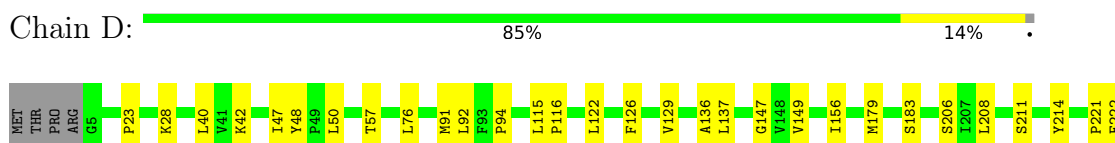
- Molecule 1: Delta-aminolevulinic acid dehydratase



- Molecule 1: Delta-aminolevulinic acid dehydratase



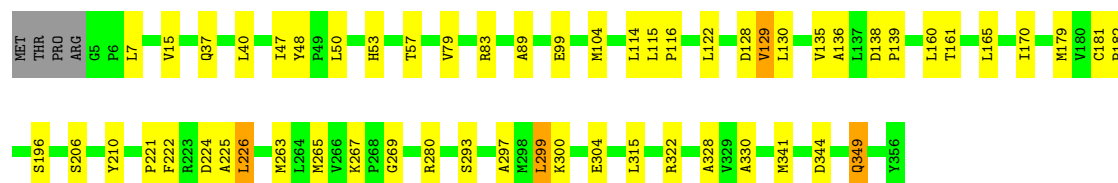
- Molecule 1: Delta-aminolevulinic acid dehydratase





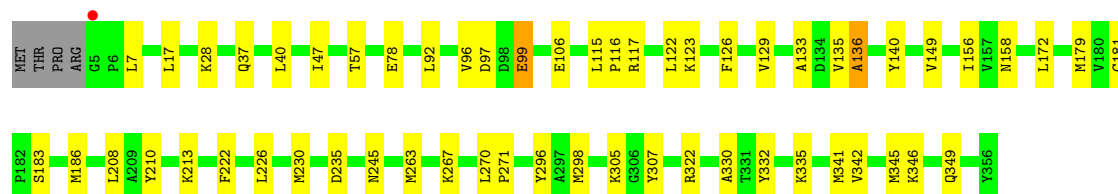
- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain E: 83% 15% ..



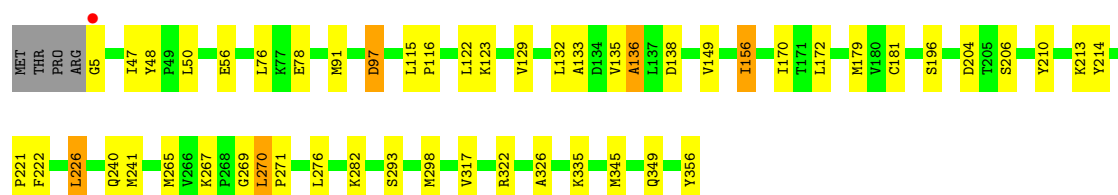
- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain F: 83% 15% ..



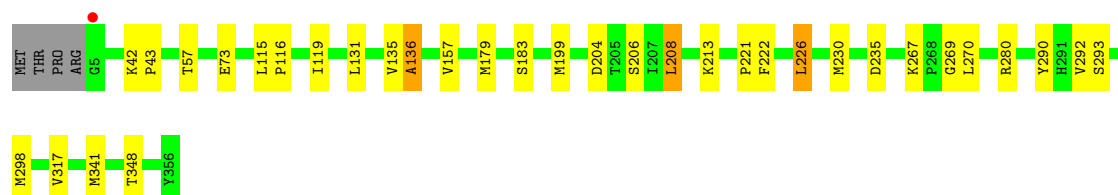
- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain G: 84% 13% ..



- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain H: 89% 9% ..



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 49.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.93-2.50) 98.3 (49.93-2.50)	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 (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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: CL, EDO, PBG, 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	0.90	1/2748 (0.0%)	0.95	3/3716 (0.1%)
1	B	0.88	0/2728	0.91	1/3691 (0.0%)
1	C	0.85	0/2729	0.91	1/3696 (0.0%)
1	D	0.87	0/2726	0.93	2/3690 (0.1%)
1	E	0.87	0/2757	0.92	2/3727 (0.1%)
1	F	0.84	0/2747	0.92	3/3717 (0.1%)
1	G	0.83	0/2740	0.93	4/3706 (0.1%)
1	H	0.86	0/2728	0.93	2/3693 (0.1%)
All	All	0.86	1/21903 (0.0%)	0.92	18/29636 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	VAL	CA-CB	5.43	1.59	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	269	GLY	N-CA-C	7.79	117.30	110.21
1	G	269	GLY	N-CA-C	7.06	116.64	110.21
1	H	292	VAL	N-CA-C	6.44	117.49	110.21
1	H	269	GLY	N-CA-C	6.42	116.06	110.21
1	A	269	GLY	N-CA-C	6.13	115.79	110.21
1	E	322	ARG	CG-CD-NE	-6.12	98.54	112.00
1	A	322	ARG	CG-CD-NE	-6.04	98.71	112.00
1	E	269	GLY	N-CA-C	5.91	115.59	110.21
1	A	61	ILE	CA-C-O	5.75	122.34	119.12
1	B	322	ARG	CG-CD-NE	-5.65	99.57	112.00
1	G	322	ARG	CG-CD-NE	-5.53	99.84	112.00
1	F	322	ARG	CG-CD-NE	-5.46	99.98	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	LYS	N-CA-C	5.44	117.92	111.33
1	C	158	ASN	N-CA-C	5.44	116.90	110.97
1	F	158	ASN	N-CA-C	5.20	116.75	111.14
1	F	245	ASN	N-CA-C	5.16	117.38	109.07
1	G	270	LEU	CA-C-N	-5.12	115.61	120.83
1	G	270	LEU	C-N-CA	-5.12	115.61	120.83

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	2696	0	2653	19	0
1	B	2676	0	2608	31	0
1	C	2677	0	2601	22	0
1	D	2674	0	2609	33	0
1	E	2705	0	2663	31	0
1	F	2692	0	2632	37	0
1	G	2688	0	2619	35	0
1	H	2676	0	2616	19	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	1	0
3	G	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
4	A	16	0	12	1	0
4	B	16	0	12	2	0
4	C	16	0	12	0	0
4	D	16	0	12	4	0
4	E	16	0	12	3	0
4	F	16	0	12	4	0
4	G	16	0	12	5	0
4	H	16	0	12	1	0
5	A	12	0	18	0	0
5	B	8	0	12	0	0
5	C	8	0	12	0	0
5	D	8	0	12	0	0
5	E	8	0	12	0	0
5	F	12	0	18	0	0
5	G	12	0	18	0	0
5	H	8	0	12	0	0
6	A	101	0	0	0	0
6	B	69	0	0	0	0
6	C	81	0	0	0	0
6	D	78	0	0	0	0
6	E	76	0	0	0	0
6	F	59	0	0	0	0
6	G	58	0	0	0	0
6	H	64	0	0	1	0
All	All	22298	0	21211	211	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 5.

All (211) 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:F:126:PHE:O	1:F:129:VAL:HG12	1.72	0.90
1:D:267:LYS:HZ1	4:D:360:PBG:C4A	2.03	0.72
1:G:149:VAL:HG12	1:G:156:ILE:HD12	1.71	0.72
1:D:149:VAL:HG22	1:D:156:ILE:CD1	2.20	0.71
1:F:179:MET:HE2	1:F:208:LEU:HB2	1.74	0.69
1:B:76:LEU:HD23	1:B:122:LEU:HD23	1.75	0.68
1:F:97:ASP:CB	1:F:99:GLU:OE2	2.43	0.67
1:D:47:ILE:HG21	1:D:91:MET:CE	2.25	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:MET:HG2	1:C:206:SER:HB2	1.76	0.66
1:G:123:LYS:NZ	1:G:129:VAL:O	2.28	0.66
1:D:47:ILE:HG21	1:D:91:MET:HE3	1.78	0.65
1:E:104:MET:HE1	1:E:160:LEU:HD21	1.78	0.65
1:D:267:LYS:NZ	4:D:360:PBG:C4A	2.62	0.63
1:B:267:LYS:HZ1	4:B:360:PBG:C4A	2.12	0.62
1:G:267:LYS:HZ1	4:G:360:PBG:C4A	2.12	0.62
1:H:222:PHE:CZ	1:H:226:LEU:HD22	2.34	0.61
1:B:179:MET:HE2	1:B:208:LEU:HB2	1.82	0.61
1:B:267:LYS:NZ	4:B:360:PBG:C4A	2.63	0.61
1:C:345:MET:HE1	1:C:354:PRO:HD3	1.82	0.61
1:E:161:THR:O	1:E:165:LEU:HG	2.00	0.61
1:E:267:LYS:HZ1	4:E:360:PBG:C4A	2.14	0.61
1:B:345:MET:HE3	1:B:349:GLN:OE1	2.02	0.60
1:D:149:VAL:HG22	1:D:156:ILE:HD12	1.83	0.59
1:G:76:LEU:HD22	1:G:122:LEU:HD23	1.85	0.58
1:D:47:ILE:CG2	1:D:91:MET:HE3	2.33	0.57
1:D:179:MET:HE1	1:D:263:MET:HE3	1.84	0.57
1:B:310:GLU:O	1:B:314:VAL:HG23	2.05	0.57
1:G:181:CYS:HB3	1:G:210:TYR:HE1	1.70	0.57
1:D:115:LEU:HB3	1:D:116:PRO:HD3	1.86	0.56
1:B:123:LYS:NZ	1:B:129:VAL:O	2.38	0.56
1:F:92:LEU:HD11	1:F:122:LEU:HD12	1.86	0.56
1:G:115:LEU:HB3	1:G:116:PRO:HD3	1.87	0.56
1:B:76:LEU:CD2	1:B:122:LEU:HD23	2.35	0.56
1:A:299:LEU:HG	1:B:298:MET:HE3	1.88	0.56
1:F:267:LYS:NZ	4:F:360:PBG:C4A	2.69	0.56
1:G:149:VAL:HG12	1:G:156:ILE:CD1	2.36	0.55
1:H:179:MET:HE1	1:H:208:LEU:HB2	1.88	0.55
1:H:179:MET:HG2	1:H:206:SER:HB2	1.88	0.55
1:D:214:TYR:CE2	1:D:241:MET:HE2	2.41	0.55
1:G:48:TYR:CE2	1:G:50:LEU:HD21	2.42	0.55
1:E:179:MET:HE1	1:E:263:MET:HE3	1.89	0.55
1:F:345:MET:HE2	3:F:397:CL:CL	2.44	0.55
1:F:7:LEU:HD23	1:F:17:LEU:HD13	1.89	0.54
1:A:36:VAL:CG1	1:C:263:MET:HE2	2.38	0.54
1:B:191:SER:HB2	1:B:259:GLU:HG2	1.88	0.54
1:E:300:LYS:O	1:E:304:GLU:HG3	2.08	0.54
1:E:344:ASP:OD2	1:E:349:GLN:HA	2.07	0.54
1:B:76:LEU:HD23	1:B:122:LEU:CD2	2.37	0.54
1:F:179:MET:HE1	1:F:263:MET:HE3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:PHE:O	1:C:129:VAL:HG12	2.08	0.53
1:E:179:MET:HE3	1:E:206:SER:HB3	1.89	0.53
1:A:298:MET:HB3	1:B:298:MET:HB3	1.89	0.53
1:B:222:PHE:CE1	1:B:226:LEU:HD22	2.44	0.53
1:F:115:LEU:HB3	1:F:116:PRO:HD3	1.90	0.53
1:C:268:PRO:HD2	1:C:272:TYR:CE2	2.44	0.53
1:D:40:LEU:HD11	1:H:42:LYS:HD3	1.91	0.53
1:H:115:LEU:HB3	1:H:116:PRO:HD3	1.91	0.53
1:F:78:GLU:OE2	1:F:335:LYS:NZ	2.32	0.52
1:F:267:LYS:HZ1	4:F:360:PBG:C4A	2.22	0.52
1:B:179:MET:HE1	1:B:263:MET:HE3	1.91	0.52
1:G:267:LYS:NZ	4:G:360:PBG:C4A	2.72	0.52
1:H:230:MET:HE3	1:H:235:ASP:HA	1.92	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:149:VAL:HG22	1:F:156:ILE:HD12	1.90	0.51
1:F:230:MET:HE3	1:F:235:ASP:HA	1.92	0.51
1:G:47:ILE:HG21	1:G:91:MET:HE3	1.91	0.51
1:A:47:ILE:HB	1:A:330:ALA:HA	1.92	0.51
1:F:213:LYS:HZ2	1:F:267:LYS:NZ	2.09	0.51
1:F:222:PHE:CE1	1:F:226:LEU:HD22	2.46	0.51
1:B:170:ILE:HD11	1:B:196:SER:HB2	1.91	0.51
1:D:310:GLU:O	1:D:314:VAL:HG23	2.11	0.51
1:G:78:GLU:OE2	1:G:335:LYS:NZ	2.39	0.51
1:F:99:GLU:H	1:F:99:GLU:CD	2.19	0.51
1:F:117[B]:ARG:HG2	1:F:117[B]:ARG:HH11	1.76	0.51
1:D:94:PRO:HG3	1:D:115:LEU:HD22	1.92	0.50
1:B:156:ILE:N	1:B:156:ILE:HD12	2.27	0.50
1:C:221:PRO:HB2	1:C:293:SER:HB2	1.93	0.50
1:D:230:MET:HE3	1:D:235:ASP:HA	1.94	0.50
1:H:267:LYS:HG3	1:H:290:TYR:HB3	1.93	0.50
1:D:126:PHE:O	1:D:129:VAL:HG12	2.12	0.49
1:F:183:SER:OG	4:F:360:PBG:N1	2.41	0.49
1:G:213:LYS:HE2	1:G:240:GLN:NE2	2.28	0.49
1:D:42:LYS:HA	1:D:341:MET:HE1	1.93	0.49
1:E:48:TYR:CE2	1:E:50:LEU:HD21	2.48	0.49
1:E:181:CYS:HB3	1:E:210:TYR:HE1	1.78	0.49
1:G:138:ASP:OD2	4:G:360:PBG:HHA1	2.13	0.49
1:B:48:TYR:CE2	1:B:50:LEU:HD21	2.47	0.49
1:E:79:VAL:HG21	1:E:122:LEU:CD2	2.43	0.49
1:D:222:PHE:CZ	1:D:226:LEU:HD22	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:GLN:NE2	1:E:40:LEU:HD23	2.28	0.48
1:E:83:ARG:HH12	1:E:128:ASP:CG	2.21	0.48
1:D:179:MET:HE1	1:D:263:MET:CE	2.43	0.48
1:F:341:MET:HE3	1:G:356:TYR:HD2	1.77	0.48
1:G:270:LEU:HD11	1:G:317:VAL:HG22	1.95	0.48
1:F:179:MET:HE1	1:F:263:MET:SD	2.52	0.48
1:A:211:SER:OG	1:A:264:LEU:HD22	2.12	0.48
1:D:179:MET:HE1	1:D:263:MET:SD	2.53	0.48
1:D:183:SER:OG	4:D:360:PBG:N1	2.47	0.48
1:B:356:TYR:HD2	1:E:341:MET:HE3	1.78	0.48
1:G:222:PHE:CZ	1:G:226:LEU:HD22	2.49	0.48
1:G:345:MET:HE3	1:G:345:MET:HA	1.96	0.48
1:A:135:VAL:O	1:A:136:ALA:HB2	2.15	0.47
1:E:53:HIS:HA	1:E:114:LEU:HD21	1.95	0.47
1:C:92:LEU:HD11	1:C:131:LEU:HD22	1.95	0.47
1:G:213:LYS:HZ3	4:G:360:PBG:H12	1.62	0.47
1:E:222:PHE:CZ	1:E:226:LEU:HD22	2.49	0.47
1:G:298:MET:HE2	1:H:298:MET:HE2	1.96	0.47
1:A:135:VAL:HG12	1:A:165:LEU:HD22	1.96	0.47
1:E:138:ASP:OD2	4:E:360:PBG:HHA1	2.14	0.47
1:F:296:TYR:CD1	1:F:332:TYR:HB2	2.50	0.47
1:A:210:TYR:CD2	1:A:265:MET:HG2	2.49	0.47
1:B:115:LEU:HB3	1:B:116:PRO:HD3	1.96	0.47
1:C:247:ARG:HD2	6:H:506:HOH:O	2.14	0.47
1:F:222:PHE:CD2	4:F:360:PBG:H8A2	2.50	0.47
1:H:43:PRO:HD3	1:H:341:MET:CE	2.45	0.47
1:C:210:TYR:HA	1:C:265:MET:HB3	1.97	0.46
1:D:48:TYR:CE2	1:D:50:LEU:HD21	2.50	0.46
1:F:123:LYS:NZ	1:F:129:VAL:O	2.47	0.46
1:A:91:MET:HA	1:A:132:LEU:O	2.16	0.46
1:C:108:SER:O	1:C:168:GLN:HG3	2.16	0.46
1:D:208:LEU:HD11	1:D:265:MET:HB2	1.97	0.46
1:D:345:MET:HE3	1:D:349:GLN:HG2	1.96	0.46
1:G:221:PRO:HB2	1:G:293:SER:HB2	1.96	0.46
1:B:107:GLU:CD	1:B:110:ASN:HD22	2.24	0.46
1:F:133:ALA:HB1	1:F:172:LEU:HD13	1.96	0.46
1:D:270:LEU:HD21	1:D:317:VAL:HG13	1.97	0.46
1:H:221:PRO:HB2	1:H:293:SER:HB2	1.97	0.46
1:E:221:PRO:HB2	1:E:293:SER:HB2	1.96	0.46
1:H:183:SER:HB2	1:H:213:LYS:HZ2	1.82	0.46
1:G:48:TYR:CZ	1:G:50:LEU:HD21	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:ILE:HB	1:E:330:ALA:HA	1.98	0.45
1:G:133:ALA:HB1	1:G:172:LEU:HD13	1.98	0.45
1:B:35:LEU:HD22	1:E:328:ALA:HB2	1.98	0.45
1:E:170:ILE:HD11	1:E:196:SER:HB3	1.98	0.45
1:G:76:LEU:HD22	1:G:122:LEU:CD2	2.45	0.45
1:B:270:LEU:N	1:B:271:PRO:CD	2.80	0.45
1:H:179:MET:CE	1:H:208:LEU:HB2	2.46	0.45
1:E:299:LEU:HG	1:F:298:MET:HE3	1.98	0.45
1:H:119:ILE:HG23	1:H:131:LEU:HD12	1.99	0.45
1:E:267:LYS:NZ	4:E:360:PBG:C4A	2.80	0.45
1:E:115:LEU:HB3	1:E:116:PRO:HD3	1.99	0.44
1:E:7:LEU:HD13	1:E:15:VAL:CG1	2.47	0.44
1:A:299:LEU:HG	1:B:298:MET:CE	2.47	0.44
1:C:298:MET:HB3	1:D:298:MET:HB3	2.00	0.44
1:A:222:PHE:CE1	1:A:226:LEU:HD22	2.53	0.44
1:C:345:MET:HE1	1:C:354:PRO:CD	2.47	0.44
1:B:53:HIS:HA	1:B:114:LEU:HD21	1.98	0.43
1:G:5:GLY:HA2	1:H:199:MET:HE1	2.00	0.43
1:C:57:THR:HG22	1:C:58:SER:O	2.18	0.43
1:C:70:LEU:HD13	1:C:75:LEU:HA	2.00	0.43
1:A:356:TYR:CZ	1:C:315:LEU:HD22	2.54	0.43
1:H:135:VAL:O	1:H:136:ALA:HB2	2.18	0.43
1:A:36:VAL:HG11	1:C:263:MET:HE2	2.00	0.43
1:H:42:LYS:HA	1:H:341:MET:HE1	2.00	0.43
1:A:138:ASP:N	1:A:139:PRO:CD	2.82	0.43
1:C:19:ILE:HD12	1:C:21:ALA:O	2.19	0.43
1:F:37:GLN:NE2	1:F:40:LEU:HD23	2.34	0.43
1:A:183:SER:HB2	1:A:213:LYS:HZ2	1.84	0.43
1:D:253:ALA:CB	1:D:279:ILE:HD12	2.49	0.43
1:F:342:VAL:CG1	1:F:346:LYS:HE2	2.49	0.43
1:H:267:LYS:HZ1	4:H:360:PBG:C4A	2.32	0.42
1:A:43:PRO:HD3	1:A:341:MET:CE	2.49	0.42
1:A:210:TYR:HA	1:A:265:MET:HB3	2.02	0.42
1:C:17:LEU:HG	1:C:19:ILE:HG23	2.01	0.42
1:D:267:LYS:HZ3	4:D:360:PBG:C3A	2.32	0.42
1:G:213:LYS:NZ	4:G:360:PBG:H12	2.16	0.42
1:H:179:MET:HE2	1:H:179:MET:HB3	1.90	0.42
1:B:265:MET:HA	1:B:288:VAL:O	2.20	0.42
1:G:214:TYR:CE2	1:G:241:MET:HE2	2.53	0.42
1:C:191:SER:HB2	1:C:259:GLU:HG2	2.02	0.42
1:F:181:CYS:HB3	1:F:210:TYR:HE1	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:VAL:HG21	1:F:140:TYR:CE1	2.55	0.42
1:D:137:LEU:HD12	1:D:147:GLY:HA2	2.01	0.42
1:E:297:ALA:HB1	1:F:307:TYR:CD2	2.54	0.42
1:G:170:ILE:HD11	1:G:196:SER:HB3	2.01	0.42
1:A:307:TYR:CD1	1:B:63:SER:HA	2.55	0.41
1:B:221:PRO:HB2	1:B:293:SER:HB2	2.00	0.41
1:D:179:MET:HE3	1:D:206:SER:HB3	2.01	0.41
1:E:83:ARG:HH11	1:E:129:VAL:HG23	1.84	0.41
1:B:186:MET:HE2	1:B:186:MET:HA	2.02	0.41
1:B:210:TYR:CE2	1:B:265:MET:HG2	2.56	0.41
1:C:270:LEU:N	1:C:271:PRO:CD	2.83	0.41
1:D:211:SER:OG	1:D:264:LEU:HD22	2.20	0.41
1:E:135:VAL:O	1:E:182:PRO:HA	2.20	0.41
1:B:213:LYS:HE2	1:B:240:GLN:NE2	2.35	0.41
1:C:348:THR:HG22	1:C:348:THR:O	2.20	0.41
1:F:156:ILE:HD13	1:F:156:ILE:N	2.35	0.41
1:D:221:PRO:HB2	1:D:293:SER:HB2	2.02	0.41
1:G:276:LEU:HD21	1:G:326:ALA:HB2	2.02	0.41
1:F:270:LEU:N	1:F:271:PRO:CD	2.83	0.41
1:G:179:MET:HG2	1:G:206:SER:HB2	2.02	0.41
1:E:210:TYR:HA	1:E:265:MET:HB3	2.01	0.41
1:F:47:ILE:HB	1:F:330:ALA:HA	2.03	0.41
1:G:97:ASP:OD1	1:G:97:ASP:N	2.51	0.41
1:B:210:TYR:CD2	1:B:265:MET:HG2	2.56	0.41
1:C:181:CYS:HB3	1:C:210:TYR:HE1	1.85	0.41
1:E:89:ALA:HA	1:E:130:LEU:HB3	2.03	0.41
1:G:91:MET:HE2	1:G:132:LEU:HD23	2.03	0.41
1:G:135:VAL:O	1:G:136:ALA:HB2	2.21	0.41
1:E:138:ASP:OD1	1:E:139:PRO:HD3	2.21	0.41
1:F:135:VAL:O	1:F:136:ALA:HB2	2.21	0.41
1:E:224:ASP:O	1:E:225:ALA:C	2.64	0.40
1:F:186:MET:HA	1:F:186:MET:HE2	2.03	0.40
1:H:270:LEU:HD11	1:H:317:VAL:HG22	2.02	0.40
1:D:76:LEU:CD2	1:D:122:LEU:HD23	2.51	0.40
1:D:76:LEU:HD22	1:D:122:LEU:HD23	2.02	0.40
1:F:179:MET:HE1	1:F:263:MET:CE	2.50	0.40
1:G:210:TYR:HA	1:G:265:MET:HB3	2.04	0.40
1:G:156:ILE:HD13	1:G:156:ILE:N	2.36	0.40
1:F:222:PHE:CZ	1:F:226:LEU:HD22	2.57	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%)	36	55
1	B	350/356 (98%)	337 (96%)	12 (3%)	1 (0%)	36	55
1	C	350/356 (98%)	340 (97%)	10 (3%)	0	100	100
1	D	350/356 (98%)	336 (96%)	13 (4%)	1 (0%)	36	55
1	E	350/356 (98%)	339 (97%)	10 (3%)	1 (0%)	36	55
1	F	351/356 (99%)	340 (97%)	10 (3%)	1 (0%)	36	55
1	G	350/356 (98%)	335 (96%)	14 (4%)	1 (0%)	36	55
1	H	350/356 (98%)	338 (97%)	11 (3%)	1 (0%)	36	55
All	All	2801/2848 (98%)	2705 (97%)	89 (3%)	7 (0%)	36	63

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%)	281 (98%)	6 (2%)	47	74
1	B	280/299 (94%)	275 (98%)	5 (2%)	51	77
1	C	281/299 (94%)	277 (99%)	4 (1%)	59	81
1	D	281/299 (94%)	276 (98%)	5 (2%)	51	77
1	E	289/299 (97%)	281 (97%)	8 (3%)	38	66
1	F	284/299 (95%)	278 (98%)	6 (2%)	47	74
1	G	284/299 (95%)	277 (98%)	7 (2%)	42	69
1	H	282/299 (94%)	274 (97%)	8 (3%)	38	66
All	All	2268/2392 (95%)	2219 (98%)	49 (2%)	45	73

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	88	LYS
1	A	204	ASP
1	A	208	LEU
1	A	282	LYS
1	A	348	THR
1	B	196	SER
1	B	211	SER
1	B	309	SER
1	B	339	LYS
1	B	349	GLN
1	C	20	GLN
1	C	56	GLU
1	C	157	VAL
1	C	278	LYS
1	D	23	PRO
1	D	57	THR
1	D	92	LEU
1	D	226	LEU
1	D	348	THR
1	E	57	THR
1	E	99	GLU
1	E	129	VAL
1	E	226	LEU
1	E	280	ARG
1	E	299	LEU
1	E	315	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	349	GLN
1	F	28	LYS
1	F	57	THR
1	F	99	GLU
1	F	106	GLU
1	F	305	LYS
1	F	349	GLN
1	G	56	GLU
1	G	97	ASP
1	G	156	ILE
1	G	204	ASP
1	G	226	LEU
1	G	282	LYS
1	G	349	GLN
1	H	57	THR
1	H	73	GLU
1	H	157	VAL
1	H	204	ASP
1	H	208	LEU
1	H	226	LEU
1	H	280	ARG
1	H	348	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	67	GLN
1	A	163	HIS
1	C	163	HIS
1	C	164	GLN
1	E	349	GLN
1	F	9	ASN
1	F	349	GLN
1	G	20	GLN
1	G	163	HIS
1	H	164	GLN
1	H	349	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	H	360	-	16,16,16	1.12	2 (12%)	18,21,21	1.65	4 (22%)
5	EDO	A	385	-	3,3,3	0.67	0	2,2,2	0.13	0
5	EDO	C	375	-	3,3,3	0.40	0	2,2,2	0.41	0
5	EDO	D	375	-	3,3,3	0.35	0	2,2,2	0.20	0
5	EDO	B	370	-	3,3,3	0.38	0	2,2,2	0.50	0
4	PBG	C	360	-	16,16,16	1.15	1 (6%)	18,21,21	1.53	4 (22%)
5	EDO	G	375	-	3,3,3	0.36	0	2,2,2	0.28	0
5	EDO	A	375	-	3,3,3	0.50	0	2,2,2	0.23	0
4	PBG	D	360	-	16,16,16	0.93	0	18,21,21	1.76	5 (27%)
5	EDO	H	385	-	3,3,3	0.33	0	2,2,2	0.50	0
5	EDO	F	375	-	3,3,3	0.44	0	2,2,2	0.35	0
4	PBG	B	360	-	16,16,16	1.04	1 (6%)	18,21,21	1.63	4 (22%)
5	EDO	E	375	-	3,3,3	0.38	0	2,2,2	0.13	0
4	PBG	G	360	-	16,16,16	1.07	1 (6%)	18,21,21	1.61	3 (16%)
5	EDO	D	370	-	3,3,3	0.66	0	2,2,2	0.23	0
5	EDO	E	390	-	3,3,3	0.72	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	G	385	-	3,3,3	0.49	0	2,2,2	0.15	0
5	EDO	C	370	-	3,3,3	0.35	0	2,2,2	0.47	0
5	EDO	B	375	-	3,3,3	0.19	0	2,2,2	0.29	0
4	PBG	F	360	-	16,16,16	0.96	1 (6%)	18,21,21	1.86	3 (16%)
5	EDO	H	375	-	3,3,3	0.41	0	2,2,2	0.30	0
5	EDO	F	385	-	3,3,3	0.57	0	2,2,2	0.10	0
4	PBG	E	360	-	16,16,16	1.05	1 (6%)	18,21,21	2.12	5 (27%)
5	EDO	F	370	-	3,3,3	0.29	0	2,2,2	0.49	0
5	EDO	A	380	-	3,3,3	0.48	0	2,2,2	0.31	0
4	PBG	A	360	-	16,16,16	1.27	2 (12%)	18,21,21	1.63	4 (22%)
5	EDO	G	390	-	3,3,3	0.77	0	2,2,2	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	PBG	H	360	-	-	1/9/11/11	0/1/1/1
5	EDO	A	385	-	-	0/1/1/1	-
5	EDO	C	375	-	-	1/1/1/1	-
5	EDO	D	375	-	-	0/1/1/1	-
5	EDO	B	370	-	-	1/1/1/1	-
4	PBG	C	360	-	-	0/9/11/11	0/1/1/1
5	EDO	G	375	-	-	0/1/1/1	-
5	EDO	A	375	-	-	0/1/1/1	-
4	PBG	D	360	-	-	2/9/11/11	0/1/1/1
5	EDO	H	385	-	-	1/1/1/1	-
5	EDO	F	375	-	-	0/1/1/1	-
4	PBG	B	360	-	-	1/9/11/11	0/1/1/1
5	EDO	E	375	-	-	1/1/1/1	-
4	PBG	G	360	-	-	2/9/11/11	0/1/1/1
5	EDO	D	370	-	-	0/1/1/1	-
5	EDO	E	390	-	-	1/1/1/1	-
5	EDO	G	385	-	-	0/1/1/1	-
5	EDO	C	370	-	-	0/1/1/1	-
5	EDO	B	375	-	-	1/1/1/1	-
4	PBG	F	360	-	-	3/9/11/11	0/1/1/1
5	EDO	H	375	-	-	0/1/1/1	-
5	EDO	F	385	-	-	0/1/1/1	-
4	PBG	E	360	-	-	1/9/11/11	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	F	370	-	-	1/1/1/1	-
5	EDO	A	380	-	-	1/1/1/1	-
4	PBG	A	360	-	-	1/9/11/11	0/1/1/1
5	EDO	G	390	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	360	PBG	C1A-NA	-2.79	1.33	1.37
4	B	360	PBG	C1A-NA	-2.67	1.33	1.37
4	G	360	PBG	C1A-NA	-2.53	1.34	1.37
4	A	360	PBG	C5A-C6A	-2.52	1.47	1.51
4	H	360	PBG	C1A-NA	-2.46	1.34	1.37
4	F	360	PBG	C1A-NA	-2.27	1.34	1.37
4	E	360	PBG	C1A-NA	-2.24	1.34	1.37
4	A	360	PBG	C1A-NA	-2.20	1.34	1.37
4	H	360	PBG	O1A-C6A	2.04	1.28	1.22

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	360	PBG	C1A-CHA-N1	5.13	122.86	112.50
4	F	360	PBG	C8A-C7A-C3A	4.12	121.31	112.94
4	F	360	PBG	C1A-CHA-N1	3.98	120.53	112.50
4	H	360	PBG	C1A-CHA-N1	3.77	120.11	112.50
4	D	360	PBG	C1A-CHA-N1	3.58	119.72	112.50
4	G	360	PBG	C1A-CHA-N1	3.41	119.38	112.50
4	G	360	PBG	C6A-C5A-C2A	3.23	121.88	113.76
4	C	360	PBG	C1A-CHA-N1	3.16	118.88	112.50
4	E	360	PBG	C6A-C5A-C2A	3.16	121.70	113.76
4	B	360	PBG	C1A-CHA-N1	3.14	118.84	112.50
4	D	360	PBG	C6A-C5A-C2A	3.10	121.57	113.76
4	A	360	PBG	O4A-C9A-C8A	3.04	123.61	114.00
4	F	360	PBG	C6A-C5A-C2A	2.97	121.22	113.76
4	E	360	PBG	C8A-C7A-C3A	2.96	118.96	112.94
4	E	360	PBG	C5A-C2A-C1A	2.96	129.57	126.54
4	E	360	PBG	O4A-C9A-C8A	2.89	123.13	114.00
4	A	360	PBG	C1A-CHA-N1	2.83	118.22	112.50
4	H	360	PBG	C5A-C2A-C1A	2.76	129.36	126.54
4	B	360	PBG	C6A-C5A-C2A	2.73	120.63	113.76
4	D	360	PBG	C8A-C7A-C3A	2.53	118.09	112.94
4	D	360	PBG	O4A-C9A-C8A	2.52	121.96	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	360	PBG	C6A-C5A-C2A	2.47	119.98	113.76
4	C	360	PBG	C8A-C7A-C3A	2.40	117.82	112.94
4	A	360	PBG	O4A-C9A-O3A	-2.38	117.21	123.33
4	H	360	PBG	C8A-C7A-C3A	2.34	117.70	112.94
4	C	360	PBG	C6A-C5A-C2A	2.31	119.58	113.76
4	G	360	PBG	C8A-C7A-C3A	2.29	117.59	112.94
4	B	360	PBG	C7A-C8A-C9A	2.25	119.63	113.67
4	C	360	PBG	C5A-C2A-C1A	2.16	128.75	126.54
4	B	360	PBG	O4A-C9A-C8A	2.12	120.69	114.00
4	A	360	PBG	C5A-C2A-C1A	2.05	128.64	126.54
4	D	360	PBG	O4A-C9A-O3A	-2.05	118.07	123.33

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	360	PBG	C3A-C2A-C5A-C6A
5	H	385	EDO	O1-C1-C2-O2
5	G	390	EDO	O1-C1-C2-O2
4	D	360	PBG	C3A-C2A-C5A-C6A
5	F	370	EDO	O1-C1-C2-O2
5	B	375	EDO	O1-C1-C2-O2
5	C	375	EDO	O1-C1-C2-O2
5	E	375	EDO	O1-C1-C2-O2
5	A	380	EDO	O1-C1-C2-O2
5	B	370	EDO	O1-C1-C2-O2
5	E	390	EDO	O1-C1-C2-O2
4	F	360	PBG	C7A-C8A-C9A-O4A
4	H	360	PBG	C7A-C8A-C9A-O4A
4	G	360	PBG	C7A-C8A-C9A-O4A
4	B	360	PBG	C7A-C8A-C9A-O3A
4	A	360	PBG	C3A-C2A-C5A-C6A
4	F	360	PBG	C3A-C2A-C5A-C6A
4	G	360	PBG	C3A-C2A-C5A-C6A
4	D	360	PBG	C7A-C8A-C9A-O3A
4	F	360	PBG	C7A-C8A-C9A-O3A

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	360	PBG	1	0
4	D	360	PBG	4	0
4	B	360	PBG	2	0
4	G	360	PBG	5	0
4	F	360	PBG	4	0
4	E	360	PBG	3	0
4	A	360	PBG	1	0

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	352/356 (98%)	-0.63	2 (0%) 85 83	9, 17, 33, 60	0
1	B	352/356 (98%)	-0.48	1 (0%) 90 87	9, 22, 39, 47	0
1	C	352/356 (98%)	-0.54	3 (0%) 81 78	8, 20, 40, 52	0
1	D	352/356 (98%)	-0.47	1 (0%) 90 87	10, 23, 41, 46	0
1	E	352/356 (98%)	-0.50	0 100 100	9, 22, 43, 52	0
1	F	352/356 (98%)	-0.46	1 (0%) 90 87	10, 23, 44, 53	1 (0%)
1	G	352/356 (98%)	-0.42	1 (0%) 90 87	10, 23, 46, 57	0
1	H	352/356 (98%)	-0.43	1 (0%) 90 87	10, 24, 44, 58	0
All	All	2816/2848 (98%)	-0.49	10 (0%) 88 86	8, 22, 43, 60	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	5	GLY	3.6
1	A	6	PRO	3.2
1	A	5	GLY	3.0
1	G	5	GLY	3.0
1	C	233	GLY	2.7
1	C	5	GLY	2.5
1	F	5	GLY	2.5
1	B	231	VAL	2.3
1	C	103	VAL	2.3
1	D	233	GLY	2.2

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

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

6.3 Carbohydrates

There are no oligosaccharides 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. 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	CL	G	395	1/1	0.84	0.14	54,54,54,54	0
3	CL	C	400	1/1	0.85	0.14	59,59,59,59	0
5	EDO	A	380	4/4	0.87	0.14	54,55,55,55	0
5	EDO	H	385	4/4	0.87	0.14	34,35,38,41	0
3	CL	F	397	1/1	0.88	0.15	58,58,58,58	0
5	EDO	G	390	4/4	0.88	0.12	29,29,30,31	0
3	CL	G	400	1/1	0.88	0.12	43,43,43,43	0
5	EDO	D	370	4/4	0.89	0.11	30,33,33,34	0
5	EDO	E	390	4/4	0.90	0.12	31,32,32,34	0
3	CL	C	395	1/1	0.91	0.18	62,62,62,62	0
3	CL	D	405	1/1	0.91	0.10	40,40,40,40	0
3	CL	A	405	1/1	0.92	0.11	47,47,47,47	0
5	EDO	B	370	4/4	0.92	0.09	26,26,27,27	0
3	CL	F	400	1/1	0.92	0.12	50,50,50,50	0
3	CL	H	400	1/1	0.92	0.12	55,55,55,55	0
5	EDO	G	385	4/4	0.92	0.10	32,32,32,32	0
4	PBG	D	360	16/16	0.92	0.09	26,32,35,36	0
4	PBG	G	360	16/16	0.92	0.09	19,29,32,34	0
3	CL	E	400	1/1	0.93	0.13	57,57,57,57	0
3	CL	G	357	1/1	0.93	0.09	52,52,52,52	0
2	MG	F	365	1/1	0.94	0.10	35,35,35,35	0
5	EDO	F	385	4/4	0.94	0.08	28,32,32,34	0
4	PBG	E	360	16/16	0.94	0.08	20,26,32,34	0
3	CL	B	400	1/1	0.94	0.09	50,50,50,50	0
5	EDO	E	375	4/4	0.94	0.10	19,21,21,24	0
4	PBG	B	360	16/16	0.95	0.08	20,33,36,36	0
5	EDO	C	370	4/4	0.95	0.09	30,31,31,32	0
5	EDO	C	375	4/4	0.95	0.06	11,12,14,14	0
4	PBG	H	360	16/16	0.95	0.08	19,27,31,32	0
4	PBG	C	360	16/16	0.95	0.08	20,24,28,28	0
3	CL	A	400	1/1	0.96	0.08	49,49,49,49	0
2	MG	E	365	1/1	0.96	0.10	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	385	4/4	0.96	0.07	15,18,20,22	0
5	EDO	F	375	4/4	0.96	0.06	17,18,19,19	0
5	EDO	B	375	4/4	0.96	0.08	13,14,15,16	0
3	CL	D	400	1/1	0.96	0.08	50,50,50,50	0
4	PBG	F	360	16/16	0.96	0.07	14,27,32,32	0
5	EDO	H	375	4/4	0.96	0.07	17,19,19,19	0
3	CL	E	395	1/1	0.96	0.11	52,52,52,52	0
5	EDO	A	375	4/4	0.97	0.05	14,15,16,16	0
4	PBG	A	360	16/16	0.97	0.07	9,18,21,22	0
5	EDO	F	370	4/4	0.97	0.05	20,22,23,24	0
2	MG	G	365	1/1	0.97	0.04	34,34,34,34	0
5	EDO	D	375	4/4	0.97	0.05	11,12,12,13	0
3	CL	B	405	1/1	0.97	0.08	39,39,39,39	0
2	MG	A	365	1/1	0.97	0.03	16,16,16,16	0
2	MG	H	365	1/1	0.98	0.03	21,21,21,21	0
2	MG	D	365	1/1	0.98	0.04	32,32,32,32	0
2	MG	C	365	1/1	0.98	0.02	17,17,17,17	0
5	EDO	G	375	4/4	0.98	0.05	23,23,24,24	0
2	MG	B	365	1/1	0.99	0.04	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.