



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2025 – 06:09 PM JST

PDB ID : 8ZBC / pdb_00008zbc
Title : An acyltransferase with selective perhydrolytic activity
Authors : Yin, Z.; Jing, W.
Deposited on : 2024-04-26
Resolution : 2.97 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>.

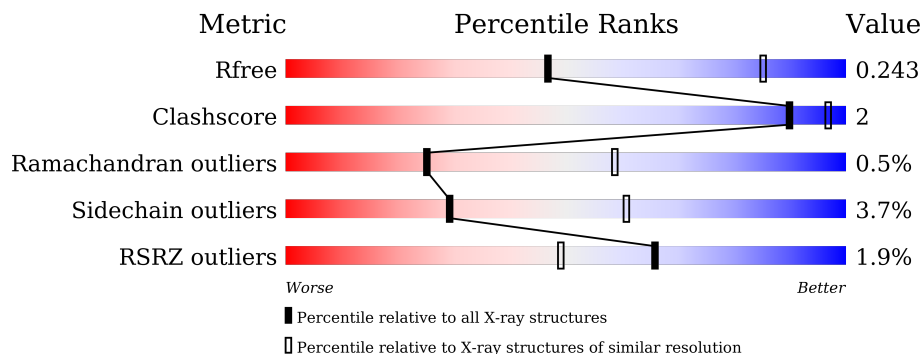
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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X-RAY DIFFRACTION

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}	164625	3360 (3.00-2.96)
Clashscore	180529	3751 (3.00-2.96)
Ramachandran outliers	177936	3628 (3.00-2.96)
Sidechain outliers	177891	3631 (3.00-2.96)
RSRZ outliers	164620	3372 (3.00-2.96)

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	233	<div> <div>3%</div> <div>92%</div> <div>• • •</div> </div>
1	B	233	<div> <div>3%</div> <div>91%</div> <div>5% • •</div> </div>
1	C	233	<div> <div>2%</div> <div>88%</div> <div>5% • 6%</div> </div>
1	D	233	<div> <div>2%</div> <div>91%</div> <div>6% • •</div> </div>
1	E	233	<div> <div></div> <div>87%</div> <div>5% • 6%</div> </div>
1	F	233	<div> <div></div> <div>89%</div> <div>• • 6%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10071 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 SGNH/GDSL hydrolase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	P	S	0	0	0
			1710	1098	281	329	1	1			
1	B	228	Total	C	N	O	P	S	0	0	0
			1719	1103	283	331	1	1			
1	C	218	Total	C	N	O	P	S	0	0	0
			1644	1055	269	318	1	1			
1	D	227	Total	C	N	O	P	S	0	0	0
			1710	1098	281	329	1	1			
1	E	218	Total	C	N	O	P	S	0	0	0
			1644	1055	269	318	1	1			
1	F	218	Total	C	N	O	P	S	0	0	0
			1644	1055	269	318	1	1			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	LYS	-	expression tag	UNP A0A967CBZ5
A	222	LEU	-	expression tag	UNP A0A967CBZ5
A	223	ALA	-	expression tag	UNP A0A967CBZ5
A	224	ALA	-	expression tag	UNP A0A967CBZ5
A	225	ALA	-	expression tag	UNP A0A967CBZ5
A	226	LEU	-	expression tag	UNP A0A967CBZ5
A	227	GLU	-	expression tag	UNP A0A967CBZ5
A	228	HIS	-	expression tag	UNP A0A967CBZ5
A	229	HIS	-	expression tag	UNP A0A967CBZ5
A	230	HIS	-	expression tag	UNP A0A967CBZ5
A	231	HIS	-	expression tag	UNP A0A967CBZ5
A	232	HIS	-	expression tag	UNP A0A967CBZ5
A	233	HIS	-	expression tag	UNP A0A967CBZ5
B	221	LYS	-	expression tag	UNP A0A967CBZ5
B	222	LEU	-	expression tag	UNP A0A967CBZ5
B	223	ALA	-	expression tag	UNP A0A967CBZ5
B	224	ALA	-	expression tag	UNP A0A967CBZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	225	ALA	-	expression tag	UNP A0A967CBZ5
B	226	LEU	-	expression tag	UNP A0A967CBZ5
B	227	GLU	-	expression tag	UNP A0A967CBZ5
B	228	HIS	-	expression tag	UNP A0A967CBZ5
B	229	HIS	-	expression tag	UNP A0A967CBZ5
B	230	HIS	-	expression tag	UNP A0A967CBZ5
B	231	HIS	-	expression tag	UNP A0A967CBZ5
B	232	HIS	-	expression tag	UNP A0A967CBZ5
B	233	HIS	-	expression tag	UNP A0A967CBZ5
C	221	LYS	-	expression tag	UNP A0A967CBZ5
C	222	LEU	-	expression tag	UNP A0A967CBZ5
C	223	ALA	-	expression tag	UNP A0A967CBZ5
C	224	ALA	-	expression tag	UNP A0A967CBZ5
C	225	ALA	-	expression tag	UNP A0A967CBZ5
C	226	LEU	-	expression tag	UNP A0A967CBZ5
C	227	GLU	-	expression tag	UNP A0A967CBZ5
C	228	HIS	-	expression tag	UNP A0A967CBZ5
C	229	HIS	-	expression tag	UNP A0A967CBZ5
C	230	HIS	-	expression tag	UNP A0A967CBZ5
C	231	HIS	-	expression tag	UNP A0A967CBZ5
C	232	HIS	-	expression tag	UNP A0A967CBZ5
C	233	HIS	-	expression tag	UNP A0A967CBZ5
D	221	LYS	-	expression tag	UNP A0A967CBZ5
D	222	LEU	-	expression tag	UNP A0A967CBZ5
D	223	ALA	-	expression tag	UNP A0A967CBZ5
D	224	ALA	-	expression tag	UNP A0A967CBZ5
D	225	ALA	-	expression tag	UNP A0A967CBZ5
D	226	LEU	-	expression tag	UNP A0A967CBZ5
D	227	GLU	-	expression tag	UNP A0A967CBZ5
D	228	HIS	-	expression tag	UNP A0A967CBZ5
D	229	HIS	-	expression tag	UNP A0A967CBZ5
D	230	HIS	-	expression tag	UNP A0A967CBZ5
D	231	HIS	-	expression tag	UNP A0A967CBZ5
D	232	HIS	-	expression tag	UNP A0A967CBZ5
D	233	HIS	-	expression tag	UNP A0A967CBZ5
E	221	LYS	-	expression tag	UNP A0A967CBZ5
E	222	LEU	-	expression tag	UNP A0A967CBZ5
E	223	ALA	-	expression tag	UNP A0A967CBZ5
E	224	ALA	-	expression tag	UNP A0A967CBZ5
E	225	ALA	-	expression tag	UNP A0A967CBZ5
E	226	LEU	-	expression tag	UNP A0A967CBZ5
E	227	GLU	-	expression tag	UNP A0A967CBZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	228	HIS	-	expression tag	UNP A0A967CBZ5
E	229	HIS	-	expression tag	UNP A0A967CBZ5
E	230	HIS	-	expression tag	UNP A0A967CBZ5
E	231	HIS	-	expression tag	UNP A0A967CBZ5
E	232	HIS	-	expression tag	UNP A0A967CBZ5
E	233	HIS	-	expression tag	UNP A0A967CBZ5
F	221	LYS	-	expression tag	UNP A0A967CBZ5
F	222	LEU	-	expression tag	UNP A0A967CBZ5
F	223	ALA	-	expression tag	UNP A0A967CBZ5
F	224	ALA	-	expression tag	UNP A0A967CBZ5
F	225	ALA	-	expression tag	UNP A0A967CBZ5
F	226	LEU	-	expression tag	UNP A0A967CBZ5
F	227	GLU	-	expression tag	UNP A0A967CBZ5
F	228	HIS	-	expression tag	UNP A0A967CBZ5
F	229	HIS	-	expression tag	UNP A0A967CBZ5
F	230	HIS	-	expression tag	UNP A0A967CBZ5
F	231	HIS	-	expression tag	UNP A0A967CBZ5
F	232	HIS	-	expression tag	UNP A0A967CBZ5
F	233	HIS	-	expression tag	UNP A0A967CBZ5

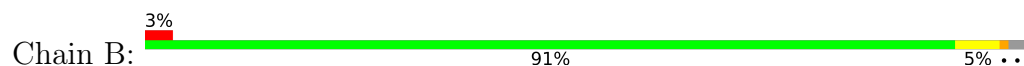
3 Residue-property plots [i](#)

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.

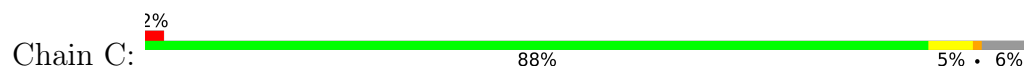
- Molecule 1: SGNH/GDSL hydrolase family protein



- Molecule 1: SGNH/GDSL hydrolase family protein



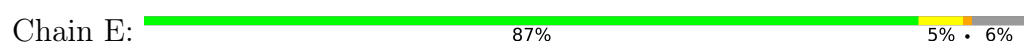
- Molecule 1: SGNH/GDSL hydrolase family protein



- Molecule 1: SGNH/GDSL hydrolase family protein



- Molecule 1: SGNH/GDSL hydrolase family protein



- Molecule 1: SGNH/GDSL hydrolase family protein

Chain F:

89%

6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	131.75Å 165.35Å 150.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.97 48.17 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.4 (48.17-2.97) 95.4 (48.17-2.97)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.239 0.214 , 0.243	Depositor DCC
R_{free} test set	1692 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 15.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10071	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 3.32% 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: SEP

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	0.48	0/1746	0.70	2/2398 (0.1%)
1	B	0.45	0/1755	0.67	1/2410 (0.0%)
1	C	0.48	0/1678	0.71	1/2305 (0.0%)
1	D	0.47	0/1746	0.69	1/2398 (0.0%)
1	E	0.47	0/1678	0.69	1/2305 (0.0%)
1	F	0.44	0/1678	0.66	1/2305 (0.0%)
All	All	0.47	0/10281	0.69	7/14121 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	SER	C-N-CD	-8.89	101.03	120.60
1	A	123	SER	C-N-CD	-8.87	101.09	120.60
1	D	123	SER	C-N-CD	-8.77	101.31	120.60
1	F	123	SER	C-N-CD	-8.65	101.56	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	SER	C-N-CD	-8.59	101.71	120.60
1	C	123	SER	C-N-CD	-8.50	101.89	120.60
1	A	127	ASP	CB-CA-C	-5.44	99.52	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	SER	Peptide
1	B	123	SER	Peptide
1	C	123	SER	Peptide
1	D	123	SER	Peptide
1	E	123	SER	Peptide
1	F	123	SER	Peptide

5.2 Too-close contacts [i](#)

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	1710	0	1691	5	0
1	B	1719	0	1702	5	0
1	C	1644	0	1621	7	0
1	D	1710	0	1691	8	0
1	E	1644	0	1621	8	0
1	F	1644	0	1621	4	0
All	All	10071	0	9947	33	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 2.

All (33) 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:13:SEP:O2P	1:F:96:ASN:ND2	2.21	0.74
1:D:13:SEP:O2P	1:D:96:ASN:ND2	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:VAL:O	1:E:123:SER:HB2	1.94	0.67
1:B:120:VAL:O	1:B:123:SER:HB2	1.94	0.67
1:D:120:VAL:O	1:D:123:SER:HB2	1.94	0.67
1:A:120:VAL:O	1:A:123:SER:HB2	1.95	0.67
1:F:120:VAL:O	1:F:123:SER:HB2	1.96	0.66
1:C:120:VAL:O	1:C:123:SER:HB2	1.95	0.65
1:C:187:VAL:HG12	1:D:220:PRO:HB2	1.83	0.60
1:B:16:TRP:CE2	1:B:29:ARG:HG3	2.38	0.58
1:D:16:TRP:CE2	1:D:29:ARG:HG3	2.39	0.58
1:C:16:TRP:CE2	1:C:29:ARG:HG3	2.39	0.57
1:A:16:TRP:CE2	1:A:29:ARG:HG3	2.39	0.57
1:E:16:TRP:CE2	1:E:29:ARG:HG3	2.39	0.56
1:D:227:GLU:O	1:D:228:HIS:C	2.44	0.56
1:F:16:TRP:CE2	1:F:29:ARG:HG3	2.39	0.56
1:D:16:TRP:CZ2	1:D:29:ARG:HG3	2.42	0.54
1:E:16:TRP:CZ2	1:E:29:ARG:HG3	2.44	0.53
1:B:16:TRP:CZ2	1:B:29:ARG:HG3	2.44	0.53
1:A:16:TRP:CZ2	1:A:29:ARG:HG3	2.44	0.53
1:E:13:SEP:HB2	1:E:56:SER:HA	1.90	0.53
1:F:16:TRP:CZ2	1:F:29:ARG:HG3	2.44	0.52
1:C:16:TRP:CZ2	1:C:29:ARG:HG3	2.44	0.52
1:C:13:SEP:HB2	1:C:56:SER:HA	1.91	0.52
1:A:13:SEP:HB2	1:A:56:SER:HA	1.92	0.51
1:B:13:SEP:HB2	1:B:56:SER:HA	1.92	0.50
1:C:2:ASP:OD2	1:E:164:GLU:OE2	2.31	0.49
1:C:100:THR:HG22	1:C:155:ILE:HA	1.94	0.48
1:D:118:ASN:OD1	1:E:108:GLU:HG3	2.17	0.43
1:E:104:ARG:HA	1:E:108:GLU:OE2	2.18	0.42
1:D:107:PHE:CZ	1:E:177:ALA:HB2	2.55	0.42
1:B:149:ASP:HA	1:B:150:PRO:HD2	1.90	0.41
1:A:228:HIS:CD2	1:A:228:HIS:C	2.95	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	224/233 (96%)	214 (96%)	9 (4%)	1 (0%)	30	63
1	B	225/233 (97%)	214 (95%)	10 (4%)	1 (0%)	30	63
1	C	215/233 (92%)	206 (96%)	8 (4%)	1 (0%)	25	59
1	D	224/233 (96%)	215 (96%)	8 (4%)	1 (0%)	30	63
1	E	215/233 (92%)	205 (95%)	9 (4%)	1 (0%)	25	59
1	F	215/233 (92%)	205 (95%)	9 (4%)	1 (0%)	25	59
All	All	1318/1398 (94%)	1259 (96%)	53 (4%)	6 (0%)	25	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	PRO
1	B	124	PRO
1	C	124	PRO
1	D	124	PRO
1	E	124	PRO
1	F	124	PRO

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	180/186 (97%)	173 (96%)	7 (4%)	27	59
1	B	181/186 (97%)	173 (96%)	8 (4%)	24	56
1	C	174/186 (94%)	169 (97%)	5 (3%)	37	68
1	D	180/186 (97%)	174 (97%)	6 (3%)	33	64
1	E	174/186 (94%)	167 (96%)	7 (4%)	27	58
1	F	174/186 (94%)	168 (97%)	6 (3%)	32	64
All	All	1063/1116 (95%)	1024 (96%)	39 (4%)	29	61

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	123	SER
1	A	126	TRP
1	A	130	ASP
1	A	151	LEU
1	A	175	GLU
1	A	228	HIS
1	B	29	ARG
1	B	123	SER
1	B	126	TRP
1	B	140	SER
1	B	151	LEU
1	B	175	GLU
1	B	189	SER
1	B	221	LYS
1	C	29	ARG
1	C	123	SER
1	C	126	TRP
1	C	130	ASP
1	C	140	SER
1	D	29	ARG
1	D	123	SER
1	D	126	TRP
1	D	130	ASP
1	D	140	SER
1	D	151	LEU
1	E	29	ARG
1	E	108	GLU
1	E	123	SER
1	E	126	TRP
1	E	130	ASP
1	E	140	SER
1	E	151	LEU
1	F	29	ARG
1	F	123	SER
1	F	126	TRP
1	F	130	ASP
1	F	151	LEU
1	F	175	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	A	13	1	8,9,10	0.78	0	8,12,14	2.51	3 (37%)
1	SEP	D	13	1	8,9,10	0.82	0	8,12,14	3.33	5 (62%)
1	SEP	C	13	1	8,9,10	0.77	0	8,12,14	2.44	3 (37%)
1	SEP	B	13	1	8,9,10	0.75	0	8,12,14	2.33	3 (37%)
1	SEP	F	13	1	8,9,10	0.83	0	8,12,14	3.09	4 (50%)
1	SEP	E	13	1	8,9,10	0.72	0	8,12,14	2.45	3 (37%)

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	SEP	A	13	1	-	1/5/8/10	-
1	SEP	D	13	1	-	5/5/8/10	-
1	SEP	C	13	1	-	1/5/8/10	-
1	SEP	B	13	1	-	1/5/8/10	-
1	SEP	F	13	1	-	5/5/8/10	-
1	SEP	E	13	1	-	1/5/8/10	-

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	SEP	OG-CB-CA	6.25	114.23	108.14
1	F	13	SEP	OG-CB-CA	6.12	114.10	108.14
1	A	13	SEP	P-OG-CB	5.62	133.78	118.30
1	E	13	SEP	P-OG-CB	5.60	133.73	118.30
1	C	13	SEP	P-OG-CB	5.50	133.44	118.30
1	B	13	SEP	P-OG-CB	5.14	132.45	118.30
1	F	13	SEP	P-OG-CB	4.79	131.48	118.30
1	D	13	SEP	P-OG-CB	4.10	129.58	118.30
1	D	13	SEP	OG-P-O1P	-3.58	96.45	106.47
1	A	13	SEP	O3P-P-O2P	2.95	118.92	107.64
1	A	13	SEP	O2P-P-OG	-2.94	98.90	106.73
1	B	13	SEP	O2P-P-OG	-2.84	99.17	106.73
1	C	13	SEP	O2P-P-OG	-2.81	99.26	106.73
1	C	13	SEP	O3P-P-O2P	2.78	118.25	107.64
1	E	13	SEP	O2P-P-OG	-2.76	99.39	106.73
1	E	13	SEP	O3P-P-O2P	2.74	118.12	107.64
1	D	13	SEP	O2P-P-O1P	2.69	121.20	110.68
1	B	13	SEP	O3P-P-O2P	2.66	117.81	107.64
1	D	13	SEP	O3P-P-O2P	2.51	117.23	107.64
1	F	13	SEP	O2P-P-O1P	-2.42	101.19	110.68
1	F	13	SEP	O3P-P-O2P	2.38	116.75	107.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	13	SEP	N-CA-CB-OG
1	D	13	SEP	CB-OG-P-O2P
1	D	13	SEP	CB-OG-P-O3P
1	F	13	SEP	N-CA-CB-OG
1	F	13	SEP	CB-OG-P-O1P
1	F	13	SEP	CB-OG-P-O2P
1	F	13	SEP	CB-OG-P-O3P
1	D	13	SEP	CB-OG-P-O1P
1	A	13	SEP	CA-CB-OG-P
1	B	13	SEP	CA-CB-OG-P
1	C	13	SEP	CA-CB-OG-P
1	D	13	SEP	CA-CB-OG-P
1	E	13	SEP	CA-CB-OG-P
1	F	13	SEP	CA-CB-OG-P

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	13	SEP	1	0
1	D	13	SEP	1	0
1	C	13	SEP	1	0
1	B	13	SEP	1	0
1	F	13	SEP	1	0
1	E	13	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	226/233 (96%)	0.01	7 (3%)	51 35	14, 21, 37, 66	0
1	B	227/233 (97%)	0.10	7 (3%)	51 35	14, 22, 38, 81	0
1	C	217/233 (93%)	0.02	4 (1%)	67 50	11, 21, 37, 84	0
1	D	226/233 (96%)	-0.01	5 (2%)	62 45	11, 21, 36, 93	0
1	E	217/233 (93%)	0.04	1 (0%)	87 77	15, 23, 40, 71	0
1	F	217/233 (93%)	0.07	1 (0%)	87 77	13, 25, 39, 61	0
All	All	1330/1398 (95%)	0.04	25 (1%)	66 49	11, 22, 39, 93	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ASP	5.2
1	A	228	HIS	5.0
1	D	228	HIS	4.9
1	C	3	LYS	4.6
1	B	228	HIS	4.6
1	A	124	PRO	3.2
1	C	4	ILE	3.1
1	B	42	GLU	2.9
1	B	1	GLN	2.8
1	D	223	ALA	2.7
1	D	225	ALA	2.5
1	A	45	GLY	2.5
1	A	3	LYS	2.4
1	B	127	ASP	2.4
1	D	226	LEU	2.3
1	C	219	GLN	2.3
1	A	159	GLY	2.3
1	D	3	LYS	2.3
1	B	227	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	125	GLY	2.2
1	B	2	ASP	2.2
1	E	2	ASP	2.2
1	A	227	GLU	2.2
1	B	125	GLY	2.1
1	F	219	GLN	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	SEP	C	13	10/11	0.82	0.23	27,39,58,60	0
1	SEP	F	13	10/11	0.82	0.19	34,46,66,69	0
1	SEP	D	13	10/11	0.83	0.18	25,35,45,47	0
1	SEP	E	13	10/11	0.87	0.19	26,36,46,47	0
1	SEP	A	13	10/11	0.88	0.17	26,37,60,63	0
1	SEP	B	13	10/11	0.89	0.17	30,39,57,57	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.