



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:06 AM UTC

PDB ID : 8SPF / pdb_00008spf
Title : Crystal structure of Bax core domain BH3-groove dimer - hexameric fraction with 2-stearoyl lysoPC
Authors : Cowan, A.D.; Miller, M.S.; Czabotar, P.E.; Colman, P.M.
Deposited on : 2023-05-03
Resolution : 2.20 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

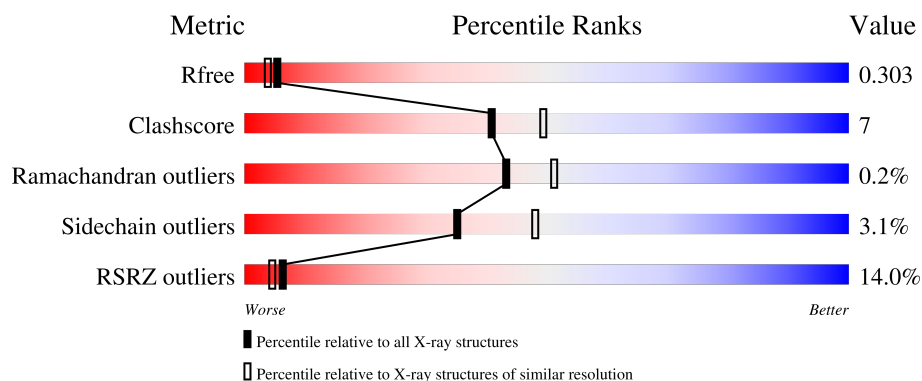
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	81	
1	B	81	
1	C	81	
1	D	81	
1	E	81	

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Mol	Chain	Length	Quality of chain
1	F	81	10%78%16%• 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3285 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 Apoptosis regulator BAX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	70	Total	C	N	O	S	0	0	0
			526	338	89	96	3			
1	D	71	Total	C	N	O	S	0	1	0
			566	363	96	104	3			
1	A	63	Total	C	N	O	S	0	0	0
			483	311	82	88	2			
1	B	62	Total	C	N	O	S	0	0	0
			455	294	75	85	1			
1	E	78	Total	C	N	O	S	0	0	0
			599	381	99	116	3			
1	F	77	Total	C	N	O	S	0	0	0
			582	370	100	109	3			

There are 42 discrepancies between the modelled and reference sequences:

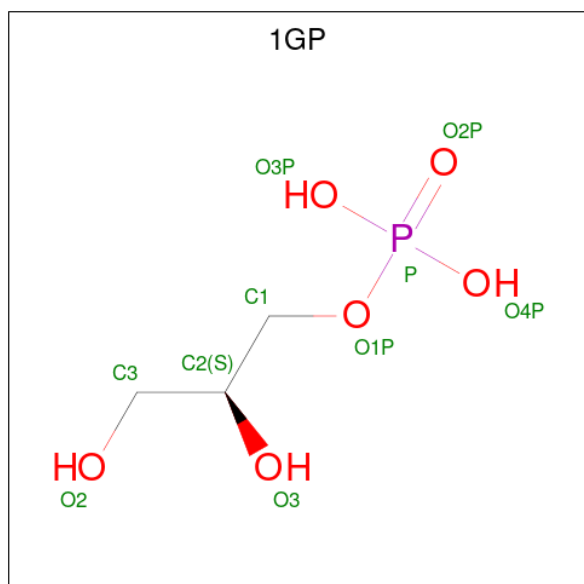
Chain	Residue	Modelled	Actual	Comment	Reference
C	48	GLY	-	expression tag	UNP Q07812
C	49	PRO	-	expression tag	UNP Q07812
C	50	LEU	-	expression tag	UNP Q07812
C	51	GLY	-	expression tag	UNP Q07812
C	52	SER	-	expression tag	UNP Q07812
C	62	SER	CYS	conflict	UNP Q07812
C	126	SER	CYS	conflict	UNP Q07812
D	48	GLY	-	expression tag	UNP Q07812
D	49	PRO	-	expression tag	UNP Q07812
D	50	LEU	-	expression tag	UNP Q07812
D	51	GLY	-	expression tag	UNP Q07812
D	52	SER	-	expression tag	UNP Q07812
D	62	SER	CYS	conflict	UNP Q07812
D	126	SER	CYS	conflict	UNP Q07812
A	48	GLY	-	expression tag	UNP Q07812
A	49	PRO	-	expression tag	UNP Q07812
A	50	LEU	-	expression tag	UNP Q07812

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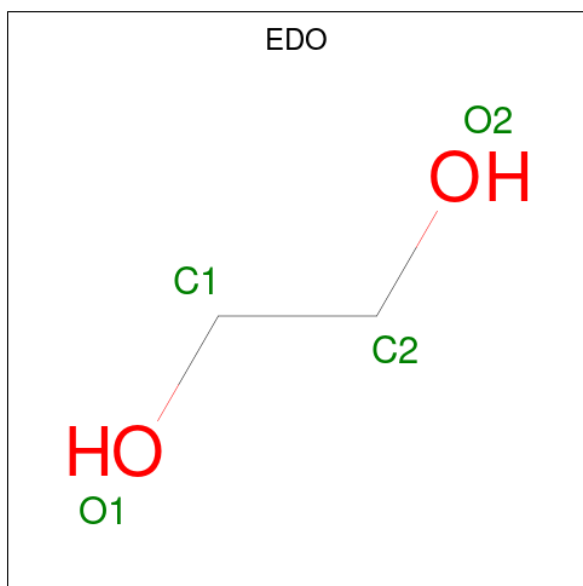
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	expression tag	UNP Q07812
A	52	SER	-	expression tag	UNP Q07812
A	62	SER	CYS	conflict	UNP Q07812
A	126	SER	CYS	conflict	UNP Q07812
B	48	GLY	-	expression tag	UNP Q07812
B	49	PRO	-	expression tag	UNP Q07812
B	50	LEU	-	expression tag	UNP Q07812
B	51	GLY	-	expression tag	UNP Q07812
B	52	SER	-	expression tag	UNP Q07812
B	62	SER	CYS	conflict	UNP Q07812
B	126	SER	CYS	conflict	UNP Q07812
E	48	GLY	-	expression tag	UNP Q07812
E	49	PRO	-	expression tag	UNP Q07812
E	50	LEU	-	expression tag	UNP Q07812
E	51	GLY	-	expression tag	UNP Q07812
E	52	SER	-	expression tag	UNP Q07812
E	62	SER	CYS	conflict	UNP Q07812
E	126	SER	CYS	conflict	UNP Q07812
F	48	GLY	-	expression tag	UNP Q07812
F	49	PRO	-	expression tag	UNP Q07812
F	50	LEU	-	expression tag	UNP Q07812
F	51	GLY	-	expression tag	UNP Q07812
F	52	SER	-	expression tag	UNP Q07812
F	62	SER	CYS	conflict	UNP Q07812
F	126	SER	CYS	conflict	UNP Q07812

- Molecule 2 is SN-GLYCEROL-1-PHOSPHATE (CCD ID: 1GP) (formula: $C_3H_9O_6P$).



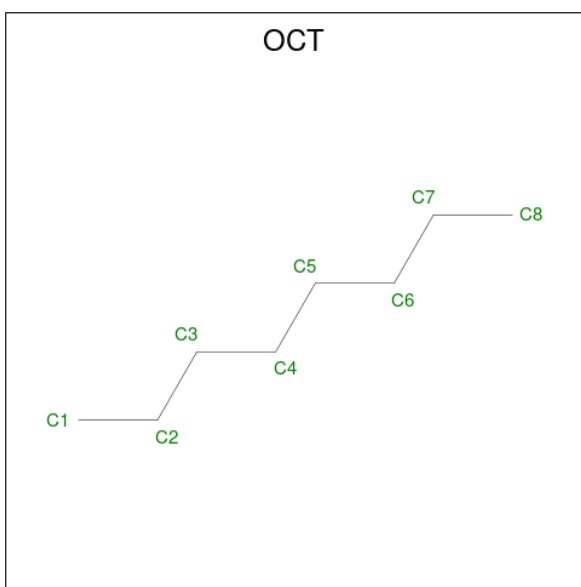
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



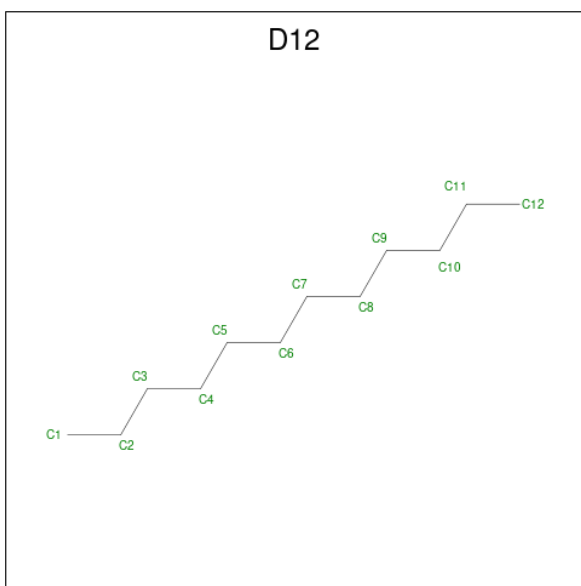
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



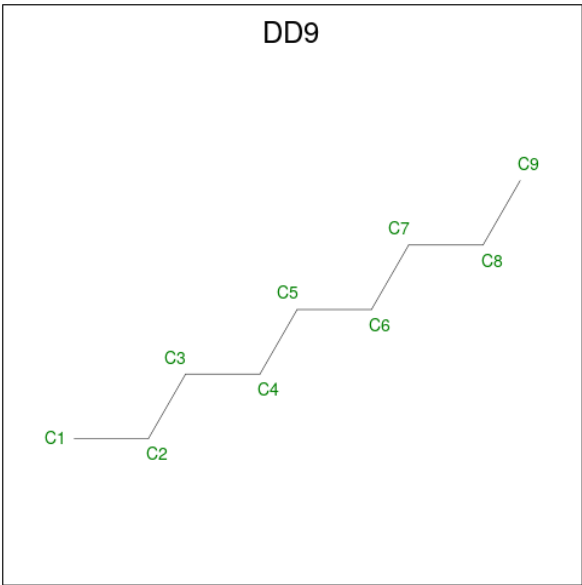
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C 8 8	0	0

- Molecule 5 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C 12 12	0	0

- Molecule 6 is nonane (CCD ID: DD9) (formula: C_9H_{20}).

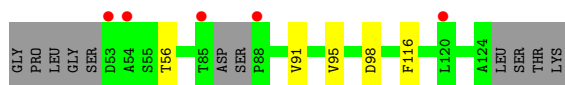


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C 9 9	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	3	Total O 3 3	0	0
7	D	2	Total O 2 2	0	0
7	A	1	Total O 1 1	0	0
7	B	1	Total O 1 1	0	0
7	E	4	Total O 4 4	0	0
7	F	4	Total O 4 4	0	0

- Molecule 1: Apoptosis regulator BAX



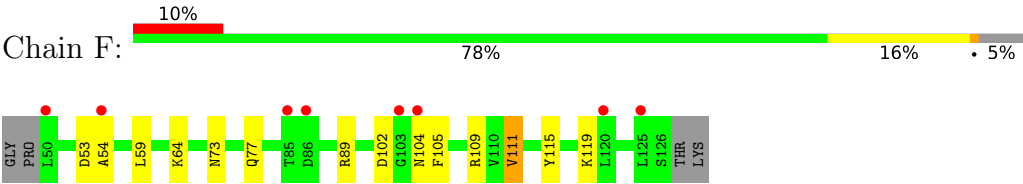
- | | | | | | | | | | | |
|------|------|------|------|------|------|------|-----|-----|-----|-----|
| GLY | PRO | LEU | GLY | SER | ASP | S54 | S55 | T56 | K57 | K58 | L59 | N73 | M74 | Q77 | V83 | D84 | T86 | D86 | E90 | F93 | R94 | Y115 | K119 | L120 | V121 | L122 | K123 | A124 | LEU | SER | THR | LVS |
|------|------|------|------|------|------|------|-----|-----|-----|-----|

- [illegible]

- [illegible]

- GLY P49 P50 L70 S72 S73 S74 S75 S76 S77 S78 S79 S80 S83 S86 S89 F92 A97 D98 M99 G103 V111 F114 V115 F116 A117 S118 S119 L120 L121 V121 A124 L125 S126 THR LVS

● Molecule 1: Apoptosis regulator BAX



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.13Å 83.88Å 100.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.32 – 2.20 44.32 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.32-2.20) 89.4 (44.32-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 2.20Å)	Xtriage
Refinement program	PHENIX (dev_3965: ???)	Depositor
R, R_{free}	0.253 , 0.305 0.252 , 0.303	Depositor DCC
R_{free} test set	1996 reflections (7.49%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3285	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: OCT, D12, 1GP, EDO, DD9

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	0.08	0/491	0.21	0/661
1	B	0.07	0/463	0.22	0/624
1	C	0.07	0/534	0.21	0/719
1	D	0.07	0/576	0.21	0/774
1	E	0.07	0/609	0.24	0/820
1	F	0.09	0/591	0.27	0/796
All	All	0.07	0/3264	0.23	0/4394

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	483	0	460	11	0
1	B	455	0	414	9	0
1	C	526	0	499	4	0
1	D	566	0	556	9	0
1	E	599	0	586	14	0
1	F	582	0	557	10	0
2	D	10	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	6	0	0
3	D	4	0	6	0	0
3	E	8	0	12	1	0
3	F	4	0	6	0	0
4	E	8	0	18	2	0
5	E	12	0	26	1	0
6	F	9	0	20	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
7	D	2	0	0	0	0
7	E	4	0	0	0	0
7	F	4	0	0	0	0
All	All	3285	0	3173	42	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 7.

All (42) 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:C:56:THR:HG21	1:D:94:ARG:HG3	1.74	0.68
1:E:70:LEU:O	1:E:77:GLN:NE2	2.31	0.62
1:E:89:ARG:HH22	3:E:204:EDO:HO1	1.52	0.56
1:E:121:VAL:HG22	5:E:203:D12:H72	1.90	0.53
1:F:104:ASN:OD1	1:F:109:ARG:NH1	2.42	0.53
1:A:98:ASP:O	1:A:101:SER:OG	2.27	0.52
1:A:70:LEU:HD13	1:B:66:ILE:HG21	1.91	0.52
1:D:83:VAL:HG11	1:D:120:LEU:HD11	1.90	0.52
1:A:114:PHE:HD2	1:B:111:VAL:HG13	1.75	0.52
1:B:102:ASP:O	1:B:104:ASN:N	2.39	0.52
1:A:115:TYR:CZ	1:A:119:LYS:HD2	2.45	0.51
1:E:115:TYR:CZ	1:E:119:LYS:HD2	2.46	0.51
1:F:89:ARG:HG2	6:F:201:DD9:H1	1.92	0.51
1:D:115:TYR:CZ	1:D:119:LYS:HD2	2.46	0.50
1:A:115:TYR:HB2	1:B:111:VAL:HG11	1.94	0.49
1:A:115:TYR:HD1	1:B:111:VAL:HG21	1.77	0.49
1:F:53:ASP:OD1	1:F:54:ALA:N	2.47	0.47
1:E:75:GLU:HG2	1:E:79:MET:HE2	1.96	0.47
1:D:93[A]:PHE:HE1	1:E:97:ALA:HA	1.80	0.47
1:E:114:PHE:HD1	4:E:202:OCT:H72	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:VAL:O	1:B:114:PHE:N	2.50	0.44
1:C:95:VAL:HG22	1:D:56:THR:HB	1.98	0.44
1:F:115:TYR:CZ	1:F:119:LYS:HD2	2.52	0.44
1:A:66:ILE:HG12	1:B:70:LEU:HD22	2.00	0.44
1:B:57:LYS:O	1:B:61:GLU:HG2	2.18	0.43
1:E:121:VAL:HG21	4:E:202:OCT:H22	2.01	0.43
1:F:73:ASN:O	1:F:77:GLN:HG2	2.19	0.43
1:D:73:ASN:O	1:D:77:GLN:HG2	2.20	0.42
1:B:116:PHE:HA	1:B:119:LYS:HD3	2.02	0.42
1:A:92:PHE:CE1	1:A:117:ALA:HB2	2.55	0.41
1:C:98:ASP:OD2	1:D:57:LYS:HD2	2.20	0.41
1:A:73:ASN:O	1:A:77:GLN:HG2	2.20	0.41
1:E:116:PHE:CE1	1:F:59:LEU:HD21	2.55	0.41
1:C:116:PHE:CE1	1:D:59:LEU:HD21	2.56	0.41
1:D:58:LYS:HE2	1:D:58:LYS:HB3	1.84	0.41
1:E:99:MET:HA	1:F:64:LYS:HE2	2.03	0.41
1:E:73:ASN:O	1:E:77:GLN:HG2	2.20	0.41
1:E:92:PHE:CE1	1:E:117:ALA:HB2	2.55	0.41
1:A:89:ARG:NH1	1:F:105:PHE:HB3	2.36	0.40
1:E:111:VAL:HG13	1:F:111:VAL:HG13	2.04	0.40
1:A:99:MET:HE2	1:A:99:MET:HB3	1.99	0.40
1:E:115:TYR:HB2	1:F:111:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	59/81 (73%)	56 (95%)	3 (5%)	0	100	100
1	B	58/81 (72%)	51 (88%)	6 (10%)	1 (2%)	7	5
1	C	66/81 (82%)	65 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	70/81 (86%)	69 (99%)	1 (1%)	0	100	100
1	E	76/81 (94%)	71 (93%)	5 (7%)	0	100	100
1	F	75/81 (93%)	72 (96%)	3 (4%)	0	100	100
All	All	404/486 (83%)	384 (95%)	19 (5%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	GLY

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	48/68 (71%)	44 (92%)	4 (8%)	10	11
1	B	43/68 (63%)	43 (100%)	0	100	100
1	C	51/68 (75%)	50 (98%)	1 (2%)	48	64
1	D	59/68 (87%)	57 (97%)	2 (3%)	32	44
1	E	64/68 (94%)	63 (98%)	1 (2%)	55	71
1	F	58/68 (85%)	56 (97%)	2 (3%)	32	44
All	All	323/408 (79%)	313 (97%)	10 (3%)	35	48

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	91	VAL
1	D	121	VAL
1	D	122	LEU
1	A	61	GLU
1	A	71	ASP
1	A	101	SER
1	A	122	LEU

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Mol	Chain	Res	Type
1	E	71	ASP
1	F	102	ASP
1	F	111	VAL

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	106	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands 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	$\# Z > 2$
2	1GP	D	201	-	9,9,9	0.88	0	10,12,12	0.67	0
3	EDO	F	202	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	D	202	-	3,3,3	0.43	0	2,2,2	0.38	0
5	D12	E	203	-	11,11,11	0.30	0	10,10,10	0.84	0
4	OCT	E	202	-	7,7,7	0.30	0	6,6,6	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	E	201	-	3,3,3	0.45	0	2,2,2	0.24	0
3	EDO	E	204	-	3,3,3	0.43	0	2,2,2	0.34	0
3	EDO	A	201	-	3,3,3	0.42	0	2,2,2	0.39	0
6	DD9	F	201	-	8,8,8	0.28	0	7,7,7	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1GP	D	201	-	-	2/8/8/8	-
3	EDO	F	202	-	-	0/1/1/1	-
3	EDO	D	202	-	-	0/1/1/1	-
5	D12	E	203	-	-	5/9/9/9	-
4	OCT	E	202	-	-	2/5/5/5	-
3	EDO	E	201	-	-	0/1/1/1	-
3	EDO	E	204	-	-	0/1/1/1	-
3	EDO	A	201	-	-	0/1/1/1	-
6	DD9	F	201	-	-	3/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	201	1GP	C1-C2-C3-O2
5	E	203	D12	C2-C3-C4-C5
4	E	202	OCT	C4-C5-C6-C7
6	F	201	DD9	C3-C4-C5-C6
5	E	203	D12	C5-C6-C7-C8
6	F	201	DD9	C4-C5-C6-C7
2	D	201	1GP	O3-C2-C3-O2
6	F	201	DD9	C2-C3-C4-C5
5	E	203	D12	C1-C2-C3-C4
5	E	203	D12	C7-C8-C9-C10
4	E	202	OCT	C3-C4-C5-C6
5	E	203	D12	C3-C4-C5-C6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	203	D12	1	0
4	E	202	OCT	2	0
3	E	204	EDO	1	0
6	F	201	DD9	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 ⓘ

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	63/81 (77%)	1.20	10 (15%) 5 3	77, 114, 164, 174	0
1	B	62/81 (76%)	1.41	18 (29%) 1 1	86, 125, 170, 186	0
1	C	70/81 (86%)	0.65	5 (7%) 22 19	53, 76, 131, 165	0
1	D	71/81 (87%)	0.87	9 (12%) 8 6	39, 72, 128, 151	1 (1%)
1	E	78/81 (96%)	0.92	9 (11%) 9 7	54, 88, 148, 251	0
1	F	77/81 (95%)	0.73	8 (10%) 11 9	54, 76, 147, 169	0
All	All	421/486 (86%)	0.95	59 (14%) 6 4	39, 92, 159, 251	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	ILE	5.2
1	F	50	LEU	5.1
1	D	93[A]	PHE	4.2
1	B	78	ARG	4.1
1	E	50	LEU	4.0
1	B	107	TRP	3.8
1	B	114	PHE	3.5
1	D	54	ALA	3.5
1	A	103	GLY	3.5
1	C	88	PRO	3.1
1	B	120	LEU	3.0
1	B	104	ASN	3.0
1	A	59	LEU	2.9
1	D	90	GLU	2.9
1	A	87	SER	2.7
1	F	125	LEU	2.7
1	A	66	ILE	2.7
1	C	85	THR	2.7
1	C	120	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	83	VAL	2.7
1	A	82	ALA	2.6
1	A	114	PHE	2.6
1	B	86	ASP	2.6
1	B	121	VAL	2.6
1	B	88	PRO	2.6
1	B	110	VAL	2.5
1	A	62	SER	2.5
1	D	85	THR	2.5
1	C	53	ASP	2.4
1	E	49	PRO	2.4
1	B	74	MET	2.4
1	B	89	ARG	2.4
1	B	106	ASN	2.4
1	E	86	ASP	2.3
1	D	121	VAL	2.3
1	B	76	LEU	2.3
1	B	75	GLU	2.3
1	B	97	ALA	2.3
1	D	74	MET	2.3
1	E	121	VAL	2.3
1	E	124	ALA	2.3
1	F	86	ASP	2.3
1	D	120	LEU	2.2
1	D	86	ASP	2.2
1	F	103	GLY	2.2
1	A	70	LEU	2.2
1	B	79	MET	2.2
1	E	114	PHE	2.2
1	F	104	ASN	2.1
1	E	103	GLY	2.1
1	C	54	ALA	2.1
1	F	85	THR	2.1
1	E	80	ILE	2.1
1	D	124	ALA	2.0
1	A	112	ALA	2.0
1	B	54	ALA	2.0
1	B	111	VAL	2.0
1	F	54	ALA	2.0
1	F	120	LEU	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	1GP	D	201	10/10	0.42	0.16	131,134,142,149	0
3	EDO	A	201	4/4	0.67	0.12	101,104,108,110	0
5	D12	E	203	12/12	0.71	0.25	86,90,105,105	0
4	OCT	E	202	8/8	0.75	0.26	81,91,100,101	0
3	EDO	F	202	4/4	0.81	0.12	91,95,100,104	0
3	EDO	D	202	4/4	0.86	0.12	84,89,91,98	0
6	DD9	F	201	9/9	0.89	0.23	69,75,85,86	0
3	EDO	E	204	4/4	0.90	0.13	71,81,86,93	0
3	EDO	E	201	4/4	0.93	0.17	76,81,82,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.