



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2020 – 08:10 AM EDT

PDB ID : 6ODH
Title : BH3 domain swapped dimer of a BAK fragment
Authors : Liu, L.-K.
Deposited on : 2019-03-26
Resolution : 2.30 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 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) : 1.13
EDS : 2.14.6
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

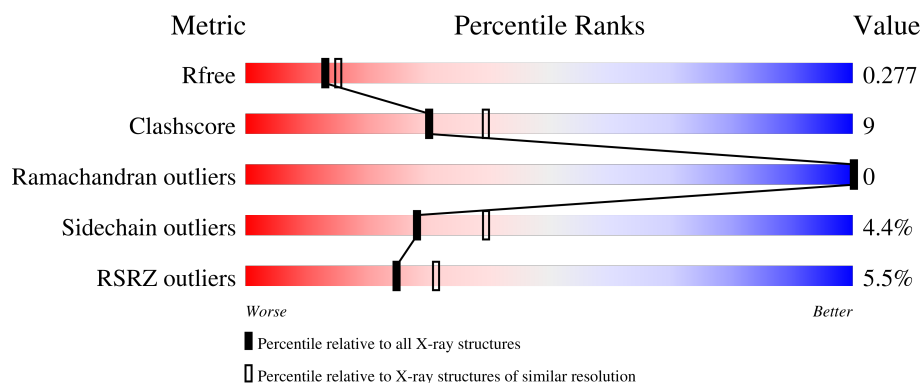
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	84	<div> <div>4%</div> <div>65% 24% 10%</div> </div>
1	B	84	<div> <div>64% 23% 12%</div> </div>
1	C	84	<div> <div>5%</div> <div>83% 10% 7%</div> </div>
1	D	84	<div> <div>8%</div> <div>75% 12% 11%</div> </div>
1	E	84	<div> <div>6%</div> <div>69% 19% 11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	84	<div><div></div><div>7%</div><div>65%</div><div>21%</div><div>•</div><div>12%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3794 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 Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	76	Total	C	N	O	S	0	0	0
			606	386	108	110	2			
1	B	74	Total	C	N	O	S	0	0	0
			599	384	104	109	2			
1	C	78	Total	C	N	O	S	0	0	0
			622	399	110	112	1			
1	D	75	Total	C	N	O	S	0	0	0
			591	375	105	109	2			
1	E	75	Total	C	N	O	S	0	0	0
			609	390	107	110	2			
1	F	74	Total	C	N	O	S	0	0	0
			589	379	100	108	2			

There are 42 discrepancies between the modelled and reference sequences:

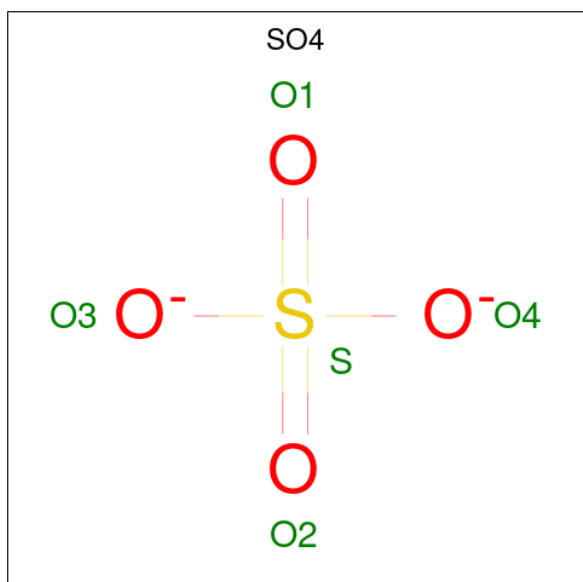
Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLU	-	expression tag	UNP Q16611
A	149	GLU	-	expression tag	UNP Q16611
A	150	ASN	-	expression tag	UNP Q16611
A	151	LEU	-	expression tag	UNP Q16611
A	152	TYR	-	expression tag	UNP Q16611
A	153	PHE	-	expression tag	UNP Q16611
A	154	GLN	-	expression tag	UNP Q16611
B	148	GLU	-	expression tag	UNP Q16611
B	149	GLU	-	expression tag	UNP Q16611
B	150	ASN	-	expression tag	UNP Q16611
B	151	LEU	-	expression tag	UNP Q16611
B	152	TYR	-	expression tag	UNP Q16611
B	153	PHE	-	expression tag	UNP Q16611
B	154	GLN	-	expression tag	UNP Q16611
C	148	GLU	-	expression tag	UNP Q16611
C	149	GLU	-	expression tag	UNP Q16611
C	150	ASN	-	expression tag	UNP Q16611

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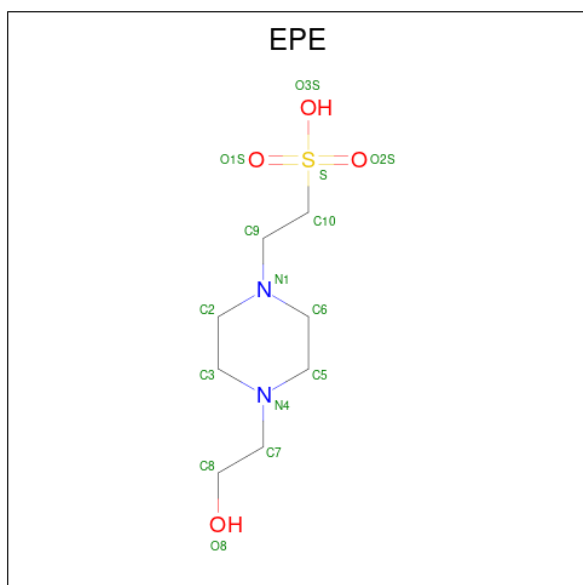
Chain	Residue	Modelled	Actual	Comment	Reference
C	151	LEU	-	expression tag	UNP Q16611
C	152	TYR	-	expression tag	UNP Q16611
C	153	PHE	-	expression tag	UNP Q16611
C	154	GLN	-	expression tag	UNP Q16611
D	148	GLU	-	expression tag	UNP Q16611
D	149	GLU	-	expression tag	UNP Q16611
D	150	ASN	-	expression tag	UNP Q16611
D	151	LEU	-	expression tag	UNP Q16611
D	152	TYR	-	expression tag	UNP Q16611
D	153	PHE	-	expression tag	UNP Q16611
D	154	GLN	-	expression tag	UNP Q16611
E	148	GLU	-	expression tag	UNP Q16611
E	149	GLU	-	expression tag	UNP Q16611
E	150	ASN	-	expression tag	UNP Q16611
E	151	LEU	-	expression tag	UNP Q16611
E	152	TYR	-	expression tag	UNP Q16611
E	153	PHE	-	expression tag	UNP Q16611
E	154	GLN	-	expression tag	UNP Q16611
F	148	GLU	-	expression tag	UNP Q16611
F	149	GLU	-	expression tag	UNP Q16611
F	150	ASN	-	expression tag	UNP Q16611
F	151	LEU	-	expression tag	UNP Q16611
F	152	TYR	-	expression tag	UNP Q16611
F	153	PHE	-	expression tag	UNP Q16611
F	154	GLN	-	expression tag	UNP Q16611

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			30	16	4	8	2		
3	A	1	Total	C	N	O	S	0	1
			30	16	4	8	2		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	E	1	Total	C	N	O	S	0	1
			30	16	4	8	2		
3	E	1	Total	C	N	O	S	0	1
			30	16	4	8	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

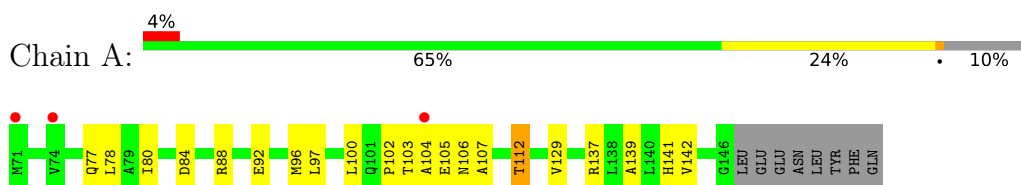
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	3	Total	O	0	0
			3	3		
5	C	1	Total	O	0	0
			1	1		
5	D	2	Total	O	0	0
			2	2		
5	E	4	Total	O	0	0
			4	4		
5	F	6	Total	O	0	0
			6	6		

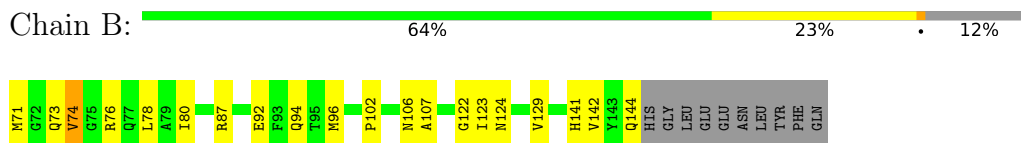
3 Residue-property plots [i](#)

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.

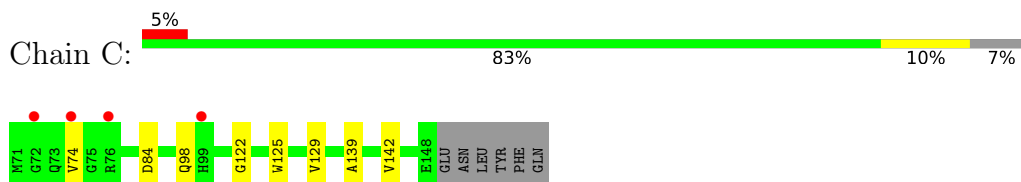
- Molecule 1: Bcl-2 homologous antagonist/killer



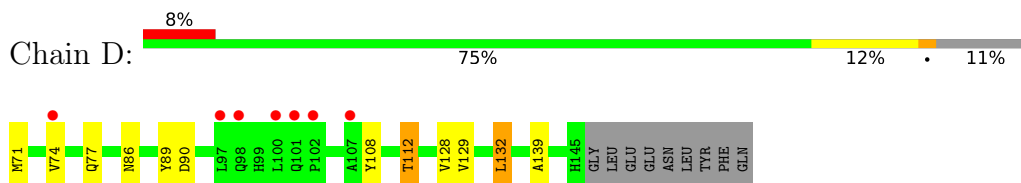
- Molecule 1: Bcl-2 homologous antagonist/killer



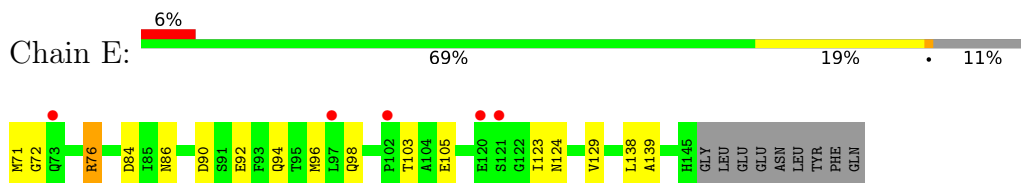
- Molecule 1: Bcl-2 homologous antagonist/killer



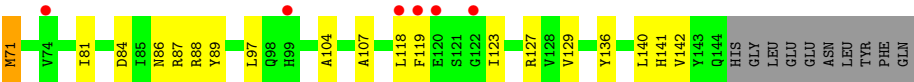
- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 1: Bcl-2 homologous antagonist/killer



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.04Å 55.04Å 55.68Å 117.13° 107.97° 97.55°	Depositor
Resolution (Å)	32.52 – 2.30 46.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.1 (32.52-2.30) 97.1 (46.94-2.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.214 , 0.271 0.219 , 0.277	Depositor DCC
R_{free} test set	882 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3794	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.44% 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: PEG, EPE, SO4

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	0.27	0/619	0.43	0/836
1	B	0.28	0/612	0.47	0/827
1	C	0.26	0/636	0.41	0/861
1	D	0.25	0/603	0.42	0/815
1	E	0.28	0/623	0.43	0/842
1	F	0.30	0/602	0.48	0/815
All	All	0.27	0/3695	0.44	0/4996

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	606	0	585	16	0
1	B	599	0	582	13	0
1	C	622	0	595	6	0
1	D	591	0	559	7	0
1	E	609	0	589	15	0
1	F	589	0	565	17	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
3	A	60	0	68	8	0
3	C	15	0	17	2	0
3	E	60	0	68	14	0
4	D	7	0	10	1	0
4	F	7	0	10	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	4	0	0	1	0
5	F	6	0	0	0	0
All	All	3794	0	3648	69	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 9.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:THR:HG23	1:A:105:GLU:H	1.47	0.77
1:B:102:PRO:HA	1:B:106:ASN:HD21	1.54	0.72
3:A:203[B]:EPE:H21	1:B:123:ILE:HG12	1.74	0.69
1:E:124:ASN:HA	3:E:202[B]:EPE:H101	1.75	0.67
1:E:123:ILE:HG12	3:E:202[B]:EPE:H22	1.77	0.66
1:E:71:MET:N	5:E:301:HOH:O	2.28	0.66
1:C:129:VAL:HG22	1:D:129:VAL:HB	1.79	0.65
1:A:107:ALA:HB1	3:E:201[A]:EPE:H32	1.80	0.64
1:E:84:ASP:OD2	1:F:89:TYR:OH	2.14	0.64
1:A:139:ALA:HA	3:E:201[B]:EPE:H21	1.79	0.63
1:A:84:ASP:OD2	1:A:88:ARG:NH2	2.32	0.62
3:A:203[A]:EPE:H92	1:B:124:ASN:HA	1.80	0.62
1:F:84:ASP:OD1	1:F:87:ARG:NH2	2.32	0.61
3:A:202[A]:EPE:H52	1:C:139:ALA:HA	1.83	0.60
3:E:201[A]:EPE:H61	1:F:123:ILE:HG12	1.86	0.58
1:E:129:VAL:HB	1:F:129:VAL:HB	1.86	0.56
1:F:118:LEU:HD11	1:F:127:ARG:HB3	1.86	0.56
1:D:139:ALA:HA	3:E:202[A]:EPE:H61	1.87	0.56
1:B:122:GLY:HA2	1:E:105:GLU:HA	1.88	0.56
1:B:71:MET:HB2	1:B:74:VAL:HG22	1.87	0.55
1:F:104:ALA:HA	1:F:142:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG13	1:B:129:VAL:HB	1.90	0.54
1:E:103:THR:HG23	1:E:105:GLU:H	1.72	0.54
1:F:71:MET:SD	1:F:71:MET:N	2.81	0.53
1:B:102:PRO:HD2	1:B:141:HIS:CE1	2.43	0.52
3:A:203[A]:EPE:H62	1:B:123:ILE:HG23	1.91	0.52
1:A:103:THR:N	1:A:106:ASN:OD1	2.30	0.52
3:A:203[A]:EPE:H32	1:E:139:ALA:HB2	1.93	0.49
1:A:142:VAL:HB	3:E:201[B]:EPE:H22	1.95	0.49
1:A:92:GLU:O	1:A:96:MET:HG3	2.13	0.49
1:E:86:ASN:O	1:E:90:ASP:HB2	2.12	0.49
1:E:90:ASP:O	1:E:94:GLN:HG2	2.13	0.48
1:A:112:THR:HG21	3:C:201:EPE:H22	1.95	0.48
1:B:92:GLU:O	1:B:96:MET:HG3	2.13	0.48
1:D:128:VAL:O	1:D:132:LEU:HD12	2.14	0.47
1:D:108:TYR:O	1:D:112:THR:OG1	2.31	0.47
1:F:84:ASP:O	1:F:88:ARG:HG3	2.14	0.47
1:B:107:ALA:HB2	1:B:142:VAL:HG21	1.95	0.46
1:D:86:ASN:O	1:D:90:ASP:HB2	2.15	0.46
3:E:201[B]:EPE:H52	1:F:123:ILE:HG12	1.98	0.46
1:F:107:ALA:HB2	1:F:142:VAL:HG21	1.98	0.45
1:A:139:ALA:HA	3:E:201[A]:EPE:H21	1.98	0.45
1:A:139:ALA:HA	3:E:201[A]:EPE:C2	2.48	0.44
1:A:102:PRO:HA	1:A:106:ASN:HD21	1.83	0.44
3:C:201:EPE:H81	3:C:201:EPE:H32	1.74	0.44
1:A:104:ALA:O	1:F:123:ILE:HG22	2.18	0.44
1:F:97:LEU:HD13	1:F:141:HIS:HB2	1.99	0.44
3:E:202[B]:EPE:H92	1:F:136:TYR:OH	2.18	0.43
3:A:203[B]:EPE:H82	1:E:138:LEU:HD23	2.00	0.43
1:F:136:TYR:CZ	1:F:140:LEU:HD11	2.54	0.43
1:B:141:HIS:O	1:B:144:GLN:HG3	2.18	0.43
3:A:202[B]:EPE:O2S	3:A:202[B]:EPE:H61	2.19	0.42
1:B:71:MET:HB3	1:B:73:GLN:H	1.85	0.42
1:E:96:MET:HB3	1:E:96:MET:HE2	1.83	0.41
1:A:97:LEU:HD13	1:A:141:HIS:HB2	2.01	0.41
1:C:122:GLY:HA2	1:F:104:ALA:O	2.20	0.41
1:E:123:ILE:O	3:E:202[B]:EPE:H21	2.19	0.41
1:E:72:GLY:O	1:E:76:ARG:HD3	2.19	0.41
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.89	0.41
1:C:125:TRP:HA	4:D:201:PEG:H41	2.02	0.41
3:E:202[A]:EPE:N1	3:E:202[A]:EPE:O1S	2.53	0.41
3:A:202[B]:EPE:H31	1:C:142:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:GLU:CD	1:F:81:ILE:HD11	2.41	0.41
1:A:77:GLN:HA	1:A:80:ILE:HD12	2.02	0.41
1:C:84:ASP:OD2	1:D:89:TYR:OH	2.26	0.41
1:D:71:MET:O	1:D:74:VAL:HG12	2.21	0.41
1:F:119:PHE:CD1	1:F:123:ILE:HD12	2.55	0.41
1:B:76:ARG:O	1:B:80:ILE:HD13	2.20	0.41
3:E:201[A]:EPE:H21	3:E:201[A]:EPE:H102	1.71	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	74/84 (88%)	74 (100%)	0	0	100	100
1	B	72/84 (86%)	70 (97%)	2 (3%)	0	100	100
1	C	76/84 (90%)	75 (99%)	1 (1%)	0	100	100
1	D	73/84 (87%)	73 (100%)	0	0	100	100
1	E	73/84 (87%)	70 (96%)	3 (4%)	0	100	100
1	F	72/84 (86%)	72 (100%)	0	0	100	100
All	All	440/504 (87%)	434 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	61/70 (87%)	58 (95%)	3 (5%)	25	35
1	B	61/70 (87%)	57 (93%)	4 (7%)	16	22
1	C	61/70 (87%)	59 (97%)	2 (3%)	38	53
1	D	58/70 (83%)	55 (95%)	3 (5%)	23	32
1	E	62/70 (89%)	60 (97%)	2 (3%)	39	54
1	F	59/70 (84%)	57 (97%)	2 (3%)	37	51
All	All	362/420 (86%)	346 (96%)	16 (4%)	28	39

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	112	THR
1	A	137	ARG
1	B	74	VAL
1	B	78	LEU
1	B	87	ARG
1	B	94	GLN
1	C	74	VAL
1	C	98	GLN
1	D	77	GLN
1	D	112	THR
1	D	132	LEU
1	E	76	ARG
1	E	98	GLN
1	F	71	MET
1	F	86	ASN

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 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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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$
3	EPE	E	201[A]	-	15,15,15	0.88	1 (6%)	18,20,20	1.94	5 (27%)
3	EPE	E	201[B]	-	15,15,15	0.76	1 (6%)	18,20,20	1.74	5 (27%)
3	EPE	A	202[B]	-	15,15,15	0.87	1 (6%)	18,20,20	2.19	8 (44%)
3	EPE	A	202[A]	-	15,15,15	0.64	0	18,20,20	1.69	5 (27%)
3	EPE	A	203[B]	-	15,15,15	0.87	1 (6%)	18,20,20	1.79	5 (27%)
4	PEG	D	201	-	6,6,6	0.49	0	5,5,5	0.29	0
4	PEG	F	201	-	6,6,6	0.48	0	5,5,5	0.30	0
3	EPE	E	202[B]	-	15,15,15	0.72	1 (6%)	18,20,20	1.43	3 (16%)
2	SO4	B	201	-	4,4,4	0.14	0	6,6,6	0.09	0
3	EPE	E	202[A]	-	15,15,15	0.91	1 (6%)	18,20,20	2.13	6 (33%)
2	SO4	A	201	-	4,4,4	0.13	0	6,6,6	0.08	0
3	EPE	A	203[A]	-	15,15,15	0.77	1 (6%)	18,20,20	1.93	5 (27%)
3	EPE	C	201	-	15,15,15	0.85	1 (6%)	18,20,20	2.10	6 (33%)

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
3	EPE	E	201[A]	-	-	6/9/19/19	0/1/1/1
3	EPE	E	201[B]	-	-	6/9/19/19	0/1/1/1
3	EPE	A	202[B]	-	-	7/9/19/19	0/1/1/1
3	EPE	A	202[A]	-	-	2/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	203[B]	-	-	4/9/19/19	0/1/1/1
4	PEG	D	201	-	-	0/4/4/4	-
3	EPE	E	202[B]	-	-	5/9/19/19	0/1/1/1
4	PEG	F	201	-	-	3/4/4/4	-
3	EPE	E	202[A]	-	-	5/9/19/19	0/1/1/1
3	EPE	A	203[A]	-	-	6/9/19/19	0/1/1/1
3	EPE	C	201	-	-	2/9/19/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	202[A]	EPE	C10-S	3.15	1.82	1.77
3	E	201[A]	EPE	C10-S	2.94	1.81	1.77
3	A	203[B]	EPE	C10-S	2.94	1.81	1.77
3	A	202[B]	EPE	C10-S	2.92	1.81	1.77
3	C	201	EPE	C10-S	2.69	1.81	1.77
3	E	201[B]	EPE	C10-S	2.54	1.81	1.77
3	A	203[A]	EPE	C10-S	2.51	1.81	1.77
3	E	202[B]	EPE	C10-S	2.09	1.80	1.77

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	202[A]	EPE	C5-N4-C3	5.58	121.38	108.83
3	A	202[B]	EPE	C5-N4-C3	5.12	120.35	108.83
3	A	203[A]	EPE	C5-N4-C3	4.69	119.39	108.83
3	E	201[A]	EPE	C5-N4-C3	4.40	118.74	108.83
3	A	203[B]	EPE	C5-N4-C3	4.39	118.70	108.83
3	C	201	EPE	C6-N1-C2	4.35	118.63	108.83
3	E	201[B]	EPE	C5-N4-C3	4.30	118.51	108.83
3	E	201[A]	EPE	C7-N4-C3	3.64	120.54	111.23
3	A	202[A]	EPE	C5-N4-C3	3.61	116.95	108.83
3	A	203[A]	EPE	C7-N4-C3	3.59	120.42	111.23
3	C	201	EPE	C5-N4-C3	3.58	116.89	108.83
3	A	202[B]	EPE	C2-C3-N4	3.49	117.80	110.64
3	A	203[A]	EPE	C7-N4-C5	3.34	119.79	111.23
3	A	202[B]	EPE	O3S-S-C10	3.33	111.16	105.77
3	C	201	EPE	C7-N4-C5	3.31	119.69	111.23
3	A	202[A]	EPE	C7-N4-C3	3.29	119.64	111.23
3	E	201[A]	EPE	C7-N4-C5	3.27	119.61	111.23
3	A	202[A]	EPE	O2S-S-C10	3.16	110.72	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	202[A]	EPE	C7-N4-C5	3.11	119.18	111.23
3	E	202[A]	EPE	O3S-S-C10	3.02	110.64	105.77
3	E	202[A]	EPE	C7-N4-C3	2.99	118.89	111.23
3	E	201[A]	EPE	O1S-S-C10	2.95	110.47	106.92
3	A	203[B]	EPE	C7-N4-C5	2.95	118.78	111.23
3	C	201	EPE	O2S-S-C10	2.90	110.40	106.92
3	A	202[B]	EPE	C7-N4-C3	2.87	118.57	111.23
3	C	201	EPE	C7-N4-C3	2.70	118.15	111.23
3	A	203[B]	EPE	O2S-S-C10	2.69	110.16	106.92
3	E	201[B]	EPE	C7-N4-C5	2.66	118.03	111.23
3	E	202[B]	EPE	C5-N4-C3	2.62	114.73	108.83
3	E	201[B]	EPE	C7-N4-C3	2.58	117.83	111.23
3	A	202[B]	EPE	C7-N4-C5	2.57	117.80	111.23
3	A	203[B]	EPE	O3S-S-C10	2.50	109.81	105.77
3	A	202[A]	EPE	C7-N4-C5	2.49	117.60	111.23
3	E	201[B]	EPE	O3S-S-C10	2.48	109.78	105.77
3	E	202[B]	EPE	C7-N4-C5	2.38	117.33	111.23
3	A	202[A]	EPE	C9-N1-C2	-2.37	105.17	111.23
3	A	202[B]	EPE	C5-C6-N1	-2.34	105.83	110.64
3	A	203[B]	EPE	C7-N4-C3	2.31	117.14	111.23
3	A	202[B]	EPE	O1S-S-C10	2.30	109.69	106.92
3	E	202[A]	EPE	C6-C5-N4	2.24	115.25	110.64
3	A	203[A]	EPE	O1S-S-C10	2.21	109.57	106.92
3	A	202[B]	EPE	O2S-S-C10	2.17	109.53	106.92
3	C	201	EPE	O1S-S-C10	2.17	109.53	106.92
3	E	202[A]	EPE	O2S-S-C10	2.15	109.50	106.92
3	E	201[B]	EPE	O2S-S-C10	2.13	109.48	106.92
3	E	201[A]	EPE	O2S-S-C10	2.13	109.47	106.92
3	A	203[A]	EPE	O2S-S-C10	2.09	109.43	106.92
3	E	202[B]	EPE	C7-N4-C3	2.07	116.52	111.23

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	201[A]	EPE	N4-C7-C8-O8
3	E	201[A]	EPE	S-C10-C9-N1
3	E	201[A]	EPE	C9-C10-S-O1S
3	E	201[A]	EPE	C9-C10-S-O3S
3	A	202[B]	EPE	C8-C7-N4-C5
3	A	202[A]	EPE	C10-C9-N1-C6
3	A	202[A]	EPE	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
3	A	203[B]	EPE	C9-C10-S-O1S
3	A	203[B]	EPE	C9-C10-S-O2S
3	A	203[B]	EPE	C9-C10-S-O3S
3	E	202[B]	EPE	S-C10-C9-N1
3	E	202[A]	EPE	C8-C7-N4-C3
3	A	203[A]	EPE	C8-C7-N4-C3
3	A	203[A]	EPE	N4-C7-C8-O8
3	A	203[A]	EPE	C9-C10-S-O2S
3	C	201	EPE	C8-C7-N4-C3
3	C	201	EPE	S-C10-C9-N1
3	A	202[B]	EPE	N4-C7-C8-O8
4	F	201	PEG	O2-C3-C4-O4
3	A	202[B]	EPE	C9-C10-S-O3S
3	E	202[B]	EPE	C9-C10-S-O3S
3	E	201[B]	EPE	N4-C7-C8-O8
3	E	202[A]	EPE	N4-C7-C8-O8
3	E	202[A]	EPE	S-C10-C9-N1
3	E	202[B]	EPE	C8-C7-N4-C3
3	E	201[B]	EPE	C10-C9-N1-C2
3	E	201[B]	EPE	C10-C9-N1-C6
3	E	201[A]	EPE	C9-C10-S-O2S
3	A	202[B]	EPE	C9-C10-S-O1S
3	A	202[B]	EPE	C9-C10-S-O2S
3	A	203[A]	EPE	C9-C10-S-O1S
4	F	201	PEG	O1-C1-C2-O2
3	A	203[B]	EPE	N4-C7-C8-O8
3	E	201[A]	EPE	C8-C7-N4-C5
3	E	201[B]	EPE	C8-C7-N4-C5
4	F	201	PEG	C1-C2-O2-C3
3	A	202[B]	EPE	C10-C9-N1-C2
3	A	202[B]	EPE	C10-C9-N1-C6
3	E	202[A]	EPE	C10-C9-N1-C2
3	E	202[A]	EPE	C10-C9-N1-C6
3	E	202[B]	EPE	C8-C7-N4-C5
3	E	201[B]	EPE	C8-C7-N4-C3
3	A	203[A]	EPE	C9-C10-S-O3S
3	A	203[A]	EPE	C8-C7-N4-C5
3	E	201[B]	EPE	C9-C10-S-O2S
3	E	202[B]	EPE	C9-C10-S-O1S

There are no ring outliers.

10 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	201[A]	EPE	5	0
3	E	201[B]	EPE	3	0
3	A	202[B]	EPE	2	0
3	A	202[A]	EPE	1	0
3	A	203[B]	EPE	2	0
4	D	201	PEG	1	0
3	E	202[B]	EPE	4	0
3	E	202[A]	EPE	2	0
3	A	203[A]	EPE	3	0
3	C	201	EPE	2	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	76/84 (90%)	0.30	3 (3%) 39 46	45, 78, 120, 137	0
1	B	74/84 (88%)	0.00	0 100 100	43, 75, 116, 157	0
1	C	78/84 (92%)	0.14	4 (5%) 28 35	39, 66, 116, 136	0
1	D	75/84 (89%)	0.44	7 (9%) 8 11	50, 80, 124, 156	0
1	E	75/84 (89%)	0.21	5 (6%) 17 23	43, 75, 115, 139	0
1	F	74/84 (88%)	0.34	6 (8%) 12 16	47, 74, 119, 187	0
All	All	452/504 (89%)	0.24	25 (5%) 25 31	39, 75, 120, 187	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	100	LEU	6.4
1	A	71	MET	5.2
1	D	101	GLN	4.2
1	C	74	VAL	4.1
1	F	120	GLU	3.7
1	F	122	GLY	3.5
1	D	98	GLN	3.4
1	E	97	LEU	3.3
1	F	74	VAL	3.2
1	D	102	PRO	2.9
1	E	121	SER	2.7
1	D	97	LEU	2.6
1	F	118	LEU	2.6
1	D	74	VAL	2.6
1	E	73	GLN	2.6
1	E	102	PRO	2.5
1	E	120	GLU	2.5
1	C	72	GLY	2.4
1	C	76	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	107	ALA	2.3
1	C	99	HIS	2.2
1	A	74	VAL	2.1
1	F	99	HIS	2.1
1	F	119	PHE	2.1
1	A	104	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	201	5/5	0.53	0.18	142,147,151,154	0
3	EPE	C	201	15/15	0.69	0.18	103,130,167,171	0
4	PEG	F	201	7/7	0.71	0.26	87,100,107,114	0
4	PEG	D	201	7/7	0.75	0.21	77,81,87,93	0
3	EPE	A	203[A]	15/15	0.77	0.29	51,69,74,75	15
3	EPE	A	203[B]	15/15	0.77	0.29	50,67,72,73	15
3	EPE	E	201[A]	15/15	0.82	0.28	61,74,83,83	15
3	EPE	E	201[B]	15/15	0.82	0.28	56,76,83,86	15
3	EPE	A	202[A]	15/15	0.84	0.29	45,64,69,69	15
3	EPE	A	202[B]	15/15	0.84	0.29	62,65,74,75	15
2	SO4	B	201	5/5	0.84	0.20	122,130,132,133	0
3	EPE	E	202[A]	15/15	0.86	0.28	50,70,80,81	15
3	EPE	E	202[B]	15/15	0.86	0.28	52,69,79,80	15

6.5 Other polymers [i](#)

There are no such residues in this entry.