



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:48 AM UTC

PDB ID : 6EOP / pdb_00006eop
Title : DPP8 - SLRFLYEG, space group 20
Authors : Ross, B.R.; Huber, R.
Deposited on : 2017-10-10
Resolution : 2.40 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

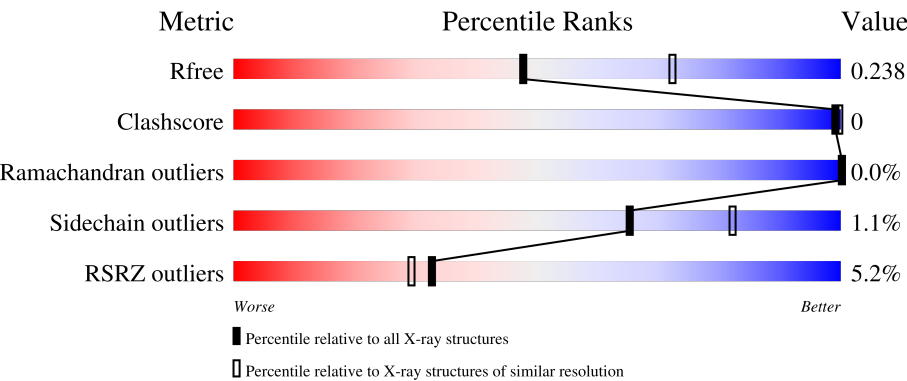
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	898	4% 91% 6%
1	B	898	5% 91% 7%
1	C	898	5% 92% 7%
2	D	8	25% 100%
2	E	8	38% 100%

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Mol	Chain	Length	Quality of chain
2	F	8	12% 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21351 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.

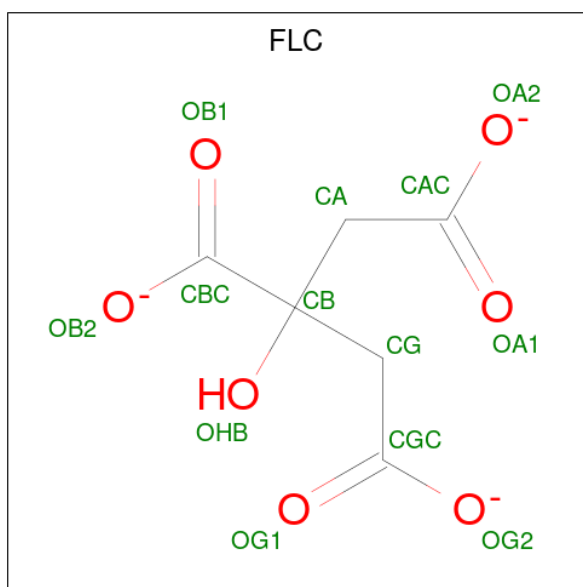
- Molecule 1 is a protein called Dipeptidyl peptidase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6849	4398	1151	1271	29			
1	B	838	Total	C	N	O	S	0	0	0
			6821	4380	1146	1266	29			
1	C	837	Total	C	N	O	S	0	0	0
			6815	4377	1145	1264	29			

- Molecule 2 is a protein called SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	8	Total	C	N	O	0	0	0
			69	46	11	12			
2	E	8	Total	C	N	O	0	0	0
			69	46	11	12			
2	F	8	Total	C	N	O	0	0	0
			69	46	11	12			

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $\text{C}_6\text{H}_5\text{O}_7$).

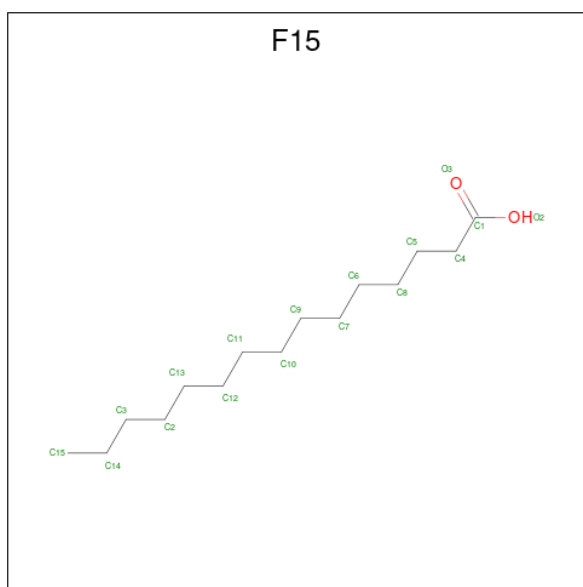


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is PENTADECANOIC ACID (CCD ID: F15) (formula: C₁₅H₃₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			17	15	2		
5	E	1	Total	C	O	0	0
			17	15	2		
5	F	1	Total	C	O	0	0
			17	15	2		

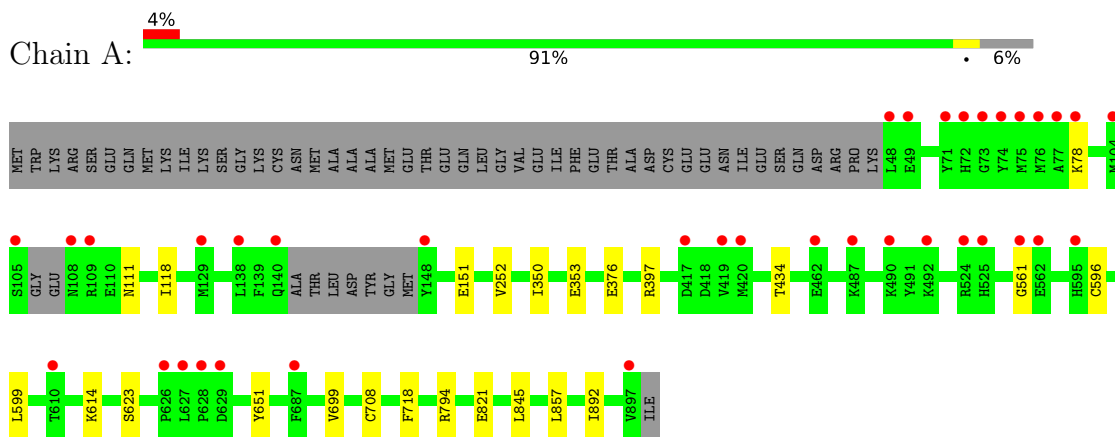
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	214	Total	O	0	0
			214	214		
6	B	215	Total	O	0	0
			215	215		
6	C	158	Total	O	0	0
			158	158		
6	D	2	Total	O	0	0
			2	2		
6	E	1	Total	O	0	0
			1	1		
6	F	2	Total	O	0	0
			2	2		

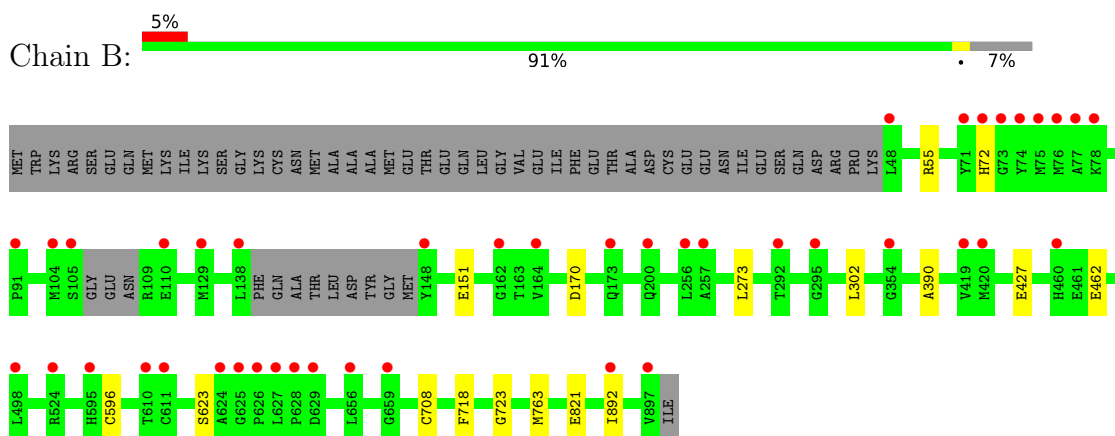
3 Residue-property plots [i](#)

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.

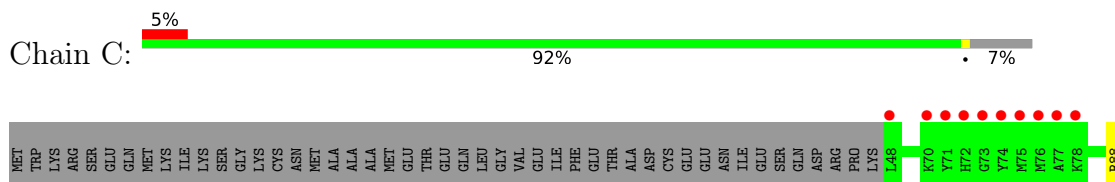
- Molecule 1: Dipeptidyl peptidase 8

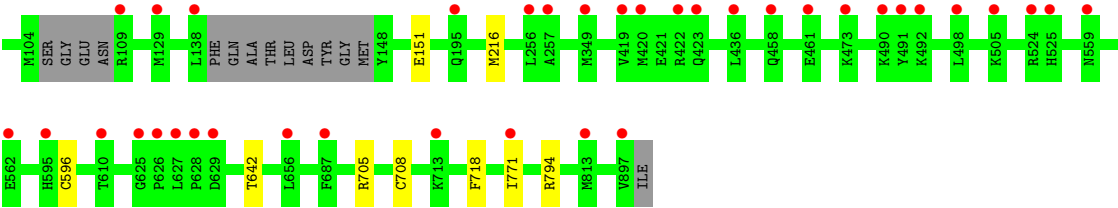


- Molecule 1: Dipeptidyl peptidase 8



- Molecule 1: Dipeptidyl peptidase 8

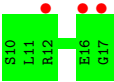




● Molecule 2: SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY



● Molecule 2: SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY



● Molecule 2: SER-LEU-ARG-PHE-LEU-TYR-GLU-GLY



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	162.83Å 246.37Å 261.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.62 – 2.40 44.62 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.62-2.40) 99.9 (44.62-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.214 , 0.237 0.216 , 0.238	Depositor DCC
R_{free} test set	10161 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21351	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: CME, F15, CA, FLC

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	0.51	0/7027	0.73	0/9528
1	B	0.50	0/6998	0.73	0/9489
1	C	0.51	0/6992	0.73	0/9481
2	D	0.51	0/70	0.56	0/92
2	E	0.45	0/70	0.54	0/92
2	F	0.54	0/70	0.55	0/92
All	All	0.51	0/21227	0.73	0/28774

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	6849	0	6668	7	0
1	B	6821	0	6646	5	0
1	C	6815	0	6640	2	0
2	D	69	0	66	0	0
2	E	69	0	66	0	0
2	F	69	0	66	0	0
3	A	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	D	17	0	29	0	0
5	E	17	0	29	0	0
5	F	17	0	29	0	0
6	A	214	0	0	1	0
6	B	215	0	0	0	0
6	C	158	0	0	1	0
6	D	2	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	0	0
All	All	21351	0	20244	14	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 0.

All (14) 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:B:723:GLY:HA3	1:B:763:MET:HE2	1.97	0.47
1:C:642:THR:HG21	1:C:705:ARG:NH1	2.30	0.46
1:B:55:ARG:HE	1:B:892:ILE:HG21	1.81	0.46
1:B:302:LEU:HD22	1:B:390:ALA:HB1	2.00	0.44
1:C:794:ARG:NH2	6:C:1002:HOH:O	2.51	0.43
1:B:596:CYS:SG	1:B:623:SER:HB2	2.59	0.42
1:B:72:HIS:O	1:B:72:HIS:CG	2.72	0.42
1:A:794:ARG:NH2	6:A:1004:HOH:O	2.53	0.42
1:A:376:GLU:HG3	1:A:397:ARG:HB2	2.01	0.42
1:A:651:TYR:HB2	1:A:699:VAL:HB	2.02	0.42
1:A:118:ILE:HD12	1:A:599:LEU:CD2	2.50	0.41
1:A:596:CYS:SG	1:A:623:SER:HB2	2.60	0.41
1:A:118:ILE:HD12	1:A:599:LEU:HD22	2.02	0.41
1:A:845:LEU:HD11	1:A:857:LEU:HD22	2.03	0.41

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	834/898 (93%)	809 (97%)	24 (3%)	1 (0%)	48	64
1	B	831/898 (92%)	805 (97%)	26 (3%)	0	100	100
1	C	830/898 (92%)	803 (97%)	27 (3%)	0	100	100
2	D	6/8 (75%)	6 (100%)	0	0	100	100
2	E	6/8 (75%)	6 (100%)	0	0	100	100
2	F	6/8 (75%)	6 (100%)	0	0	100	100
All	All	2513/2718 (92%)	2435 (97%)	77 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	561	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	746/794 (94%)	735 (98%)	11 (2%)	57	77
1	B	743/794 (94%)	736 (99%)	7 (1%)	70	85
1	C	742/794 (94%)	736 (99%)	6 (1%)	73	86
2	D	7/7 (100%)	7 (100%)	0	100	100
2	E	7/7 (100%)	7 (100%)	0	100	100
2	F	7/7 (100%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2252/2403 (94%)	2228 (99%)	24 (1%)	65 82

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LYS
1	A	111	ASN
1	A	151	GLU
1	A	252	VAL
1	A	350	ILE
1	A	353	GLU
1	A	434	THR
1	A	614	LYS
1	A	718	PHE
1	A	821	GLU
1	A	892	ILE
1	B	151	GLU
1	B	170	ASP
1	B	273	LEU
1	B	427	GLU
1	B	462	GLU
1	B	718	PHE
1	B	821	GLU
1	C	88	ARG
1	C	151	GLU
1	C	216	MET
1	C	596	CYS
1	C	718	PHE
1	C	771	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	111	ASN
1	A	123	ASN
1	A	173	GLN
1	A	188	HIS
1	A	195	GLN
1	A	232	HIS
1	A	403	GLN

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Mol	Chain	Res	Type
1	A	448	ASN
1	A	460	HIS
1	A	579	GLN
1	A	673	GLN
1	A	882	HIS
1	B	173	GLN
1	B	181	GLN
1	B	366	GLN
1	B	458	GLN
1	B	579	GLN
1	B	801	GLN
1	B	814	GLN
1	B	862	GLN
1	B	879	HIS
1	C	60	GLN
1	C	72	HIS
1	C	123	ASN
1	C	188	HIS
1	C	232	HIS
1	C	315	HIS
1	C	403	GLN
1	C	654	HIS
1	C	801	GLN
1	C	858	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	CME	A	708	1	8,9,10	0.87	0	6,9,11	1.41	2 (33%)
1	CME	C	708	1	8,9,10	0.88	0	6,9,11	1.48	1 (16%)
1	CME	B	708	1	8,9,10	0.99	1 (12%)	6,9,11	1.95	2 (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
1	CME	A	708	1	-	5/5/8/10	-
1	CME	C	708	1	-	3/5/8/10	-
1	CME	B	708	1	-	4/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	708	CME	CB-SG	-2.03	1.74	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	708	CME	CB-SG-SD	-3.43	94.99	103.86
1	B	708	CME	CB-CA-C	2.75	118.26	110.80
1	C	708	CME	CB-SG-SD	-2.60	97.13	103.86
1	A	708	CME	CB-SG-SD	-2.58	97.20	103.86
1	A	708	CME	CB-CA-C	2.10	116.49	110.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	708	CME	N-CA-CB-SG
1	A	708	CME	SD-CE-CZ-OH
1	B	708	CME	N-CA-CB-SG
1	B	708	CME	CZ-CE-SD-SG
1	A	708	CME	CE-SD-SG-CB
1	C	708	CME	SD-CE-CZ-OH
1	B	708	CME	SD-CE-CZ-OH
1	A	708	CME	CZ-CE-SD-SG

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Mol	Chain	Res	Type	Atoms
1	C	708	CME	CE-SD-SG-CB
1	A	708	CME	CA-CB-SG-SD
1	B	708	CME	CA-CB-SG-SD
1	C	708	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
5	F15	F	101	-	16,16,16	0.56	0	16,16,16	0.73	0
5	F15	D	101	-	16,16,16	0.57	0	16,16,16	0.71	0
3	FLC	A	901	-	12,12,12	1.00	0	17,17,17	1.39	1 (5%)
5	F15	E	101	-	16,16,16	0.54	0	16,16,16	0.78	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
5	F15	F	101	-	-	5/14/14/14	-
5	F15	D	101	-	-	7/14/14/14	-
3	FLC	A	901	-	-	9/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	F15	E	101	-	-	7/14/14/14	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FLC	OB2-CBC-CB	3.89	120.61	113.14

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	FLC	CG-CB-CBC-OB1
3	A	901	FLC	CG-CB-CBC-OB2
3	A	901	FLC	OHB-CB-CBC-OB1
3	A	901	FLC	OHB-CB-CBC-OB2
5	F	101	F15	C8-C6-C7-C9
5	E	101	F15	C7-C6-C8-C5
3	A	901	FLC	CAC-CA-CB-OHB
5	F	101	F15	C10-C11-C12-C13
5	E	101	F15	C4-C5-C8-C6
3	A	901	FLC	CAC-CA-CB-CBC
5	D	101	F15	C10-C11-C12-C13
5	E	101	F15	C1-C4-C5-C8
5	D	101	F15	C12-C13-C2-C3
3	A	901	FLC	CAC-CA-CB-CG
5	D	101	F15	C6-C7-C9-C10
5	D	101	F15	C1-C4-C5-C8
5	D	101	F15	C4-C5-C8-C6
5	E	101	F15	C8-C6-C7-C9
5	E	101	F15	O3-C1-C4-C5
5	E	101	F15	C9-C10-C11-C12
5	F	101	F15	O3-C1-C4-C5
5	E	101	F15	O2-C1-C4-C5
3	A	901	FLC	CA-CB-CBC-OB2
5	F	101	F15	O2-C1-C4-C5
5	F	101	F15	C9-C10-C11-C12
5	D	101	F15	C9-C10-C11-C12
5	D	101	F15	C13-C2-C3-C14
3	A	901	FLC	CA-CB-CBC-OB1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	840/898 (93%)	0.33	37 (4%)	39	34	42, 59, 96, 165	0
1	B	837/898 (93%)	0.34	43 (5%)	33	30	42, 59, 95, 152	0
1	C	836/898 (93%)	0.54	47 (5%)	30	26	46, 63, 99, 163	0
2	D	8/8 (100%)	1.15	2 (25%)	2	1	57, 63, 88, 89	0
2	E	8/8 (100%)	1.60	3 (37%)	1	0	60, 67, 92, 94	0
2	F	8/8 (100%)	1.17	1 (12%)	8	6	64, 69, 88, 90	0
All	All	2537/2718 (93%)	0.41	133 (5%)	33	29	42, 61, 97, 165	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	LEU	6.4
1	C	897	VAL	6.4
1	B	627	LEU	6.3
1	B	74	TYR	5.7
1	A	897	VAL	5.4
1	A	72	HIS	5.1
1	A	71	TYR	5.0
1	C	419	VAL	4.9
1	B	76	MET	4.8
1	C	48	LEU	4.8
1	A	627	LEU	4.7
1	B	626	PRO	4.6
1	A	74	TYR	4.6
1	C	74	TYR	4.5
1	B	71	TYR	4.4
2	E	17	GLY	4.4
1	C	627	LEU	4.4
1	C	71	TYR	4.3
1	C	76	MET	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	17	GLY	4.1
1	B	72	HIS	3.8
1	A	140	GLN	3.8
1	C	75	MET	3.8
1	A	138	LEU	3.7
1	A	78	LYS	3.7
1	A	626	PRO	3.6
1	C	72	HIS	3.6
1	B	77	ALA	3.6
1	C	129	MET	3.6
1	C	626	PRO	3.6
1	A	129	MET	3.5
1	A	628	PRO	3.5
1	A	104	MET	3.5
1	B	75	MET	3.5
1	B	138	LEU	3.5
1	B	419	VAL	3.5
1	C	687	PHE	3.4
1	B	105	SER	3.4
1	B	48	LEU	3.4
1	A	75	MET	3.4
1	A	76	MET	3.4
1	B	524	ARG	3.4
1	B	625	GLY	3.3
2	D	17	GLY	3.3
1	B	897	VAL	3.3
1	B	420	MET	3.2
1	C	109	ARG	3.2
1	A	487	LYS	3.2
1	B	256	LEU	3.2
1	B	656	LEU	3.2
1	A	524	ARG	3.1
1	C	77	ALA	3.0
1	B	78	LYS	3.0
1	A	419	VAL	3.0
1	C	610	THR	3.0
1	B	104	MET	3.0
1	A	525	HIS	3.0
1	B	628	PRO	3.0
1	C	813	MET	2.9
1	B	129	MET	2.9
1	A	687	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	524	ARG	2.8
1	B	610	THR	2.7
1	C	420	MET	2.7
1	C	73	GLY	2.7
1	C	498	LEU	2.7
1	A	77	ALA	2.7
1	B	73	GLY	2.7
1	B	659	GLY	2.7
1	C	78	LYS	2.6
1	A	109	ARG	2.6
1	B	624	ALA	2.6
1	C	595	HIS	2.6
2	E	16	GLU	2.6
1	A	105	SER	2.6
2	E	12	ARG	2.5
1	A	595	HIS	2.5
1	B	611	CYS	2.5
1	A	73	GLY	2.5
1	B	148	TYR	2.5
1	A	48	LEU	2.4
1	B	595	HIS	2.4
1	B	164	VAL	2.4
1	A	462	GLU	2.4
1	C	256	LEU	2.4
1	C	491	TYR	2.4
1	B	91	PRO	2.4
1	C	70	LYS	2.4
1	C	629	ASP	2.4
1	C	490	LYS	2.4
1	A	417	ASP	2.3
1	B	110	GLU	2.3
1	B	292	THR	2.3
2	D	12	ARG	2.3
1	C	525	HIS	2.3
1	B	173	GLN	2.3
1	B	629	ASP	2.3
1	C	656	LEU	2.2
1	C	562	GLU	2.2
1	A	108	ASN	2.2
1	A	492	LYS	2.2
1	C	628	PRO	2.2
1	C	625	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	562	GLU	2.2
1	C	473	LYS	2.2
1	A	610	THR	2.2
1	C	771	ILE	2.2
1	A	629	ASP	2.2
1	C	713	LYS	2.2
1	B	460	HIS	2.1
1	A	420	MET	2.1
1	C	458	GLN	2.1
1	C	461	GLU	2.1
1	C	195	GLN	2.1
1	C	423	GLN	2.1
1	C	349	MET	2.1
1	B	498	LEU	2.1
1	C	422	ARG	2.1
1	B	892	ILE	2.1
1	A	148	TYR	2.1
1	C	492	LYS	2.1
1	B	200	GLN	2.1
1	B	257	ALA	2.1
1	C	257	ALA	2.1
1	B	162	GLY	2.1
1	C	505	LYS	2.1
1	A	490	LYS	2.0
1	A	49	GLU	2.0
1	C	436	LEU	2.0
1	A	561	GLY	2.0
1	B	295	GLY	2.0
1	B	354	GLY	2.0
1	C	559	ASN	2.0

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

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	CME	B	708	10/11	0.87	0.18	51,62,92,96	0
1	CME	C	708	10/11	0.88	0.18	57,72,100,103	0
1	CME	A	708	10/11	0.89	0.17	59,71,97,98	0

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
3	FLC	A	901	13/13	0.50	0.25	110,120,123,124	0
5	F15	D	101	17/17	0.89	0.26	74,80,99,103	0
5	F15	F	101	17/17	0.91	0.25	83,95,103,104	0
5	F15	E	101	17/17	0.92	0.21	72,77,91,93	0
4	CA	B	901	1/1	0.93	0.13	96,96,96,96	0
4	CA	C	901	1/1	0.96	0.13	85,85,85,85	0
4	CA	A	902	1/1	0.97	0.16	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.