WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 1, 2022 – 12:44 pm GMT

PDB ID : 4UU8

Title : Crystal structure of zebrafish Sirtuin 5 in complex with 3,3-dimethyl- succiny-lated CPS1-peptide

Authors : Pannek, M.; Gertz, M.; Steegborn, C.

Deposited on : 2014-07-24

Resolution : 2.90 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.90 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	Percentile Ranks	Value
Rfree		0.250
Clashscore		7
Ramachandran outliers		0.6%
Sidechain outliers		7.4%
RSRZ outliers		1.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
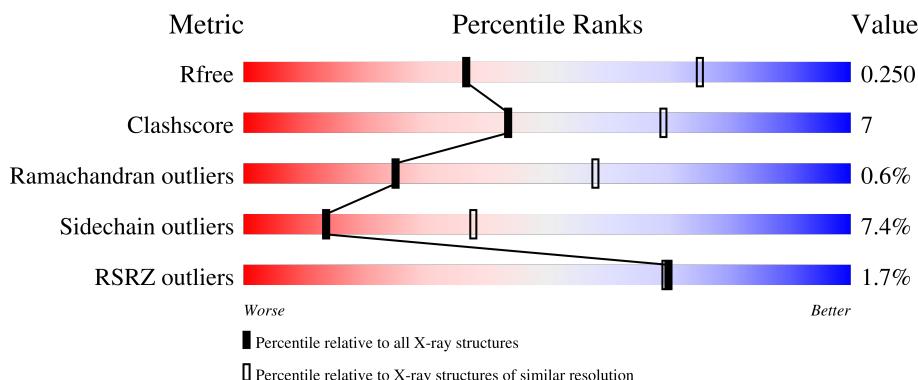
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	275	73% 20% • 5%
1	B	275	3% 79% 16% • •
2	D	9	78% 22%
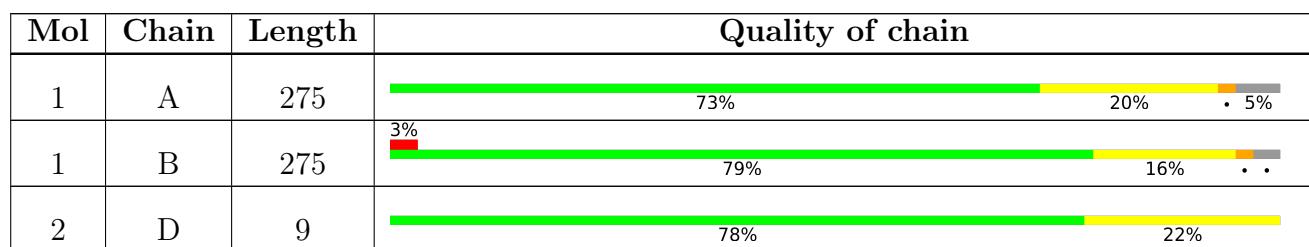
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

W O R L D W I D E
wwPDB
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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	WOC	A	1300	-	X	-	-

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 4268 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 NAD-DEPENDENT PROTEIN DEACYLASE SIRTUIN-5, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	1	0
			2038	1286	367	370	15			
1	B	266	Total	C	N	O	S	0	1	0
			2073	1307	375	376	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP Q6DHI5
A	25	ILE	-	expression tag	UNP Q6DHI5
A	26	ASP	-	expression tag	UNP Q6DHI5
A	27	PRO	-	expression tag	UNP Q6DHI5
A	28	PHE	-	expression tag	UNP Q6DHI5
A	29	THR	-	expression tag	UNP Q6DHI5
B	24	GLY	-	expression tag	UNP Q6DHI5
B	25	ILE	-	expression tag	UNP Q6DHI5
B	26	ASP	-	expression tag	UNP Q6DHI5
B	27	PRO	-	expression tag	UNP Q6DHI5
B	28	PHE	-	expression tag	UNP Q6DHI5
B	29	THR	-	expression tag	UNP Q6DHI5

- Molecule 2 is a protein called CARBAMOYLPHOSPHATE SYNTHETASE I.

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	9	Total	C	N	O	0	0	0
			68	47	9	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	BEZ	-	modified residue	UNP Q5R209

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0

- Molecule 4 is 2,2-dimethylbutanedioic acid (three-letter code: WOC) (formula: $C_6H_{10}O_4$).
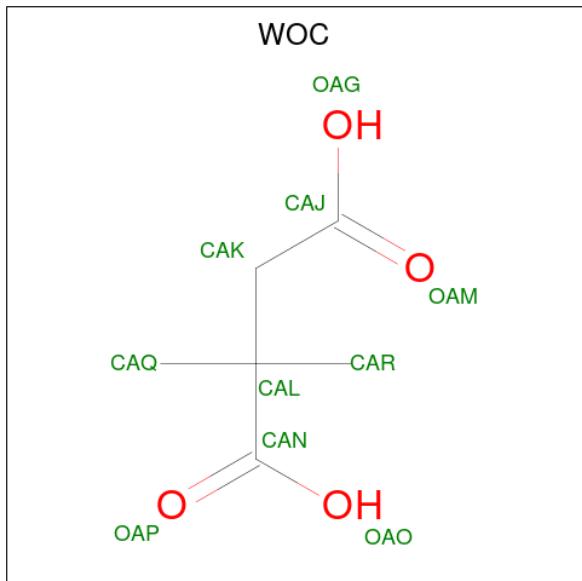
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 9	C 6	O 3	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

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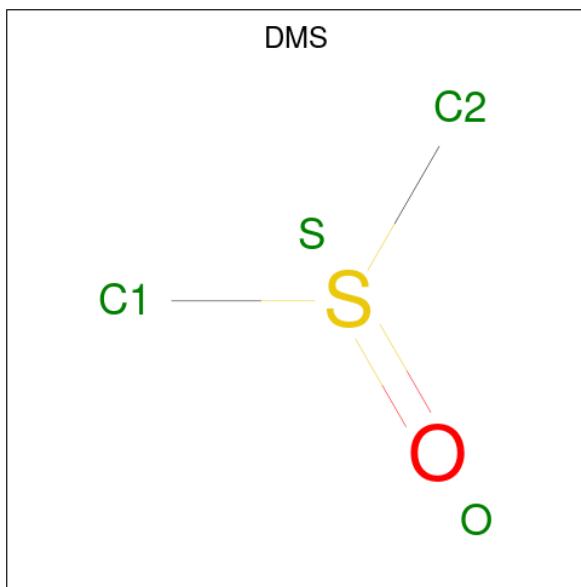
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	A	1	4	2	1	1	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).

EPE
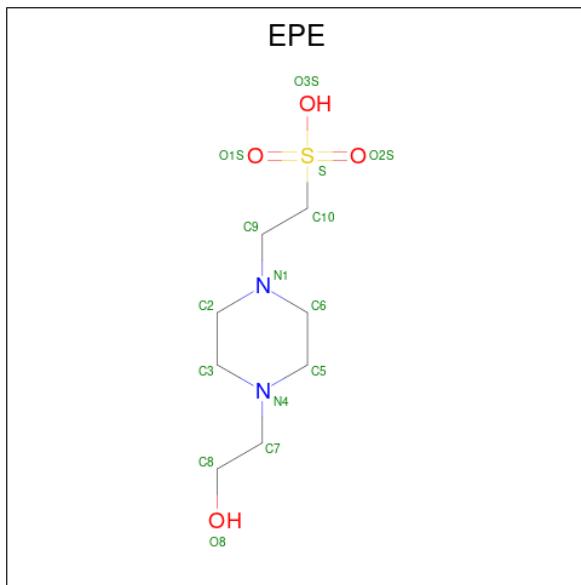
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	B	1	15	8	2	4	1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO
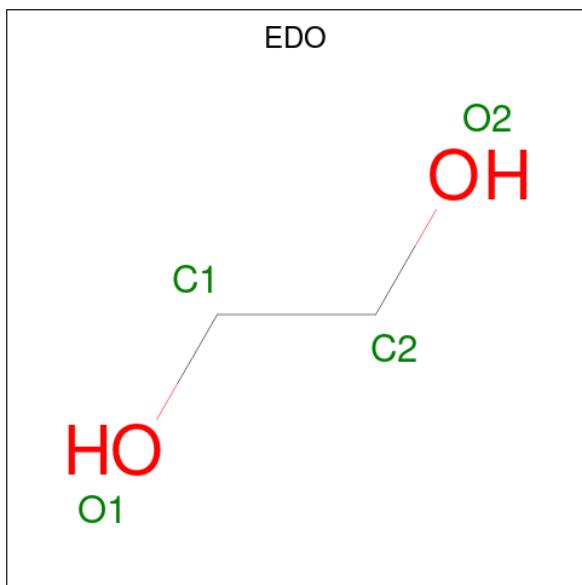
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 4	C 2	O 2	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Na 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	39	Total 39	O 39	0	0
9	B	15	Total 15	O 15	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NAD-DEPENDENT PROTEIN DEACYLASE SIRTUIN-5, MITOCHONDRIAL

Chain A:

• Molecule 1: NAD-DEPENDENT PROTEIN DEACYLASE SIRTUIN-5, MITOCHONDRIAL

Chain B:
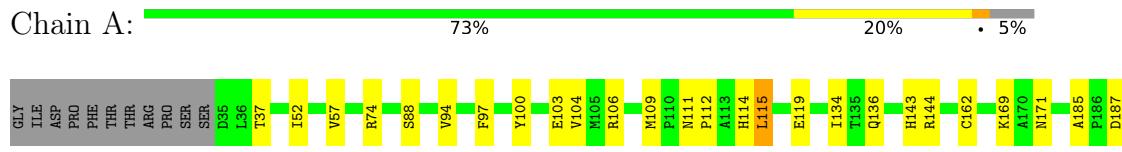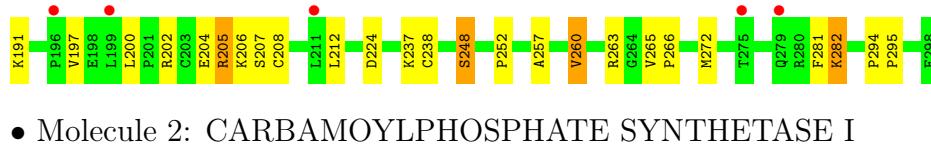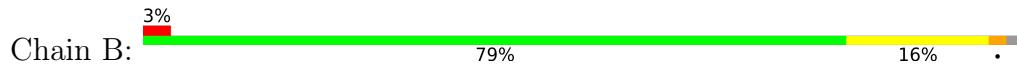
• Molecule 2: CARBAMOYLPHOSPHATE SYNTHETASE I

Chain D:
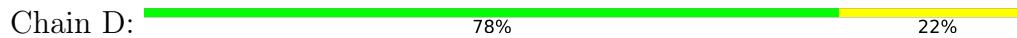
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	87.49Å　87.49Å　314.77Å 90.00°　90.00°　120.00°	Depositor
Resolution (Å)	48.42　–　2.90 48.42　–　2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.42-2.90) 100.0 (48.42-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.192　,　0.252 0.198　,　0.250	Depositor DCC
R_{free} test set	826 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	72.4	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4268	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ 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: DMS, EPE, BEZ, EDO, ZN, WOC, NA

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	0.69	0/2095	0.83	4/2840 (0.1%)
1	B	0.63	0/2131	0.83	1/2888 (0.0%)
2	D	0.85	0/60	1.17	0/79
All	All	0.66	0/4286	0.83	5/5807 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	115	LEU	CA-CB-CG	-6.17	101.11	115.30
1	A	202	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	115	LEU	CA-CB-CG	-5.79	101.98	115.30
1	A	202	ARG	NE-CZ-NH1	5.26	122.93	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2038	0	2002	34	0
1	B	2073	0	2041	24	0
2	D	68	0	66	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	9	0	8	1	0
5	A	4	0	6	0	0
6	B	15	0	18	0	0
7	B	4	0	6	0	0
8	B	1	0	0	0	0
9	A	39	0	0	3	0
9	B	15	0	0	0	0
All	All	4268	0	4147	56	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 (56) 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:74:ARG:HA	1:A:188:PRO:HA	1.81	0.61
1:B:272:MET:O	1:B:272:MET:HG3	2.01	0.61
1:A:235:LEU:HD13	1:A:256:PHE:HB3	1.86	0.56
1:A:249:ILE:O	1:A:249:ILE:HG22	2.05	0.56
1:A:143[B]:HIS:CD2	9:A:2018:HOH:O	2.58	0.55
1:A:143[B]:HIS:CE1	9:A:2018:HOH:O	2.59	0.55
1:A:185:ALA:HB3	1:A:190:THR:HG21	1.89	0.55
1:A:273:GLU:O	1:A:286:GLU:HG3	2.08	0.54
1:B:111:ASN:HB2	1:B:112:PRO:HD2	1.89	0.54
1:B:74:ARG:HA	1:B:188:PRO:HA	1.89	0.54
1:A:103:GLU:OE1	1:A:106:ARG:NH1	2.41	0.53
1:A:225:SER:O	1:A:229:THR:HG22	2.09	0.53
1:B:185:ALA:HB3	1:B:190:THR:HG21	1.91	0.53
1:A:111:ASN:HB2	1:A:112:PRO:HD2	1.90	0.52
1:B:248:SER:HB3	1:B:257:ALA:HB3	1.92	0.52
1:A:278:THR:O	1:A:279:GLN:HG3	2.09	0.52
1:A:100:TYR:O	1:A:104:VAL:HG13	2.11	0.51
1:B:79:GLN:HG2	1:B:80:ASP:N	2.25	0.50
1:A:162:CYS:HA	1:A:212:LEU:HD23	1.94	0.49
1:B:204:GLU:O	1:B:206:LYS:N	2.44	0.49
1:B:266:PRO:HA	1:B:282:LYS:HD2	1.95	0.49
1:A:111:ASN:H	1:A:114:HIS:HD2	1.61	0.49
1:B:100:TYR:O	1:B:104:VAL:HG13	2.13	0.49
1:A:278:THR:O	1:A:279:GLN:CG	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:O	1:A:206:LYS:N	2.47	0.48
1:B:162:CYS:HA	1:B:212:LEU:HD23	1.96	0.48
1:A:205:ARG:O	1:A:208:CYS:HB3	2.15	0.47
1:A:193:ALA:O	1:A:194:ARG:C	2.53	0.47
1:A:200:LEU:O	1:A:202:ARG:HG2	2.16	0.46
1:A:257:ALA:N	1:A:258:PRO:CD	2.79	0.45
1:B:205:ARG:O	1:B:208:CYS:HB3	2.16	0.45
1:A:52:ILE:HA	1:A:134:ILE:O	2.17	0.45
1:A:57:VAL:HG23	1:A:114:HIS:CE1	2.52	0.45
1:A:206:LYS:O	1:A:206:LYS:HG3	2.17	0.44
1:B:171:ASN:OD1	1:B:171:ASN:C	2.56	0.44
1:A:283:TYR:CD1	1:A:283:TYR:N	2.86	0.44
1:A:115:LEU:HB3	1:B:109:MET:HE2	1.99	0.44
4:A:1300:WOC:OAM	4:A:1300:WOC:HAQA	2.17	0.44
1:B:281:PHE:O	1:B:282:LYS:C	2.56	0.44
1:A:171:ASN:OD1	1:A:171:ASN:C	2.56	0.43
1:B:57:VAL:HG12	1:B:114:HIS:CE1	2.52	0.43
1:A:94:VAL:O	1:A:97:PHE:HB3	2.18	0.43
1:A:109:MET:HE2	1:B:115:LEU:CB	2.49	0.43
1:B:200:LEU:O	1:B:202:ARG:HG2	2.19	0.42
1:A:119:GLU:OE1	1:B:144:ARG:NH2	2.53	0.42
1:B:111:ASN:H	1:B:114:HIS:HD2	1.67	0.41
1:B:204:GLU:O	1:B:205:ARG:C	2.59	0.41
1:A:100:TYR:CE2	1:A:104:VAL:HG11	2.56	0.41
1:A:204:GLU:O	1:A:205:ARG:C	2.59	0.41
1:A:256:PHE:O	1:A:259:GLN:HB3	2.20	0.41
1:B:52:ILE:HA	1:B:134:ILE:O	2.20	0.41
1:B:206:LYS:O	1:B:206:LYS:HG3	2.21	0.41
1:B:260:VAL:HG13	1:B:265:VAL:HB	2.02	0.40
1:A:143[B]:HIS:NE2	9:A:2018:HOH:O	2.36	0.40
1:A:251:TYR:CD1	2:D:5:GLU:HG3	2.56	0.40
1:B:294:PRO:HB2	1:B:295:PRO:HD3	2.02	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	259/275 (94%)	244 (94%)	14 (5%)	1 (0%)	34	66
1	B	265/275 (96%)	246 (93%)	17 (6%)	2 (1%)	19	51
2	D	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	531/559 (95%)	496 (93%)	32 (6%)	3 (1%)	25	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	ARG
1	B	282	LYS
1	A	205	ARG

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	218/229 (95%)	202 (93%)	16 (7%)	14	38
1	B	222/229 (97%)	205 (92%)	17 (8%)	13	35
2	D	6/6 (100%)	5 (83%)	1 (17%)	2	6
All	All	446/464 (96%)	412 (92%)	34 (8%)	13	36

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	88	SER
1	A	136	GLN
1	A	169	LYS
1	A	187	ASP
1	A	197	VAL

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Mol	Chain	Res	Type
1	A	207	SER
1	A	224	ASP
1	A	226	ASP
1	A	238	CYS
1	A	248	SER
1	A	250	VAL
1	A	260	VAL
1	A	272	MET
1	A	278	THR
1	A	283	TYR
1	B	37	THR
1	B	79	GLN
1	B	88	SER
1	B	106	ARG
1	B	173	LYS
1	B	187	ASP
1	B	191	LYS
1	B	197	VAL
1	B	207	SER
1	B	224	ASP
1	B	237	LYS
1	B	238	CYS
1	B	248	SER
1	B	252	PRO
1	B	260	VAL
1	B	263[A]	ARG
1	B	263[B]	ARG
2	D	8	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	136	GLN
1	A	189	ASN
1	B	114	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	DMS	A	1301	-	3,3,3	0.54	0	3,3,3	1.11	0
4	WOC	A	1300	2	8,8,9	1.86	2 (25%)	11,11,13	2.46	4 (36%)
7	EDO	B	1301	-	3,3,3	0.59	0	2,2,2	0.15	0
6	EPE	B	1300	-	15,15,15	1.93	1 (6%)	18,20,20	2.05	8 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	WOC	A	1300	2	-	6/10/10/11	-
7	EDO	B	1301	-	-	1/1/1/1	-
6	EPE	B	1300	-	-	4/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1300	EPE	C10-S	-7.01	1.67	1.77
4	A	1300	WOC	CAL-CAN	3.85	1.56	1.52
4	A	1300	WOC	CAK-CAL	-2.90	1.52	1.55

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1300	WOC	OAP-CAN-CAL	-4.84	115.97	122.87
4	A	1300	WOC	CAL-CAK-CAJ	-4.49	106.81	113.49
6	B	1300	EPE	C5-C6-N1	3.96	118.77	110.64
6	B	1300	EPE	O3S-S-O2S	3.30	119.33	111.27
6	B	1300	EPE	O2S-S-O1S	-2.93	103.82	113.95
6	B	1300	EPE	O1S-S-C10	2.89	110.39	106.92
4	A	1300	WOC	OAO-CAN-CAL	2.85	120.24	114.30
6	B	1300	EPE	C9-N1-C2	-2.43	105.01	111.23
6	B	1300	EPE	C2-C3-N4	-2.34	105.85	110.64
4	A	1300	WOC	CAR-CAL-CAN	2.33	113.96	109.05
6	B	1300	EPE	C7-N4-C5	2.26	117.02	111.23
6	B	1300	EPE	C5-N4-C3	-2.18	103.92	108.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1300	EPE	N4-C7-C8-O8
4	A	1300	WOC	CAQ-CAL-CAN-OAO
7	B	1301	EDO	O1-C1-C2-O2
6	B	1300	EPE	C9-C10-S-O3S
4	A	1300	WOC	CAQ-CAL-CAN-OAP
6	B	1300	EPE	C9-C10-S-O1S
6	B	1300	EPE	C9-C10-S-O2S
4	A	1300	WOC	CAK-CAL-CAN-OAO
4	A	1300	WOC	CAK-CAL-CAN-OAP
4	A	1300	WOC	OAM-CAJ-CAK-CAL
4	A	1300	WOC	CAR-CAL-CAN-OAP

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1300	WOC	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(Å²)	Q<0.9
1	A	262/275 (95%)	0.09	0	100	100	41, 61, 95, 128	0
1	B	266/275 (96%)	0.39	9 (3%)	45	40	45, 75, 129, 161	0
2	D	8/9 (88%)	0.14	0	100	100	55, 67, 73, 92	0
All	All	536/559 (95%)	0.24	9 (1%)	70	69	41, 65, 121, 161	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	GLN	3.3
1	B	76	TRP	3.2
1	B	199	LEU	3.1
1	B	196	PRO	3.0
1	B	180	LEU	2.9
1	B	275	THR	2.7
1	B	34	SER	2.2
1	B	81	LEU	2.2
1	B	211	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	B	1301	4/4	0.92	0.39	61,70,78,78	0
6	EPE	B	1300	15/15	0.94	0.29	67,74,83,85	0
3	ZN	B	1299	1/1	0.94	0.07	113,113,113,113	0
8	NA	B	1302	1/1	0.94	0.33	94,94,94,94	1
4	WOC	A	1300	9/10	0.95	0.26	52,63,71,77	0
3	ZN	A	1299	1/1	0.97	0.12	56,56,56,56	0
5	DMS	A	1301	4/4	0.98	0.21	55,63,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.