



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:09 PM UTC

PDB ID : 6YFV / pdb_00006yfv
Title : Crystal structure of Mtr4-Red1 minimal complex from *Chaetomium thermophilum*
Authors : Dobrev, N.; Ahmed, Y.L.; Sinning, I.
Deposited on : 2020-03-26
Resolution : 2.75 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

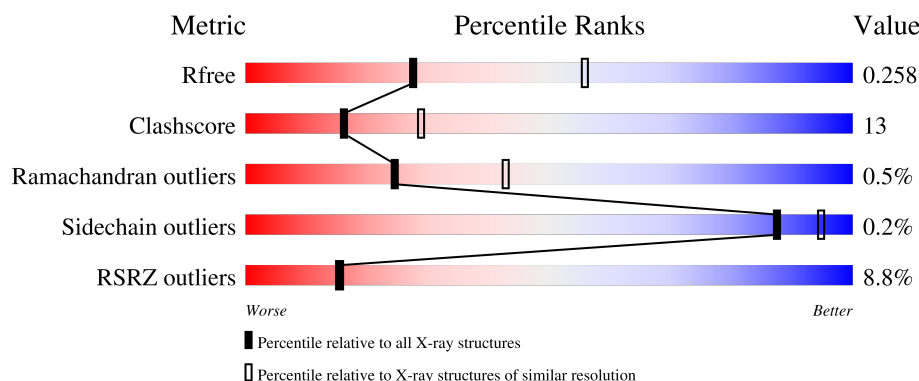
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	213	4% 80% 19%
1	C	213	10% 65% 31% ..
2	B	89	7% 83% 6% 11%
2	D	89	16% 46% 30% • 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4599 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 ATP dependent RNA helicase (Dob1)-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1699	1061	308	319	11			
1	C	209	Total	C	N	O	S	0	1	0
			1685	1052	307	315	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	653	MET	-	initiating methionine	UNP G0RZ64
C	653	MET	-	initiating methionine	UNP G0RZ64

- Molecule 2 is a protein called Red1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	0	0
			637	406	109	118	4			
2	D	69	Total	C	N	O	S	0	0	0
			561	359	96	101	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1011	GLY	-	expression tag	UNP G0S1V1
B	1012	ALA	-	expression tag	UNP G0S1V1
B	1013	MET	-	expression tag	UNP G0S1V1
B	1081	ALA	-	insertion	UNP G0S1V1
B	1092	GLY	-	expression tag	UNP G0S1V1
B	1093	SER	-	expression tag	UNP G0S1V1
B	1094	HIS	-	expression tag	UNP G0S1V1
B	1095	HIS	-	expression tag	UNP G0S1V1
B	1096	HIS	-	expression tag	UNP G0S1V1
B	1097	HIS	-	expression tag	UNP G0S1V1

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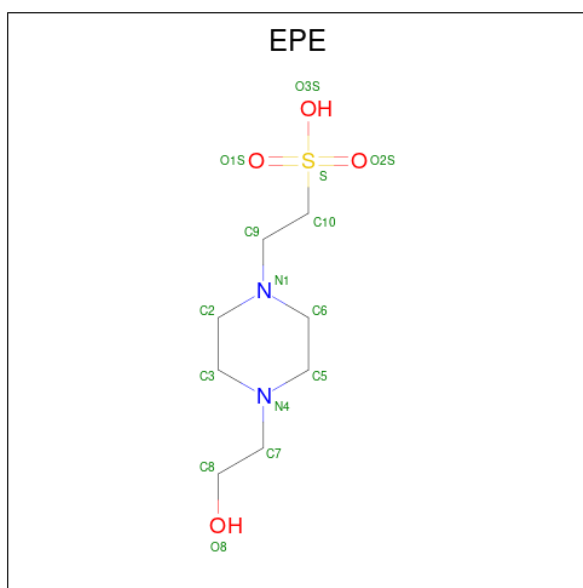
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1098	HIS	-	expression tag	UNP G0S1V1
B	1099	HIS	-	expression tag	UNP G0S1V1
D	1011	GLY	-	expression tag	UNP G0S1V1
D	1012	ALA	-	expression tag	UNP G0S1V1
D	1013	MET	-	expression tag	UNP G0S1V1
D	1081	ALA	-	insertion	UNP G0S1V1
D	1092	GLY	-	expression tag	UNP G0S1V1
D	1093	SER	-	expression tag	UNP G0S1V1
D	1094	HIS	-	expression tag	UNP G0S1V1
D	1095	HIS	-	expression tag	UNP G0S1V1
D	1096	HIS	-	expression tag	UNP G0S1V1
D	1097	HIS	-	expression tag	UNP G0S1V1
D	1098	HIS	-	expression tag	UNP G0S1V1
D	1099	HIS	-	expression tag	UNP G0S1V1

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).

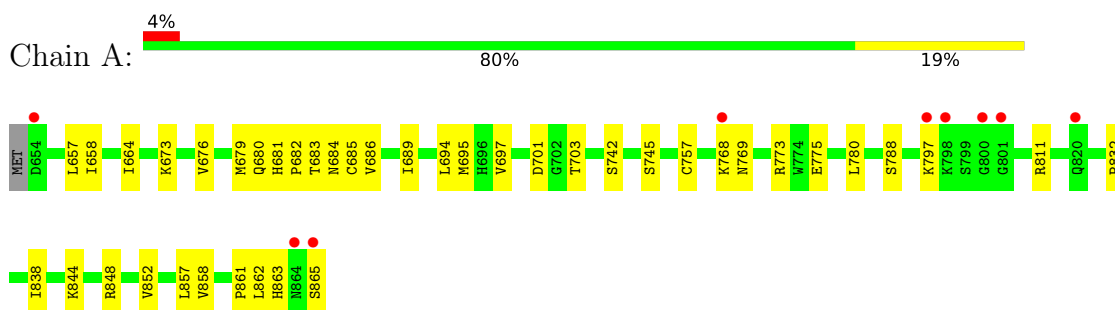


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

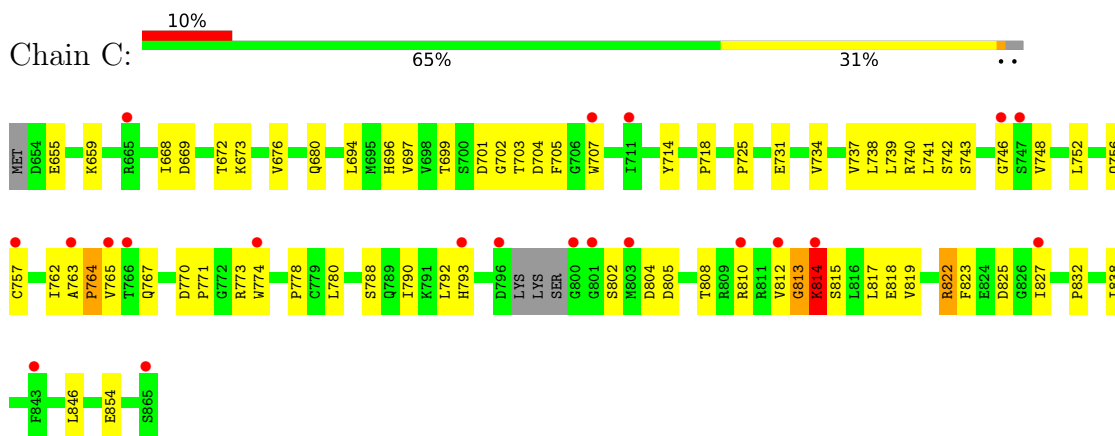
3 Residue-property plots [i](#)

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.

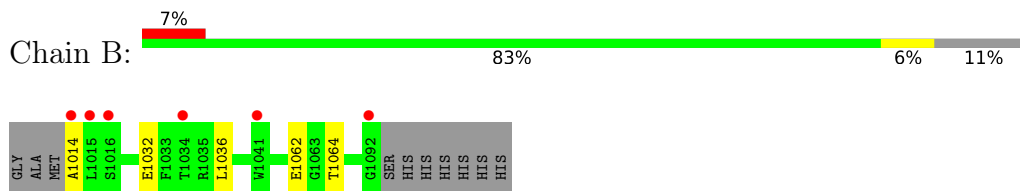
- Molecule 1: ATP dependent RNA helicase (Dob1)-like protein



- Molecule 1: ATP dependent RNA helicase (Dob1)-like protein

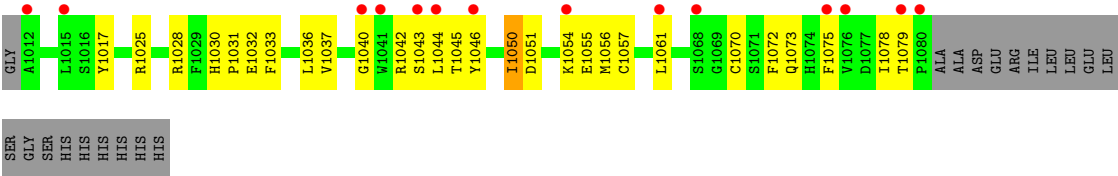


- Molecule 2: Red1



- Molecule 2: Red1





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	172.19Å 172.19Å 145.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.71 – 2.75 49.71 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.71-2.75) 100.0 (49.71-2.75)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.215 , 0.257 0.222 , 0.258	Depositor DCC
R_{free} test set	1705 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4599	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, ZN

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	0.44	0/1736	0.79	1/2348 (0.0%)
1	C	0.44	0/1721	0.83	7/2329 (0.3%)
2	B	0.39	0/656	0.59	0/888
2	D	0.34	0/580	0.70	0/785
All	All	0.42	0/4693	0.77	8/6350 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	LYS	CB-CG-CD	7.53	128.61	111.30
1	C	756	GLN	CA-C-N	-5.65	111.72	121.66
1	C	756	GLN	C-N-CA	-5.65	111.72	121.66
1	C	757	CYS	N-CA-CB	5.64	119.24	110.44
1	C	813	GLY	CA-C-N	-5.55	113.80	122.73
1	C	813	GLY	C-N-CA	-5.55	113.80	122.73
1	C	822	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	C	814	LYS	CA-CB-CG	5.18	124.46	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	814	LYS	Peptide

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	1699	0	1689	27	0
1	C	1685	0	1667	69	0
2	B	637	0	601	4	0
2	D	561	0	524	31	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	C	15	0	17	1	0
All	All	4599	0	4498	119	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 13.

All (119) 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:774:TRP:HD1	1:C:810:ARG:HD3	1.36	0.89
1:C:774:TRP:CD1	1:C:810:ARG:HD3	2.08	0.88
1:C:822:ARG:O	2:D:1044:LEU:HD13	1.77	0.84
1:A:768:LYS:HA	1:A:768:LYS:HE2	1.65	0.79
1:C:668:ILE:O	1:C:672:THR:HG23	1.84	0.77
1:A:768:LYS:HD3	1:A:769:ASN:H	1.51	0.74
1:C:740:ARG:HB2	1:C:774:TRP:CZ3	2.24	0.72
1:A:658:ILE:HG13	1:A:862:LEU:HD21	1.73	0.71
1:C:814:LYS:HB2	1:C:817:LEU:HD12	1.72	0.71
1:C:741:LEU:HD23	1:C:773:ARG:O	1.91	0.70
1:C:740:ARG:HH12	1:C:765:VAL:HG11	1.56	0.70
2:D:1057:CYS:HA	2:D:1072:PHE:HD1	1.57	0.69
1:C:812:VAL:O	1:C:815:SER:OG	2.09	0.69
1:C:707:TRP:CD2	1:C:827:ILE:HD11	2.29	0.68
1:A:679:MET:HE3	1:A:832:PRO:HB3	1.75	0.68
1:C:752:LEU:HD21	1:C:778:PRO:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:HIS:HB2	1:C:707:TRP:CE2	2.31	0.66
1:A:757:CYS:HA	1:A:780:LEU:HD22	1.78	0.66
2:D:1051:ASP:CG	2:D:1054:LYS:HG2	2.22	0.64
1:C:774:TRP:CD1	1:C:810:ARG:HA	2.32	0.64
1:C:669:ASP:OD2	1:C:673:LYS:NZ	2.31	0.63
1:C:707:TRP:CE2	1:C:827:ILE:HD11	2.34	0.63
1:C:707:TRP:CG	1:C:827:ILE:HD11	2.35	0.61
2:D:1051:ASP:H	2:D:1073:GLN:HE22	1.47	0.61
1:C:741:LEU:HD12	1:C:762:ILE:HG12	1.83	0.61
1:C:714:TYR:CZ	1:C:734:VAL:HG21	2.36	0.60
1:C:792:LEU:HD21	1:C:819:VAL:HG21	1.83	0.60
1:C:790:ILE:HG23	2:D:1050:ILE:HD11	1.83	0.59
1:A:684:ASN:HB3	1:A:838:ILE:CD1	2.33	0.59
2:D:1075:PHE:O	2:D:1079:THR:OG1	2.21	0.58
1:C:746:GLY:HA3	1:C:773:ARG:HH11	1.68	0.58
1:C:823:PHE:CD2	2:D:1044:LEU:HB3	2.39	0.58
1:C:705:PHE:HB3	1:C:739:LEU:HD13	1.85	0.58
1:C:741:LEU:HB2	1:C:762:ILE:HD11	1.84	0.58
1:C:740:ARG:NH1	1:C:765:VAL:HG11	2.19	0.57
1:C:701:ASP:OD1	1:C:703:THR:HG23	2.05	0.57
1:A:773:ARG:NH2	1:A:775:GLU:OE2	2.38	0.57
1:A:681:HIS:CE1	1:A:683:THR:HG23	2.40	0.56
1:C:738:LEU:HD11	1:C:774:TRP:HB3	1.87	0.56
1:C:694:LEU:HD23	1:C:790:ILE:HD12	1.88	0.56
2:D:1032:GLU:HB3	2:D:1036:LEU:HD11	1.87	0.56
2:D:1056:MET:HE1	2:D:1075:PHE:CZ	2.41	0.56
1:C:655:GLU:O	1:C:659:LYS:HG2	2.06	0.55
2:D:1075:PHE:HA	2:D:1078:ILE:HG13	1.88	0.55
1:A:701:ASP:OD2	1:A:703:THR:HG23	2.07	0.55
1:A:797:LYS:HD2	1:A:797:LYS:H	1.72	0.54
1:C:694:LEU:HD21	1:C:792:LEU:HG	1.89	0.54
1:C:714:TYR:CZ	1:C:734:VAL:CG2	2.91	0.54
1:C:814:LYS:CB	1:C:817:LEU:HD12	2.38	0.53
1:C:793:HIS:ND1	2:D:1055:GLU:OE1	2.35	0.53
2:D:1033:PHE:CE1	2:D:1037:VAL:HG11	2.43	0.53
1:C:741:LEU:HD23	1:C:741:LEU:H	1.73	0.53
1:C:742:SER:N	1:C:764:PRO:O	2.42	0.52
1:C:743:SER:OG	1:C:771:PRO:O	2.27	0.52
1:C:773:ARG:HA	1:C:810:ARG:NH2	2.24	0.52
1:A:694:LEU:HB2	1:A:788:SER:HB3	1.90	0.52
1:C:746:GLY:HA3	1:C:773:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1040:GLY:O	2:D:1043:SER:HB3	2.10	0.52
2:B:1032:GLU:O	2:B:1036:LEU:HD12	2.10	0.52
1:C:825:ASP:HB2	2:D:1045:THR:OG1	2.09	0.51
1:A:681:HIS:ND1	1:A:682:PRO:HD2	2.25	0.51
1:C:773:ARG:HG3	1:C:810:ARG:NH2	2.26	0.51
1:C:707:TRP:CD1	1:C:827:ILE:HD11	2.46	0.51
1:C:805:ASP:OD2	1:C:808:THR:OG1	2.14	0.50
1:C:707:TRP:CD2	1:C:827:ILE:CD1	2.93	0.50
1:C:762:ILE:HD12	1:C:763:ALA:H	1.75	0.50
1:C:731:GLU:HG2	1:C:780:LEU:HD23	1.92	0.50
1:C:854:GLU:OE2	2:D:1017:TYR:OH	2.28	0.50
1:C:815:SER:HB2	2:D:1061:LEU:HD11	1.93	0.49
1:A:768:LYS:HA	1:A:768:LYS:CE	2.40	0.49
1:C:793:HIS:HA	2:D:1055:GLU:OE1	2.13	0.49
2:D:1032:GLU:O	2:D:1036:LEU:HD12	2.13	0.49
1:C:802:SER:C	1:C:804:ASP:H	2.18	0.49
2:D:1028:ARG:HA	2:D:1033:PHE:CD1	2.48	0.49
2:D:1051:ASP:H	2:D:1073:GLN:NE2	2.11	0.48
1:A:848:ARG:O	1:A:852:VAL:HG12	2.14	0.48
1:C:748:VAL:O	1:C:748:VAL:HG23	2.14	0.47
2:D:1042:ARG:O	2:D:1042:ARG:HG2	2.14	0.47
1:A:695:MET:HE2	1:A:697:VAL:HG22	1.97	0.47
2:B:1062:GLU:HB3	2:B:1064:THR:HG23	1.97	0.47
2:D:1032:GLU:CB	2:D:1036:LEU:HD11	2.45	0.47
1:C:699:THR:HG23	1:C:701:ASP:OD1	2.14	0.46
1:C:676:VAL:O	1:C:680:GLN:HG3	2.16	0.46
1:A:682:PRO:O	1:A:686:VAL:HG13	2.16	0.46
1:A:811:ARG:NH2	2:B:1062:GLU:OE2	2.49	0.46
1:A:858:VAL:HG12	1:A:863:HIS:CD2	2.51	0.46
1:C:740:ARG:HB2	1:C:774:TRP:CH2	2.50	0.46
1:C:696:HIS:HE2	1:C:704:ASP:CG	2.24	0.46
1:C:774:TRP:NE1	1:C:813:GLY:HA3	2.30	0.46
1:C:790:ILE:CG2	2:D:1050:ILE:HD11	2.46	0.46
1:C:818:GLU:O	1:C:822:ARG:HG2	2.16	0.46
2:D:1045:THR:HG22	2:D:1046:TYR:H	1.81	0.46
1:A:768:LYS:CD	1:A:769:ASN:H	2.25	0.45
1:C:822:ARG:O	2:D:1044:LEU:CD1	2.60	0.45
1:C:767:GLN:O	1:C:770:ASP:HB2	2.17	0.45
2:D:1030:HIS:CG	2:D:1031:PRO:HD2	2.53	0.44
1:C:697:VAL:HG21	1:C:737:VAL:HG11	1.99	0.44
1:C:741:LEU:CD1	1:C:762:ILE:HG12	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:HIS:HE1	1:A:683:THR:HG23	1.82	0.44
4:C:901:EPE:H51	4:C:901:EPE:H82	1.68	0.43
1:C:694:LEU:HB2	1:C:788:SER:HB3	2.00	0.43
1:C:832:PRO:O	1:C:838:ILE:HD12	2.18	0.43
1:A:865:SER:O	2:B:1014:ALA:HA	2.19	0.43
1:A:676:VAL:O	1:A:680:GLN:HG3	2.19	0.42
1:C:815:SER:HB2	2:D:1061:LEU:CD1	2.50	0.42
2:D:1051:ASP:HB3	2:D:1054:LYS:HG2	2.01	0.42
1:C:718:PRO:HB3	1:C:725:PRO:HG3	2.01	0.42
1:C:819:VAL:O	1:C:822:ARG:HB2	2.19	0.42
1:C:846:LEU:HD12	1:C:846:LEU:HA	1.86	0.42
1:A:664:ILE:HG21	1:A:857:LEU:HB2	2.02	0.42
1:C:773:ARG:HA	1:C:810:ARG:CZ	2.50	0.42
1:C:701:ASP:OD1	1:C:702:GLY:N	2.53	0.42
2:D:1051:ASP:CB	2:D:1054:LYS:HG2	2.50	0.42
1:A:685:CYS:O	1:A:689:ILE:HG12	2.20	0.41
1:A:742:SER:O	1:A:745:SER:HB3	2.20	0.41
2:D:1057:CYS:O	2:D:1061:LEU:HD23	2.20	0.41
1:A:657:LEU:HD21	1:A:861:PRO:HG2	2.03	0.41
1:A:679:MET:HE3	1:A:832:PRO:CB	2.47	0.41
2:D:1025:ARG:O	2:D:1028:ARG:HG3	2.22	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	210/213 (99%)	208 (99%)	2 (1%)	0	100	100
1	C	206/213 (97%)	199 (97%)	6 (3%)	1 (0%)	24	43
2	B	77/89 (86%)	77 (100%)	0	0	100	100
2	D	67/89 (75%)	53 (79%)	12 (18%)	2 (3%)	3	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	560/604 (93%)	537 (96%)	20 (4%)	3 (0%)	24	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	764	PRO
2	D	1050	ILE
2	D	1070	CYS

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	195/196 (100%)	194 (100%)	1 (0%)	81	89
1	C	193/196 (98%)	193 (100%)	0	100	100
2	B	70/78 (90%)	70 (100%)	0	100	100
2	D	62/78 (80%)	62 (100%)	0	100	100
All	All	520/548 (95%)	519 (100%)	1 (0%)	87	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	844	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	837	HIS
2	B	1065	GLN
1	C	667	GLN
1	C	721	ASN
1	C	785	HIS
1	C	837	HIS

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Mol	Chain	Res	Type
1	C	863	HIS
1	C	864	ASN
2	D	1073	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
4	EPE	C	901	-	15,15,15	0.85	1 (6%)	19,20,20	1.87	4 (21%)

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	EPE	C	901	-	-	8/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	901	EPE	C10-S	2.65	1.81	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	901	EPE	C5-N4-C3	4.33	118.16	108.84
4	C	901	EPE	C7-N4-C3	4.06	122.06	111.24
4	C	901	EPE	C7-N4-C5	3.16	119.67	111.24
4	C	901	EPE	O1S-S-C10	2.49	110.49	106.73

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	901	EPE	C10-C9-N1-C6
4	C	901	EPE	C8-C7-N4-C5
4	C	901	EPE	S-C10-C9-N1
4	C	901	EPE	C9-C10-S-O1S
4	C	901	EPE	N4-C7-C8-O8
4	C	901	EPE	C9-C10-S-O3S
4	C	901	EPE	C10-C9-N1-C2
4	C	901	EPE	C9-C10-S-O2S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	901	EPE	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	212/213 (99%)	0.08	9 (4%) 40 39	56, 80, 131, 152	0
1	C	209/213 (98%)	0.72	21 (10%) 12 12	45, 112, 176, 195	1 (0%)
2	B	79/89 (88%)	0.38	6 (7%) 20 19	58, 79, 127, 147	0
2	D	69/89 (77%)	1.51	14 (20%) 3 2	94, 157, 196, 204	0
All	All	569/604 (94%)	0.53	50 (8%) 15 15	45, 97, 175, 204	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1016	SER	6.3
2	D	1012	ALA	6.3
1	C	800	GLY	5.5
2	D	1080	PRO	5.2
1	C	765	VAL	4.6
2	D	1041	TRP	4.4
2	D	1040	GLY	4.3
2	B	1092	GLY	4.3
1	C	665[A]	ARG	4.1
2	D	1015	LEU	3.8
1	A	800	GLY	3.6
2	D	1075	PHE	3.6
2	B	1041	TRP	3.4
2	B	1014	ALA	3.4
1	C	796	ASP	3.3
1	C	766	THR	3.3
2	B	1015	LEU	3.3
2	D	1044	LEU	3.3
2	D	1076	VAL	3.2
2	D	1046	TYR	3.1
2	B	1034	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	810	ARG	2.9
1	C	827	ILE	2.8
1	A	797	LYS	2.8
1	C	793	HIS	2.8
1	A	768	LYS	2.7
1	C	865	SER	2.7
1	C	803	MET	2.7
1	C	747	SER	2.7
1	C	757	CYS	2.6
1	A	820	GLN	2.6
1	C	707	TRP	2.6
1	C	711	ILE	2.4
2	D	1079	THR	2.4
1	A	864	ASN	2.4
1	C	814	LYS	2.3
1	A	801	GLY	2.3
1	C	801	GLY	2.3
2	D	1061	LEU	2.3
1	A	654	ASP	2.3
1	C	774	TRP	2.3
1	A	798	LYS	2.3
1	C	746	GLY	2.2
1	C	763	ALA	2.2
1	A	865	SER	2.2
1	C	843	PHE	2.2
2	D	1043	SER	2.2
1	C	812	VAL	2.2
2	D	1068	SER	2.1
2	D	1054	LYS	2.1

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 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
4	EPE	C	901	15/15	0.82	0.24	90,139,162,166	0
3	ZN	D	1101	1/1	0.98	0.04	190,190,190,190	0
3	ZN	B	1101	1/1	1.00	0.05	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.