



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:36 AM UTC

PDB ID : 4XB6 / pdb_00004xb6
Title : Structure of the E. coli C-P lyase core complex
Authors : Brodersen, D.E.
Deposited on : 2014-12-16
Resolution : 1.70 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

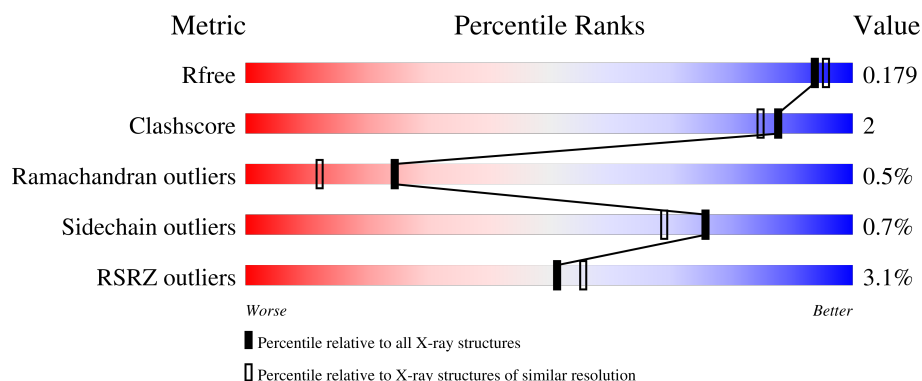
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	150	3% 85% 9% .
1	E	150	5% 94% 5% .
2	B	194	2% 92% 6% ..
2	F	194	2% 93% 6% ..
3	C	354	2% 96% .

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Mol	Chain	Length	Quality of chain
3	G	354	2% 95% 5%
4	D	281	4% 93% 5%
4	H	281	4% 96% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31865 atoms, of which 14894 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 Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	144	Total	C	H	N	O	S	0	1	0
			2233	692	1109	216	209	7			
1	E	149	Total	C	H	N	O	S	0	1	0
			2286	709	1130	223	218	6			

- Molecule 2 is a protein called Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	194	Total	C	H	N	O	S	0	3	0
			3027	947	1528	261	280	11			
2	F	193	Total	C	H	N	O	S	0	1	0
			2977	935	1496	258	278	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	152	ARG	GLN	engineered mutation	UNP P16686
F	152	ARG	GLN	engineered mutation	UNP P16686

- Molecule 3 is a protein called Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	353	Total	C	H	N	O	S	0	1	0
			5429	1717	2690	481	530	11			
3	G	353	Total	C	H	N	O	S	0	1	0
			5414	1714	2680	478	531	11			

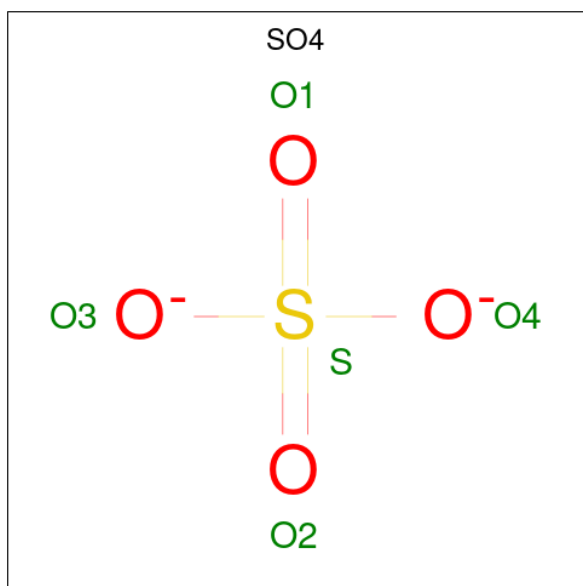
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	322	VAL	ALA	engineered mutation	UNP P16687
G	322	VAL	ALA	engineered mutation	UNP P16687

- Molecule 4 is a protein called Alpha-D-ribose 1-methylphosphonate 5-phosphate C-P lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	277	Total	C	H	N	O	S	0	2	0
			4336	1399	2124	377	421	15			
4	H	277	Total	C	H	N	O	S	0	2	0
			4347	1398	2137	376	421	15			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	Zn 1	0	0
6	D	1	Total 1	Zn 1	0	0
6	G	1	Total 1	Zn 1	0	0
6	H	1	Total 1	Zn 1	0	0

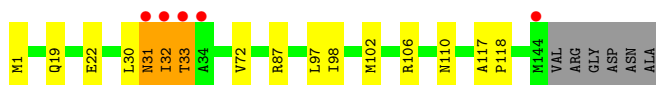
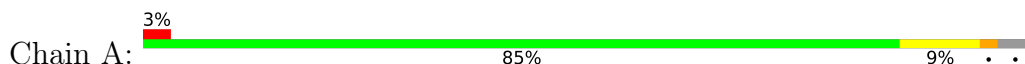
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	132	Total 132	O 132	0	0
7	B	162	Total 162	O 162	0	0
7	C	350	Total 350	O 350	0	0
7	D	259	Total 259	O 259	0	0
7	E	152	Total 152	O 152	0	0
7	F	135	Total 135	O 135	0	0
7	G	366	Total 366	O 366	0	0
7	H	236	Total 236	O 236	0	0

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.

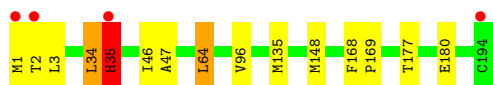
- Molecule 1: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnG



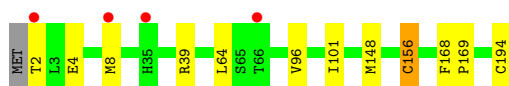
- Molecule 1: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnG



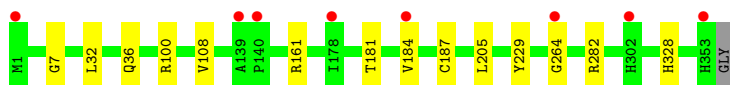
- Molecule 2: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnH



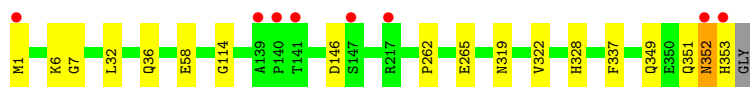
- Molecule 2: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnH



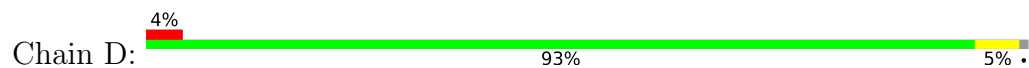
- Molecule 3: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnI



- Molecule 3: Alpha-D-ribose 1-methylphosphonate 5-triphosphate synthase subunit PhnI



- Molecule 4: Alpha-D-ribose 1-methylphosphonate 5-phosphate C-P lyase



- Molecule 4: Alpha-D-ribose 1-methylphosphonate 5-phosphate C-P lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.51Å 133.71Å 176.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.36 – 1.70 58.36 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (58.36-1.70) 94.9 (58.36-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.70Å)	Xtriage
Refinement program	PHENIX dev_1593	Depositor
R, R_{free}	0.148 , 0.176 0.153 , 0.179	Depositor DCC
R_{free} test set	12423 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31865	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: ZN, SO4, CME

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	0.49	0/1144	0.74	2/1546 (0.1%)
1	E	0.48	0/1176	0.67	0/1591
2	B	0.48	0/1515	0.77	3/2067 (0.1%)
2	F	0.44	0/1490	0.68	0/2034
3	C	0.50	0/2796	0.74	2/3791 (0.1%)
3	G	0.52	0/2791	0.75	0/3785
4	D	0.52	0/2271	0.76	0/3087
4	H	0.48	0/2269	0.72	0/3084
All	All	0.50	0/15452	0.73	7/20985 (0.0%)

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
2	B	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ILE	CA-C-N	9.98	140.61	121.54
1	A	32	ILE	C-N-CA	9.98	140.61	121.54
2	B	34	LEU	CA-C-N	-6.45	113.30	123.23
2	B	34	LEU	C-N-CA	-6.45	113.30	123.23
3	C	181	THR	CA-C-N	-6.26	115.15	119.66
3	C	181	THR	C-N-CA	-6.26	115.15	119.66
2	B	35	HIS	N-CA-C	5.56	120.20	107.48

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	34	LEU	Peptide
2	B	35	HIS	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	1124	1109	1111	9	0
1	E	1156	1130	1132	6	0
2	B	1499	1528	1539	9	0
2	F	1481	1496	1515	5	0
3	C	2739	2690	2690	13	0
3	G	2734	2680	2682	16	0
4	D	2212	2124	2153	8	0
4	H	2210	2137	2152	3	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	G	5	0	0	0	0
5	H	5	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	132	0	0	3	0
7	B	162	0	0	0	1
7	C	350	0	0	3	0
7	D	259	0	0	3	1
7	E	152	0	0	2	0
7	F	135	0	0	1	0
7	G	366	0	0	4	0
7	H	236	0	0	1	0
All	All	16971	14894	14974	61	1

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 2.

All (61) 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)
4:D:221:ARG:NH1	7:D:401:HOH:O	2.08	0.86
1:E:87:ARG:NH2	3:G:58:GLU:OE1	2.09	0.86
3:G:6:LYS:NZ	7:G:782:HOH:O	2.18	0.77
3:C:187:CYS:SG	7:C:683:HOH:O	2.51	0.67
2:F:194:CYS:SG	7:F:314:HOH:O	2.53	0.66
4:D:8[A]:ASN:OD1	7:D:617:HOH:O	2.15	0.65
4:H:18:ARG:NH2	7:H:519:HOH:O	2.32	0.62
3:G:351:GLN:O	3:G:353:HIS:N	2.33	0.62
4:D:18:ARG:NH2	7:D:611:HOH:O	2.34	0.61
2:B:1:MET:O	2:B:3:LEU:N	2.34	0.61
4:D:2:ALA:HB3	4:D:90:THR:O	2.02	0.60
1:A:87[A]:ARG:NH1	7:A:282:HOH:O	2.29	0.57
4:D:273:ARG:NH1	4:D:277:GLU:OE2	2.37	0.56
4:D:3:ASN:ND2	4:D:7:TYR:O	2.40	0.54
2:B:35:HIS:HB3	2:B:46:ILE:HG21	1.89	0.53
3:G:265:GLU:O	7:G:526:HOH:O	2.19	0.53
4:D:4:LEU:HD12	4:D:4:LEU:O	2.10	0.52
3:C:32:LEU:HD22	3:G:32:LEU:HD22	1.91	0.52
2:F:4:GLU:OE1	2:F:39:ARG:NH1	2.44	0.51
2:F:101:ILE:O	2:F:156:CME:HE3	2.11	0.51
4:H:199:MET:HG2	4:H:201:ALA:H	1.76	0.51
3:C:264:GLY:O	7:C:834:HOH:O	2.20	0.51
3:C:32:LEU:HD22	3:G:32:LEU:CD2	2.41	0.50
1:E:44:THR:HG21	1:E:87:ARG:HG2	1.93	0.50
3:C:32:LEU:CD2	3:G:32:LEU:HD22	2.41	0.50
1:A:19:GLN:O	1:A:22:GLU:HG2	2.12	0.49
3:G:262:PRO:O	7:G:526:HOH:O	2.18	0.49
1:A:106:ARG:NH2	7:A:310:HOH:O	2.45	0.48
1:A:72:VAL:HG21	1:A:97:LEU:HA	1.94	0.48
1:E:117:ALA:HB3	1:E:118:PRO:HD3	1.96	0.48
2:B:35:HIS:ND1	2:B:180:GLU:OE1	2.47	0.47
3:C:100[A]:ARG:HG2	3:C:229:TYR:HB2	1.95	0.47
1:E:126:ARG:NH1	7:E:227:HOH:O	2.41	0.47
1:A:117:ALA:HB3	1:A:118:PRO:HD3	1.97	0.46
1:A:98:ILE:O	1:A:102:MET:HG2	2.15	0.46
1:A:30:LEU:O	1:A:31:ASN:ND2	2.49	0.46
2:B:135:MET:HG3	2:B:148[A]:MET:CE	2.46	0.46
3:C:161:ARG:NH2	7:C:738:HOH:O	2.39	0.45
2:B:47:ALA:HB3	2:B:177:THR:HB	1.98	0.45
2:B:168:PHE:CG	2:B:169:PRO:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:349:GLN:NE2	7:G:866:HOH:O	2.49	0.45
3:G:351:GLN:O	3:G:352:ASN:C	2.60	0.45
1:A:110:ASN:ND2	7:A:287:HOH:O	2.43	0.44
3:C:205:LEU:HD11	3:C:282:ARG:CD	2.47	0.44
1:E:138:ARG:NH1	3:G:114:GLY:O	2.44	0.44
2:F:64:LEU:HD23	2:F:96:VAL:HB	2.00	0.44
2:F:168:PHE:CG	2:F:169:PRO:HA	2.54	0.43
2:B:64:LEU:HD23	2:B:96:VAL:HB	2.00	0.43
4:D:199:MET:HG2	4:D:201:ALA:H	1.83	0.43
2:B:168:PHE:CD1	2:B:169:PRO:HA	2.54	0.42
3:C:108:VAL:HB	3:G:337:PHE:CD2	2.55	0.42
1:A:32:ILE:HG22	1:A:33:THR:N	2.35	0.41
3:C:36:GLN:HB3	3:G:32:LEU:HD21	2.02	0.41
3:C:184:VAL:O	3:C:184:VAL:HG23	2.21	0.41
3:G:146:ASP:OD1	3:G:146:ASP:N	2.54	0.41
4:H:198:MET:HA	4:H:219:PHE:HA	2.03	0.41
3:C:32:LEU:HD21	3:G:36:GLN:HB3	2.03	0.40
1:E:149:ASN:HA	7:E:201:HOH:O	2.19	0.40
3:G:319:ASN:HA	3:G:322:VAL:HB	2.03	0.40
3:C:100[A]:ARG:CG	3:C:229:TYR:HB2	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:226:HOH:O	7:D:419:HOH:O[4_555]	2.12	0.08

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	143/150 (95%)	138 (96%)	3 (2%)	2 (1%)	9 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	148/150 (99%)	144 (97%)	3 (2%)	1 (1%)	18	7
2	B	193/194 (100%)	185 (96%)	7 (4%)	1 (0%)	24	12
2	F	190/194 (98%)	186 (98%)	4 (2%)	0	100	100
3	C	352/354 (99%)	349 (99%)	2 (1%)	1 (0%)	36	22
3	G	352/354 (99%)	348 (99%)	2 (1%)	2 (1%)	21	9
4	D	277/281 (99%)	267 (96%)	8 (3%)	2 (1%)	18	7
4	H	277/281 (99%)	268 (97%)	8 (3%)	1 (0%)	30	16
All	All	1932/1958 (99%)	1885 (98%)	37 (2%)	10 (0%)	24	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	352	ASN
2	B	2	THR
1	A	31	ASN
4	D	126	PRO
4	D	259	ALA
3	C	7	GLY
1	E	148	ASP
3	G	7	GLY
4	H	126	PRO
1	A	33	THR

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	112/115 (97%)	111 (99%)	1 (1%)	70	62
1	E	115/115 (100%)	115 (100%)	0	100	100
2	B	165/162 (102%)	164 (99%)	1 (1%)	78	72
2	F	162/162 (100%)	158 (98%)	4 (2%)	42	24
3	C	287/286 (100%)	286 (100%)	1 (0%)	86	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	287/286 (100%)	285 (99%)	2 (1%)	76	69
4	D	242/244 (99%)	239 (99%)	3 (1%)	63	51
4	H	242/244 (99%)	242 (100%)	0	100	100
All	All	1612/1614 (100%)	1600 (99%)	12 (1%)	76	69

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
2	B	64	LEU
3	C	328	HIS
4	D	4	LEU
4	D	223	GLU
4	D	230	HIS
2	F	2	THR
2	F	8[A]	MET
2	F	8[B]	MET
2	F	148	MET
3	G	1	MET
3	G	328	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	174	GLN
4	D	78	ASN
4	D	93	ASN
4	D	154	GLN
1	E	131	GLN
1	E	149	ASN
3	G	150	GLN
3	G	352	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
2	CME	F	178	2	8,9,10	1.00	0	6,9,11	0.61	0
2	CME	F	156	2	8,9,10	1.02	0	6,9,11	1.08	1 (16%)
2	CME	B	178	2	8,9,10	1.06	0	6,9,11	0.91	0
2	CME	B	156	2	8,9,10	1.01	0	6,9,11	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CME	F	178	2	-	3/5/8/10	-
2	CME	F	156	2	-	1/5/8/10	-
2	CME	B	178	2	-	0/5/8/10	-
2	CME	B	156	2	-	1/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	156	CME	CB-SG-SD	2.09	109.28	103.86

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	178	CME	SD-CE-CZ-OH
2	B	156	CME	CZ-CE-SD-SG
2	F	156	CME	CZ-CE-SD-SG

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Mol	Chain	Res	Type	Atoms
2	F	178	CME	CZ-CE-SD-SG
2	F	178	CME	CE-SD-SG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	156	CME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	SO4	G	401	-	4,4,4	0.29	0	6,6,6	0.26	0
5	SO4	C	401	-	4,4,4	0.27	0	6,6,6	0.11	0
5	SO4	H	301	-	4,4,4	0.27	0	6,6,6	0.33	0
5	SO4	D	301	-	4,4,4	0.56	0	6,6,6	0.34	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	144/150 (96%)	-0.12	5 (3%)	47	52	17, 32, 59, 96	1 (0%)
1	E	149/150 (99%)	0.02	8 (5%)	31	34	18, 34, 71, 108	1 (0%)
2	B	192/194 (98%)	-0.25	4 (2%)	63	68	17, 32, 54, 87	3 (1%)
2	F	191/194 (98%)	-0.06	4 (2%)	63	68	20, 40, 61, 81	1 (0%)
3	C	353/354 (99%)	-0.53	8 (2%)	61	65	15, 24, 55, 77	1 (0%)
3	G	353/354 (99%)	-0.56	8 (2%)	61	65	14, 24, 52, 92	1 (0%)
4	D	277/281 (98%)	-0.36	12 (4%)	40	44	16, 24, 64, 81	2 (0%)
4	H	277/281 (98%)	-0.29	11 (3%)	42	46	17, 28, 66, 96	2 (0%)
All	All	1936/1958 (98%)	-0.33	60 (3%)	51	55	14, 28, 61, 108	12 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	278	ALA	7.5
4	D	4	LEU	7.1
1	E	150	ALA	6.0
1	E	147	GLY	5.7
4	H	2	ALA	5.6
1	A	32	ILE	5.6
4	H	259	ALA	5.5
4	H	278	ALA	5.5
3	C	184	VAL	4.9
4	H	158	TYR	4.5
2	F	8[A]	MET	4.5
4	D	2	ALA	4.4
4	D	259	ALA	4.4
4	D	227	PHE	4.4
1	E	148	ASP	4.4
1	E	149	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	194	CYS	4.0
1	A	33	THR	4.0
1	E	2	HIS	3.8
4	H	4	LEU	3.7
3	C	264	GLY	3.7
2	B	35	HIS	3.7
2	F	35	HIS	3.6
4	H	258	ASP	3.6
4	D	3	ASN	3.4
4	H	227	PHE	3.3
1	E	146	ARG	3.3
4	D	230	HIS	3.3
3	G	139	ALA	3.2
4	D	231	PRO	3.2
1	A	144	MET	3.1
4	D	228	ASP	3.1
1	E	145	VAL	3.1
3	C	1	MET	3.1
4	D	260	GLY	3.0
3	G	353	HIS	2.9
2	B	2	THR	2.9
3	G	140	PRO	2.9
1	A	31	ASN	2.9
4	H	257	ASP	2.8
3	C	140	PRO	2.8
2	B	1	MET	2.8
3	G	1	MET	2.8
3	C	139	ALA	2.7
4	H	162	ALA	2.6
3	G	352	ASN	2.6
3	C	302	HIS	2.5
3	C	178	ILE	2.5
3	G	141	THR	2.4
4	D	229	ASP	2.4
4	H	3	ASN	2.3
2	F	2	THR	2.3
1	E	3	ALA	2.2
4	H	260	GLY	2.2
4	D	258	ASP	2.2
3	G	217	ARG	2.2
3	G	147	SER	2.1
3	C	353	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	34	ALA	2.1
2	F	66	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	CME	F	156	10/11	0.90	0.21	31,51,113,113	0
2	CME	B	156	10/11	0.91	0.19	32,48,115,115	0
2	CME	F	178	10/11	0.92	0.13	37,42,77,104	0
2	CME	B	178	10/11	0.96	0.12	24,36,84,106	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(Å ²)	Q<0.9
5	SO4	C	401	5/5	0.87	0.19	72,79,83,84	1
5	SO4	G	401	5/5	0.92	0.12	37,45,49,62	0
6	ZN	H	302	1/1	0.96	0.06	32,32,32,32	0
6	ZN	G	402	1/1	0.98	0.03	21,21,21,21	1
6	ZN	C	402	1/1	0.98	0.03	20,20,20,20	1
6	ZN	D	302	1/1	0.99	0.04	28,28,28,28	0
5	SO4	H	301	5/5	0.99	0.04	14,15,17,21	0
5	SO4	D	301	5/5	0.99	0.03	14,15,16,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.