WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 04:44 PM EDT

PDB ID	:	4Q3M
Title	:	Crystal structure of MGS-M4, an aldo-keto reductase enzyme from a Medee basin deep-sea metagenome library
Authors	:	Stogios, P.J.; Xu, X.; Cui, H.; Alcaide, M.; Ferrer, M.; Savchenko, A.
Deposited on	:	2014-04-11
Resolution	:	2.55 Å(reported)

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

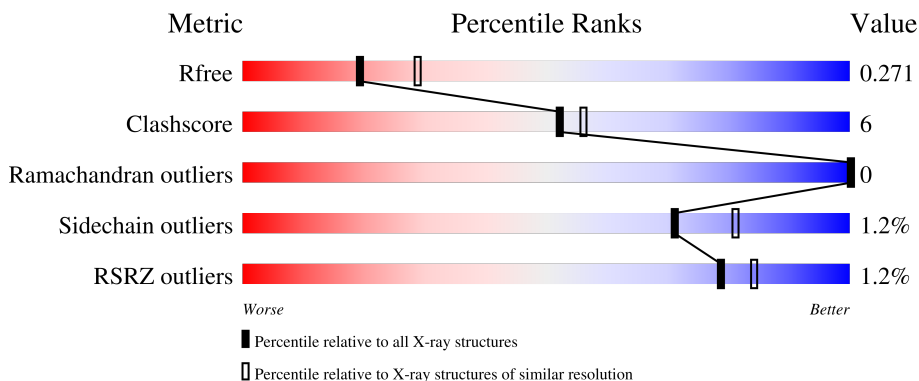|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.55 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		0.271
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		1.2%

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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	274	87% 12%
1	B	274	3% · 85% 14% ·
1	C	274	84% 15% ·
1	D	274	.% 82% 17%
1	E	274	85% 13% ··

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Mol	Chain	Length	Quality of chain
1	F	274	

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	301	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 14148 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 MGS-M4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2233	1428	375	421	9			
1	B	271	Total	C	N	O	S	0	0	0
			2218	1419	372	418	9			
1	C	273	Total	C	N	O	S	0	1	0
			2238	1432	375	421	10			
1	D	273	Total	C	N	O	S	0	0	0
			2233	1428	375	421	9			
1	E	272	Total	C	N	O	S	0	0	0
			2223	1422	372	420	9			
1	F	268	Total	C	N	O	S	0	0	0
			2190	1402	366	413	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Na 1	0	0

- Molecule 4 is water.

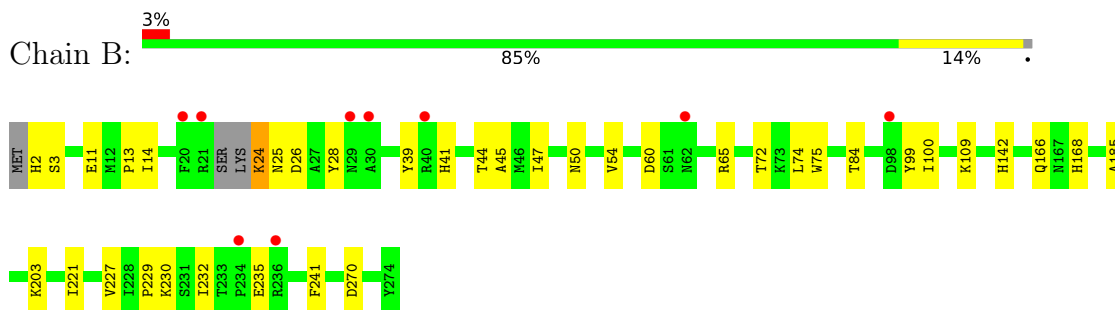| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	138	Total 138	O 138	0	0
4	B	111	Total 111	O 111	0	0
4	C	131	Total 131	O 131	0	0
4	D	113	Total 113	O 113	0	0
4	E	157	Total 157	O 157	0	0
4	F	132	Total 132	O 132	0	0

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.
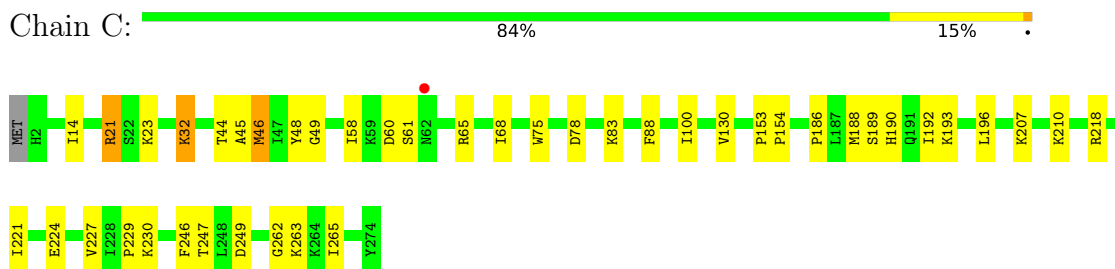
- Molecule 1: MGS-M4

Chain A:

- Molecule 1: MGS-M4

Chain B:

- Molecule 1: MGS-M4

Chain C:

- Molecule 1: MGS-M4

Chain D:
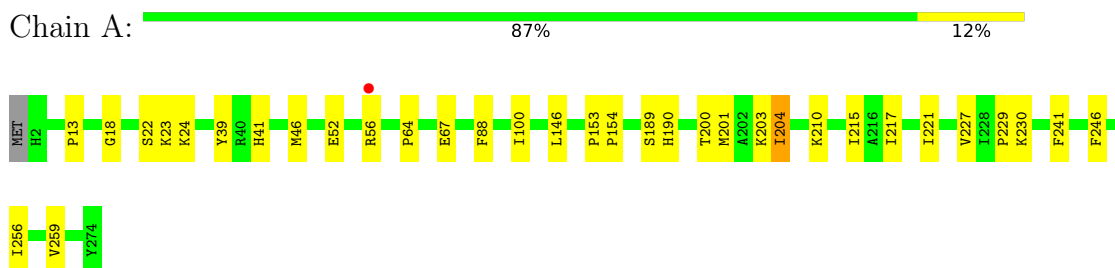
E199 T200 I221 V227 I228 P229 K230 T233 P234 E235 R236 I237 V238 Q239 N240 F241 T261 G262 K263 T267 Y274
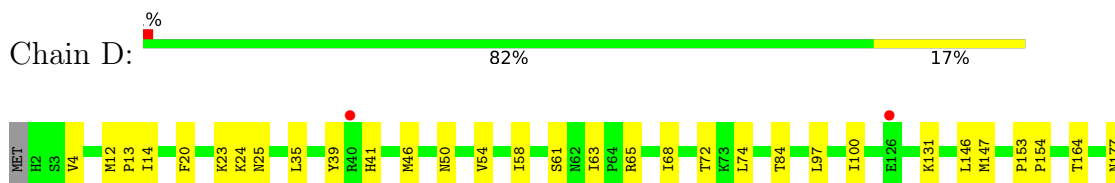
• Molecule 1: MGS-M4

Chain E:

85%   13% ••

MET HIS S3 N9 G18 T19 F20 K24 N25 Y39 R40 M46 I47 E53 R56 W75 F88 I100 D101 R119 K131 L146 A150 Q158 V163 T164 Y184 S189 H190 S197 N198 E199 T200 M201 I212 V227 I228 P229 K230

T233 P234 K254 S255 Y274

• Molecule 1: MGS-M4

2%

Chain F:

81%   16% ••

MET H2 S3 V4 K5 Y10 I14 L17 K23 K24 N25 D26 A27 Y28 K32 A33 A34 L35 E36 Y39 T44 A45 M46 R56 A57 I58 K59 D60 S61 ASN ILE PRO ARG GLU E67 L74 W75 N76 Q79 G80 Y81 E82 K83 T84 T90 D98 Y99 I100

D101 K109 R119 E127 G128 K129 D172 Y173 K176 S189 H190 E199 I204 K207 K210 V227 I228 P229 F241 F246 E251 Y274

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	172.47Å 172.47Å 113.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.58 – 2.55 24.58 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.6 (24.58-2.55) 89.2 (24.58-2.55)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1538)	Depositor
R, R_{free}	0.207 , 0.266 0.211 , 0.271	Depositor DCC
R_{free} test set	1994 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 29.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.428 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14148	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2249e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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: SO4, 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	0.24	0/2282	0.40	0/3085
1	B	0.29	0/2266	0.45	0/3063
1	C	0.30	2/2290 (0.1%)	0.47	2/3095 (0.1%)
1	D	0.27	0/2282	0.41	0/3085
1	E	0.28	0/2271	0.40	0/3070
1	F	0.32	0/2237	0.46	1/3022 (0.0%)
All	All	0.28	2/13628 (0.0%)	0.43	3/18420 (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
1	F	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46[A]	MET	CA-C	6.29	1.69	1.52
1	C	46[B]	MET	CA-C	6.29	1.69	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46[A]	MET	CA-C-O	7.55	135.95	120.10
1	C	46[B]	MET	CA-C-O	7.55	135.95	120.10
1	F	60	ASP	CA-C-N	-5.35	105.42	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	25	ASN	Mainchain
1	F	60	ASP	Mainchain

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	2233	0	2206	20	0
1	B	2218	0	2187	23	0
1	C	2238	0	2215	30	0
1	D	2233	0	2206	31	0
1	E	2223	0	2199	20	0
1	F	2190	0	2162	26	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	2	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	F	1	0	0	0	0
4	A	138	0	0	0	0
4	B	111	0	0	2	0
4	C	131	0	0	2	0
4	D	113	0	0	2	0
4	E	157	0	0	1	0
4	F	132	0	0	1	0
All	All	14148	0	13175	147	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 6.

All (147) 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:F:127:GLU:O	1:F:129:LYS:HE2	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:TYR:HA	1:F:176:LYS:HE3	1.65	0.79
1:D:153:PRO:HG2	4:D:439:HOH:O	1.86	0.74
1:C:224:GLU:HG2	4:C:441:HOH:O	1.86	0.74
1:B:24:LYS:N	1:B:24:LYS:HD2	2.03	0.73
1:A:52:GLU:HB3	1:A:56:ARG:HH12	1.58	0.69
1:D:24:LYS:O	1:D:25:ASN:HB2	1.94	0.67
1:D:14:ILE:HD13	1:D:221:ILE:HG23	1.78	0.66
1:B:227:VAL:HG22	1:B:229:PRO:HD3	1.78	0.65
1:B:24:LYS:O	1:B:25:ASN:HB2	1.97	0.65
1:B:72:THR:HG22	1:B:100:ILE:HG21	1.78	0.64
1:A:64:PRO:HB2	1:A:67:GLU:HG3	1.78	0.64
1:A:227:VAL:HG22	1:A:229:PRO:HD3	1.80	0.64
1:D:236:ARG:NH2	4:D:459:HOH:O	2.32	0.62
1:F:207:LYS:NZ	1:F:251:GLU:OE2	2.31	0.62
1:C:227:VAL:HG22	1:C:229:PRO:HD3	1.83	0.61
1:B:109:LYS:NZ	4:B:498:HOH:O	2.33	0.60
1:D:227:VAL:HG22	1:D:229:PRO:HD3	1.83	0.60
1:C:23:LYS:N	1:C:23:LYS:HD3	2.18	0.58
1:B:203:LYS:HG2	4:B:488:HOH:O	2.02	0.58
1:F:56:ARG:HA	1:F:59:LYS:HG2	1.85	0.58
1:A:201:MET:HE1	1:A:256:ILE:HG23	1.85	0.57
1:C:65:ARG:NH1	1:C:68:ILE:O	2.38	0.57
1:F:28:TYR:CE1	1:F:57:ALA:HA	2.40	0.57
1:B:47:ILE:HD13	1:B:75:TRP:CE2	2.40	0.56
1:F:82:GLU:H	1:F:82:GLU:CD	2.07	0.56
1:C:32:LYS:HZ1	1:C:60:ASP:HB3	1.71	0.56
1:C:263:LYS:HE3	4:C:448:HOH:O	2.04	0.56
1:D:236:ARG:HA	1:D:239:GLN:OE1	2.06	0.55
1:E:53:GLU:HG2	1:E:56:ARG:HH21	1.72	0.55
1:C:58:ILE:O	1:C:61:SER:OG	2.24	0.54
1:D:235:GLU:O	1:D:238:VAL:HG22	2.08	0.54
1:B:50:ASN:O	1:B:54:VAL:HG23	2.08	0.54
1:D:236:ARG:NH1	1:F:199:GLU:OE2	2.37	0.53
1:E:163:VAL:HG12	1:E:164:THR:HG23	1.90	0.53
1:F:23:LYS:HB2	1:F:26:ASP:OD2	2.08	0.53
1:D:72:THR:HG22	1:D:100:ILE:HG21	1.91	0.52
1:B:44:THR:OG1	1:B:45:ALA:N	2.43	0.52
1:D:164:THR:HB	1:D:261:THR:HG22	1.92	0.52
1:C:46[B]:MET:HE2	1:C:75:TRP:HB2	1.93	0.51
1:A:23:LYS:HZ2	1:A:24:LYS:HG2	1.75	0.51
1:B:235:GLU:HG2	1:B:235:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LEU:HD23	1:D:154:PRO:HG3	1.93	0.51
1:C:78:ASP:HA	1:C:83:LYS:HD3	1.92	0.51
1:F:10:TYR:OH	1:F:101:ASP:OD2	2.23	0.50
1:A:256:ILE:O	1:A:259:VAL:HG22	2.11	0.50
1:A:189:SER:OG	1:A:190:HIS:N	2.44	0.49
1:F:227:VAL:HG22	1:F:229:PRO:HD3	1.93	0.49
1:F:172:ASP:O	1:F:176:LYS:HG2	2.12	0.49
1:C:21:ARG:NH1	1:C:48:TYR:O	2.46	0.49
1:C:262:GLY:HA3	1:D:267:THR:HG23	1.94	0.48
1:A:204:ILE:HD11	1:A:215:ILE:CG2	2.44	0.48
1:F:99:TYR:CD2	1:F:99:TYR:C	2.86	0.48
1:C:192:ILE:HG23	1:C:193:LYS:HD3	1.95	0.48
1:D:4:VAL:N	1:D:12:MET:O	2.45	0.48
1:F:204:ILE:HA	1:F:207:LYS:HG2	1.96	0.48
1:A:203:LYS:NZ	1:A:204:ILE:HG22	2.28	0.47
1:D:39:TYR:CE1	1:D:241:PHE:HB2	2.49	0.47
1:F:28:TYR:CD1	1:F:57:ALA:HB2	2.48	0.47
1:B:26:ASP:HB3	1:B:232:ILE:HG21	1.95	0.47
1:E:227:VAL:HG22	1:E:229:PRO:HD3	1.96	0.47
1:C:207:LYS:NZ	1:C:249:ASP:OD2	2.39	0.47
1:E:101:ASP:HA	1:E:131:LYS:HB2	1.96	0.47
1:D:233:THR:O	1:D:237:ILE:HG13	2.14	0.47
1:F:189:SER:OG	1:F:190:HIS:N	2.47	0.47
1:D:74:LEU:HD13	1:D:84:THR:HG23	1.97	0.47
1:B:232:ILE:O	1:B:232:ILE:HG22	2.15	0.46
1:D:20:PHE:HE2	1:D:230:LYS:HB3	1.81	0.46
1:F:39:TYR:CE1	1:F:241:PHE:HB2	2.50	0.46
1:C:46[B]:MET:CE	1:C:75:TRP:HB2	2.46	0.46
1:C:186:PRO:HD2	2:C:301:SO4:O1	2.16	0.46
1:E:158:GLN:HG2	1:E:184:TYR:HD2	1.81	0.46
1:F:4:VAL:HG13	1:F:14:ILE:HG23	1.98	0.46
1:F:74:LEU:HD13	1:F:84:THR:HG23	1.98	0.46
1:D:20:PHE:CE2	1:D:230:LYS:HB3	2.52	0.45
1:A:52:GLU:HB3	1:A:56:ARG:NH1	2.28	0.45
1:A:217:ILE:O	1:A:221:ILE:HG12	2.17	0.45
1:B:142:HIS:NE2	1:B:270:ASP:OD1	2.48	0.45
1:D:35:LEU:HD13	1:D:61:SER:HB2	1.99	0.45
1:E:18:GLY:HA3	1:E:230:LYS:HG2	1.98	0.45
1:F:32:LYS:NZ	4:F:500:HOH:O	2.49	0.45
1:C:21:ARG:HH12	1:C:49:GLY:HA3	1.82	0.45
1:C:210:LYS:HE3	1:C:246:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:PHE:O	1:D:50:ASN:ND2	2.50	0.45
1:B:74:LEU:HD13	1:B:84:THR:HG23	1.98	0.45
1:F:44:THR:OG1	1:F:45:ALA:N	2.50	0.45
1:E:20:PHE:HB3	1:E:230:LYS:HD3	1.99	0.44
1:E:119:ARG:HH12	1:E:150:ALA:HA	1.82	0.44
1:D:147:MET:SD	1:D:177:ASN:HB3	2.57	0.44
1:A:210:LYS:HE3	1:A:246:PHE:CD2	2.53	0.44
1:C:188:MET:HB2	1:C:265:ILE:HD11	1.99	0.44
1:A:13:PRO:HB2	1:A:41:HIS:HB2	2.00	0.44
1:C:14:ILE:HD13	1:C:221:ILE:HG23	1.99	0.44
1:D:261:THR:HG23	1:D:263:LYS:H	1.82	0.44
1:F:76:ASN:HB3	1:F:109:LYS:HG3	2.00	0.44
1:D:63:ILE:HB	1:D:68:ILE:HD11	1.99	0.44
1:F:59:LYS:HE3	1:F:59:LYS:HB2	1.57	0.44
1:A:204:ILE:HD11	1:A:215:ILE:HG23	2.00	0.43
1:C:153:PRO:HA	1:C:154:PRO:HD3	1.89	0.43
1:D:131:LYS:HA	1:D:131:LYS:HD3	1.70	0.43
1:A:200:THR:O	1:A:204:ILE:HG23	2.18	0.43
1:D:65:ARG:NH1	1:D:68:ILE:O	2.51	0.43
1:F:210:LYS:HE3	1:F:246:PHE:CD1	2.54	0.43
1:B:14:ILE:HD13	1:B:221:ILE:HG23	2.00	0.43
1:C:88:PHE:CE1	1:C:100:ILE:HD12	2.53	0.43
1:D:4:VAL:O	1:D:12:MET:N	2.52	0.43
1:B:13:PRO:HB2	1:B:41:HIS:HB2	2.00	0.43
1:D:65:ARG:HE	1:D:97:LEU:HD22	1.84	0.43
1:F:76:ASN:HA	1:F:79:GLN:HG3	2.01	0.43
1:C:32:LYS:HE3	1:C:61:SER:HB3	2.01	0.43
1:C:44:THR:OG1	1:C:45:ALA:N	2.51	0.43
1:E:233:THR:HA	1:E:234:PRO:HD2	1.81	0.43
1:C:230:LYS:HE2	2:C:301:SO4:O1	2.18	0.42
1:F:17:LEU:HD22	1:F:34:ALA:HB2	2.00	0.42
1:A:88:PHE:CE1	1:A:100:ILE:HD12	2.54	0.42
1:A:39:TYR:CE1	1:A:241:PHE:HB2	2.53	0.42
1:E:39:TYR:O	1:E:40:ARG:NH1	2.48	0.42
1:E:24:LYS:HG3	1:E:25:ASN:N	2.33	0.42
1:C:32:LYS:HD3	1:C:32:LYS:HA	1.82	0.42
1:E:200:THR:HG21	1:E:255:SER:HB3	2.01	0.42
1:E:9:ASN:ND2	4:E:469:HOH:O	2.36	0.42
1:C:189:SER:OG	1:C:190:HIS:N	2.52	0.41
1:C:196:LEU:HB2	1:E:197:SER:HB2	2.01	0.41
1:E:47:ILE:HD13	1:E:75:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:TYR:OH	1:B:60:ASP:OD2	2.34	0.41
1:B:65:ARG:NH2	1:B:99:TYR:O	2.48	0.41
1:B:72:THR:HG21	1:B:100:ILE:HD13	2.00	0.41
1:A:18:GLY:HA3	1:A:230:LYS:HG2	2.03	0.41
1:F:81:TYR:HD2	1:F:119:ARG:HG3	1.85	0.41
1:C:32:LYS:NZ	1:C:60:ASP:HB3	2.34	0.41
1:D:199:GLU:HG2	1:D:200:THR:N	2.36	0.41
1:E:146:LEU:HA	1:E:146:LEU:HD12	1.87	0.41
1:D:12:MET:HA	1:D:13:PRO:HD3	1.94	0.41
1:E:199:GLU:HG3	1:E:200:THR:N	2.36	0.41
1:B:39:TYR:CE1	1:B:241:PHE:HB2	2.57	0.40
1:E:88:PHE:CE1	1:E:100:ILE:HD12	2.55	0.40
1:E:189:SER:OG	1:E:190:HIS:N	2.53	0.40
1:D:13:PRO:HB2	1:D:41:HIS:HB2	2.04	0.40
1:D:54:VAL:O	1:D:58:ILE:HG13	2.22	0.40
1:A:22:SER:OG	1:A:23:LYS:N	2.51	0.40
1:B:185:ALA:HA	2:B:301:SO4:O4	2.21	0.40
1:C:100:ILE:O	1:C:130:VAL:HA	2.22	0.40
1:A:153:PRO:HA	1:A:154:PRO:HD3	1.92	0.40
1:B:3:SER:OG	1:B:11:GLU:HB2	2.21	0.40
1:B:166:GLN:OE1	1:B:168:HIS:HE1	2.04	0.40
1:E:201:MET:HB3	1:E:212:ILE:HG23	2.03	0.40
1:C:218:ARG:NH2	1:C:247:THR:HG22	2.37	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	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
1	B	267/274 (97%)	260 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
1	D	271/274 (99%)	265 (98%)	6 (2%)	0	100	100
1	E	270/274 (98%)	266 (98%)	4 (2%)	0	100	100
1	F	264/274 (96%)	255 (97%)	9 (3%)	0	100	100
All	All	1615/1644 (98%)	1574 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	245/246 (100%)	242 (99%)	3 (1%)	71	81
1	B	243/246 (99%)	240 (99%)	3 (1%)	71	81
1	C	246/246 (100%)	244 (99%)	2 (1%)	81	88
1	D	245/246 (100%)	243 (99%)	2 (1%)	81	88
1	E	244/246 (99%)	239 (98%)	5 (2%)	55	69
1	F	240/246 (98%)	237 (99%)	3 (1%)	69	80
All	All	1463/1476 (99%)	1445 (99%)	18 (1%)	71	81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	146	LEU
1	A	204	ILE
1	B	2	HIS
1	B	24	LYS
1	B	230	LYS
1	C	21	ARG
1	C	32	LYS
1	D	23	LYS

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Mol	Chain	Res	Type
1	D	46	MET
1	E	3	SER
1	E	46	MET
1	E	131	LYS
1	E	163	VAL
1	E	254	LYS
1	F	46	MET
1	F	83	LYS
1	F	99	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	HIS
1	B	168	HIS
1	C	191	GLN
1	D	41	HIS
1	E	41	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, 1 is monoatomic - leaving 6 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	$\#|Z| > 2$
2	SO4	C	301	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	301	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	E	301	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	F	302	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.06	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	SO4	2	0
2	B	301	SO4	1	0

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(Å²)	Q<0.9
1	A	273/274 (99%)	-0.30	1 (0%)	92	96	26, 50, 86, 110	0
1	B	271/274 (98%)	-0.01	9 (3%)	46	56	32, 57, 97, 129	0
1	C	273/274 (99%)	-0.26	1 (0%)	92	96	26, 49, 84, 109	0
1	D	273/274 (99%)	-0.15	2 (0%)	87	91	33, 57, 95, 118	0
1	E	272/274 (99%)	-0.32	0	100	100	29, 46, 82, 100	0
1	F	268/274 (97%)	-0.09	6 (2%)	62	70	31, 55, 91, 131	0
All	All	1630/1644 (99%)	-0.19	19 (1%)	79	84	26, 53, 91, 131	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	98	ASP	5.0
1	B	98	ASP	4.6
1	B	20	PHE	3.6
1	F	23	LYS	3.1
1	B	62	ASN	2.8
1	B	40	ARG	2.8
1	F	24	LYS	2.7
1	F	5	LYS	2.6
1	D	40	ARG	2.6
1	B	234	PRO	2.6
1	F	90	THR	2.5
1	A	56	ARG	2.4
1	B	29	ASN	2.4
1	B	236	ARG	2.3
1	C	62	ASN	2.3
1	B	30	ALA	2.2
1	F	36	GLU	2.2
1	B	21	ARG	2.1
1	D	126	GLU	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
3	NA	F	301	1/1	0.89	0.11	57,57,57,57	0
2	SO4	C	301	5/5	0.97	0.16	56,58,60,70	0
2	SO4	A	301	5/5	0.98	0.13	53,60,62,65	0
2	SO4	E	301	5/5	0.98	0.14	54,60,61,62	0
2	SO4	B	301	5/5	0.98	0.11	48,49,53,54	0
2	SO4	F	302	5/5	0.99	0.08	44,45,51,58	0
2	SO4	D	301	5/5	0.99	0.13	48,54,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.