



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:08 AM GMT

PDB ID : 1F07
Title : STRUCTURE OF COENZYME F420 DEPENDENT TETRAHYDRO-
THANOPTERINREDUCTASE FROM METHANOBACTERIUM THER-
MOAUTOTROPHICUM
Authors : Shima, S.; Warkentin, E.; Grabarse, W.; Thauer, R.K.; Ermler, U.
Deposited on : 2000-05-15
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

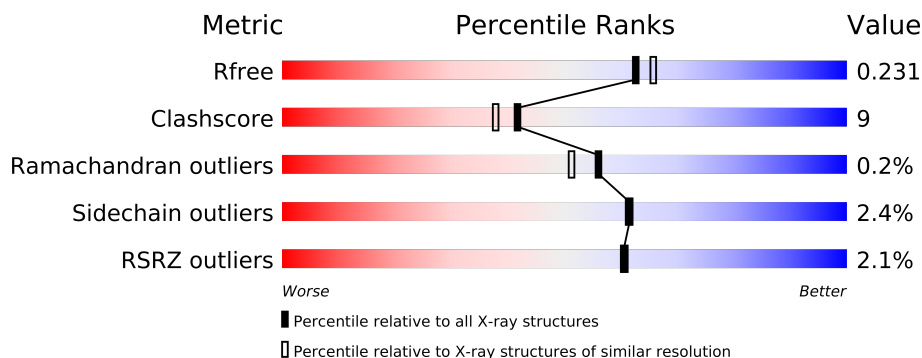
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	321	
1	B	321	
1	C	321	
1	D	321	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MPO	A	331	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11407 atoms, of which 1404 are hydrogens and 0 are deuterium.

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.

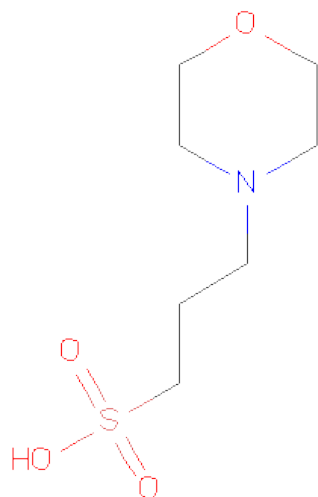
- Molecule 1 is a protein called COENZYME F420-DEPENDENT N5,N10-METHYLENETETRAHYDROMETHANOPTERINREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2353	1503	378	461	11			
1	B	321	Total	C	H	N	O	S	0	0
			2821	1503	468	378	461	11		
1	C	321	Total	C	H	N	O	S	0	0
			2821	1503	468	378	461	11		
1	D	321	Total	C	H	N	O	S	0	0
			2821	1503	468	378	461	11		

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

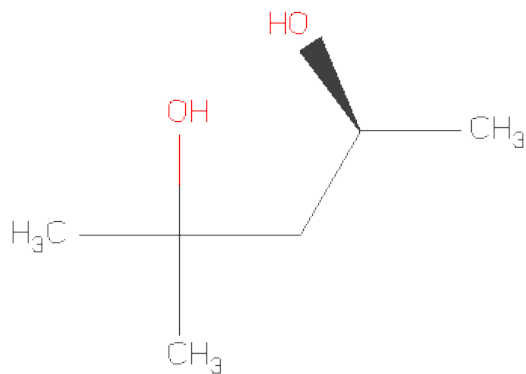
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 3[N-MORPHOLINO]PROPANESULFONIC ACID (three-letter code: MPO) (formula: C₇H₁₅NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

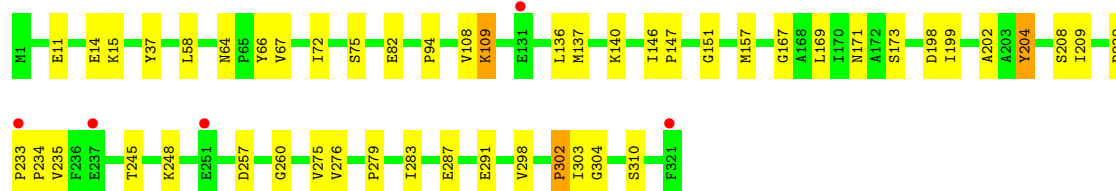
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total	O	0	0
			143	143		
5	B	97	Total	O	0	0
			97	97		
5	C	146	Total	O	0	0
			146	146		
5	D	119	Total	O	0	0
			119	119		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

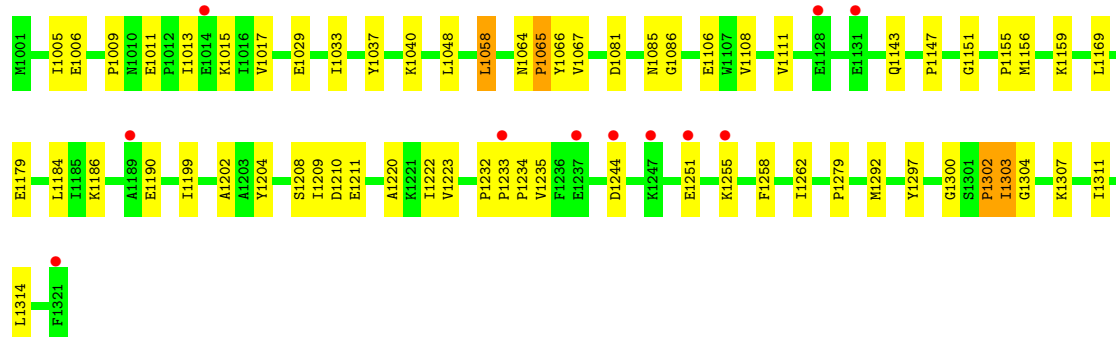
- Molecule 1: COENZYME F420-DEPENDENT N5,N10-METHYLENETETRAHYDROMETHANOPTERINREDUCTASE

Chain A: 



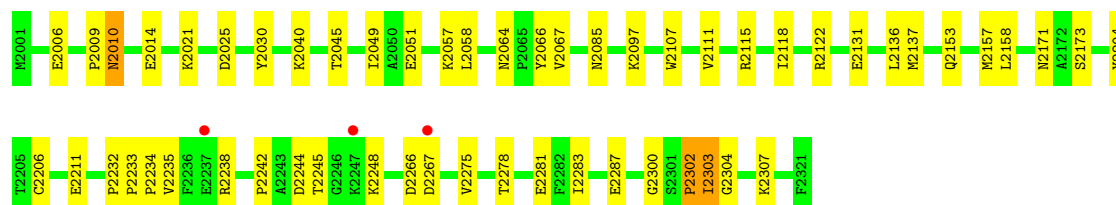
- Molecule 1: COENZYME F420-DEPENDENT N5,N10-METHYLENETETRAHYDROMETHANOPTERINREDUCTASE

Chain B: 



- Molecule 1: COENZYME F420-DEPENDENT N5,N10-METHYLENETETRAHYDROMETHANOPTERINREDUCTASE

Chain C: 



- Molecule 1: COENZYME F420-DEPENDENT N5,N10-METHYLENETETRAHYDROMETHANOPTERINREDUCTASE

Category	Item	Value	Color
Group 1	P3302	13302	Green
	I3303	13303	Yellow
	G3304	13304	Yellow
	K3309	13309	Red
Group 2	S3310	13310	Yellow
	L3314	13314	Yellow
	F3321	13321	Green
	K3189	13189	Red
Group 3	E3190	13190	Green
	I3199	13199	Yellow
	A3202	13202	Yellow
	Y3204	13204	Orange
Group 4	C3207	13207	Yellow
	S2208	13208	Yellow
	I3209	13209	Yellow
	D3210	13210	Green
Group 5	E3211	13211	Yellow
	A3217	13217	Yellow
	K3221	13221	Yellow
	V3224	13224	Yellow
Group 6	P3232	13232	Yellow
	P3233	13233	Yellow
	P3234	13234	Yellow
	V3235	13235	Yellow
Group 7	F3236	13236	Yellow
	E3237	13237	Red
	R3238	13238	Yellow
	L3241	13241	Yellow
Group 8	P3242	13242	Yellow
	A3243	13243	Green
	D3244	13244	Yellow
	T3245	13245	Yellow
Group 9	K3248	13248	Yellow
	E3251	13251	Red
	G3254	13254	Green
	K3255	13255	Yellow
Group 10	L3269	13269	Yellow
	M3270	13270	Yellow
	F3273	13273	Yellow
	V3276	13276	Yellow
Group 11	G3277	13277	Yellow
	T3278	13278	Yellow
	P3279	13279	Red
	D3280	13280	Yellow
Group 12	F3281	13281	Yellow
	F3282	13282	Yellow
	I3283	13283	Yellow
	E3287	13287	Yellow
Group 13	E3291	13291	Yellow
	K3001	13001	Red
	P3009	13009	Yellow
	K3010	13010	Yellow
Group 14	E3011	13011	Yellow
	E3014	13014	Yellow
	K3015	13015	Yellow
	K3040	13040	Yellow
Group 15	L3048	13048	Yellow
	I3049	13049	Yellow
	L3068	13068	Red
	N3064	13064	Yellow
Group 16	P3065	13065	Yellow
	Y3066	13066	Yellow
	V3067	13067	Yellow
	I3072	13072	Yellow
Group 17	A3078	13078	Yellow
	T3079	13079	Red
	L3080	13080	Yellow
	D3081	13081	Yellow
Group 18	E3082	13082	Yellow
	K3109	13109	Yellow
	I3114	13114	Yellow
	E3131	13131	Red
Group 19	Q3143	13143	Yellow
	F3144	13144	Green
	K3145	13145	Yellow
	I3146	13146	Yellow
Group 20	P3147	13147	Yellow
	Q3151	13151	Yellow
	P3155	13155	Yellow
	K3156	13156	Yellow
Group 21	M3157	13157	Yellow
	L3158	13158	Yellow
	K3159	13159	Yellow
	E3163	13163	Yellow
Group 22	D3166	13166	Yellow
	L3169	13169	Yellow
	I3170	13170	Yellow
	N3171	13171	Yellow
Group 23	L3184	13184	Yellow
	I3185	13185	Yellow
	K3186	13186	Yellow
	E3291	13291	Yellow

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.80Å 128.20Å 109.20Å 90.00° 131.40° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 9.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-2.00) 95.7 (9.99-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.01Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.208 , 0.237 0.202 , 0.231	Depositor DCC
R_{free} test set	5402 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 55.9	EDS
Estimated twinning fraction	0.002 for k+l,h+l,-l 0.000 for -k+l,-h-l,-l 0.013 for -h-2*l,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 107409 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11407	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPO, MPD, CL

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	0.39	0/2396	0.67	1/3249 (0.0%)
1	B	0.35	0/2396	0.66	1/3249 (0.0%)
1	C	0.39	0/2396	0.66	1/3249 (0.0%)
1	D	0.37	0/2396	0.67	1/3249 (0.0%)
All	All	0.38	0/9584	0.66	4/12996 (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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1151	GLY	N-CA-C	-5.62	99.05	113.10
1	A	151	GLY	N-CA-C	-5.51	99.33	113.10
1	C	2206	CYS	N-CA-C	-5.23	96.88	111.00
1	D	3151	GLY	N-CA-C	-5.13	100.27	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1297	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2353	0	2378	43	0
1	B	2353	468	1908	44	0
1	C	2353	468	1910	41	0
1	D	2353	468	1910	50	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	13	0	14	6	0
3	B	13	0	14	0	0
3	C	13	0	14	0	0
3	D	13	0	14	0	0
4	A	8	0	14	0	0
4	B	8	0	14	0	0
4	C	8	0	14	2	0
4	D	8	0	14	1	0
5	A	143	0	0	1	0
5	B	97	0	0	1	0
5	C	146	0	0	5	0
5	D	119	0	0	2	0
All	All	10003	1404	8218	173	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (173) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:64:ASN:HD22	1:A:66:TYR:H	1.06	0.99
1:B:1106:GLU:HG2	1:B:1108:VAL:HG13	1.47	0.95
1:C:2244:ASP:OD2	1:C:2248:LYS:HE2	1.76	0.84
1:C:2242:PRO:HB2	1:C:2244:ASP:OD1	1.83	0.78
1:D:3244:ASP:OD2	1:D:3248:LYS:HE2	1.86	0.75
1:A:64:ASN:HD21	1:A:67:VAL:H	1.34	0.75
1:C:2064:ASN:HD22	1:C:2066:TYR:H	1.36	0.73
1:A:64:ASN:ND2	1:A:66:TYR:H	1.84	0.72
1:A:136:LEU:O	1:A:137:MET:HE3	1.89	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2283:ILE:O	1:C:2287:GLU:HG3	1.92	0.70
1:B:1064:ASN:HD22	1:B:1066:TYR:H	1.39	0.70
1:B:1159:LYS:NZ	1:B:1184:LEU:HD22	2.07	0.69
1:D:3217:ALA:HA	1:D:3276:VAL:HG11	1.72	0.69
1:D:3064:ASN:HD21	1:D:3066:TYR:H	1.38	0.67
1:C:2242:PRO:HG2	1:C:2245:THR:OG1	1.95	0.67
1:C:2067:VAL:HG21	5:C:664:HOH:O	1.95	0.66
1:A:204:TYR:HE2	3:A:331:MPO:H11	1.60	0.66
1:C:2064:ASN:HD21	1:C:2067:VAL:H	1.45	0.64
1:B:1011:GLU:OE1	1:B:1015:LYS:HD3	1.99	0.62
1:A:233:PRO:HG2	1:A:234:PRO:CD	2.28	0.62
1:D:3058:LEU:HD13	1:D:3080:LEU:HD21	1.80	0.62
1:D:3199:ILE:N	1:D:3199:ILE:HD12	2.15	0.62
1:B:1179:GLU:HG3	1:B:1292:MET:HE1	1.82	0.61
1:C:2266:ASP:HB2	5:C:878:HOH:O	2.02	0.59
1:D:3114:ILE:HD12	1:D:3157:MET:CE	2.33	0.59
1:B:1251:GLU:HG2	1:B:1255:LYS:HE2	1.85	0.59
1:B:1009:PRO:HG3	1:B:1033:ILE:CG2	2.32	0.59
1:D:3064:ASN:HD22	1:D:3067:VAL:H	1.51	0.59
1:A:204:TYR:CE2	3:A:331:MPO:H11	2.37	0.59
1:A:283:ILE:O	1:A:287:GLU:HG3	2.02	0.58
1:D:3211:GLU:HG2	5:D:934:HOH:O	2.04	0.56
1:C:2153:GLN:HE21	1:C:2171:ASN:H	1.52	0.56
1:A:64:ASN:HD22	1:A:66:TYR:N	1.90	0.56
1:C:2051:GLU:HG3	1:D:3048:LEU:HD21	1.86	0.56
1:B:1258:PHE:O	1:B:1262:ILE:HG13	2.06	0.56
1:D:3236:PHE:CD2	1:D:3245:THR:HB	2.41	0.56
1:A:233:PRO:HG2	1:A:234:PRO:HD3	1.88	0.56
1:A:287:GLU:O	1:A:291:GLU:HG3	2.06	0.56
1:C:2045:THR:O	1:C:2049:ILE:HG13	2.05	0.55
1:D:3238:ARG:NH2	4:D:338:MPD:O2	2.40	0.55
1:C:2278:THR:OG1	1:C:2281:GLU:HG3	2.06	0.55
1:D:3270:MET:HE3	1:D:3276:VAL:HG21	1.89	0.55
1:B:1199:ILE:N	1:B:1199:ILE:HD12	2.22	0.54
1:D:3145:LYS:NZ	1:D:3166:ASP:OD1	2.39	0.54
1:A:11:GLU:OE1	1:A:15:LYS:HD2	2.08	0.54
1:A:94:PRO:HB3	1:A:157:MET:CE	2.37	0.54
1:C:2064:ASN:ND2	1:C:2067:VAL:H	2.06	0.53
1:A:209:ILE:HD11	1:A:279:PRO:HG3	1.89	0.53
1:B:1064:ASN:ND2	1:B:1066:TYR:H	2.06	0.53
1:D:3155:PRO:HA	1:D:3184:LEU:HD13	1.90	0.53
1:B:1013:ILE:O	1:B:1017:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:64:ASN:ND2	1:A:67:VAL:H	2.06	0.52
1:C:2137:MET:HE2	1:C:2137:MET:HA	1.91	0.52
1:C:2307:LYS:HE2	5:C:416:HOH:O	2.07	0.52
1:D:3114:ILE:HD12	1:D:3157:MET:HE1	1.92	0.52
1:B:1155:PRO:O	1:B:1159:LYS:HG2	2.10	0.52
1:B:1159:LYS:HD3	1:B:1184:LEU:O	2.10	0.51
1:D:3251:GLU:O	1:D:3255:LYS:HG3	2.09	0.51
1:C:2238:ARG:NH1	4:C:337:MPD:O2	2.44	0.51
1:A:137:MET:HE2	1:A:137:MET:HA	1.93	0.51
1:B:1233:PRO:N	1:B:1234:PRO:HD2	2.26	0.50
1:B:1169:LEU:HD23	1:B:1202:ALA:HB3	1.93	0.50
1:C:2173:SER:HB3	1:C:2275:VAL:HG23	1.94	0.50
1:B:1064:ASN:HD21	1:B:1067:VAL:H	1.58	0.50
1:D:3171:ASN:HD21	1:D:3204:TYR:HB3	1.77	0.50
1:B:1058:LEU:HD12	1:B:1058:LEU:H	1.77	0.50
1:B:1143:GLN:HE22	1:B:1147:PRO:HD3	1.76	0.50
1:A:304:GLY:HA3	1:A:310:SER:OG	2.12	0.49
1:D:3011:GLU:O	1:D:3040:LYS:HE3	2.12	0.49
1:A:232:PRO:HG2	1:A:235:VAL:HG23	1.95	0.49
1:D:3278:THR:OG1	1:D:3281:GLU:HG3	2.12	0.49
1:C:2064:ASN:HD22	1:C:2066:TYR:N	2.09	0.49
1:D:3217:ALA:O	1:D:3221:LYS:HG3	2.13	0.49
1:D:3302:PRO:O	1:D:3303:ILE:HB	2.13	0.49
1:A:171:ASN:ND2	3:A:331:MPO:H31	2.28	0.48
1:C:2115:ARG:NE	5:C:463:HOH:O	2.37	0.48
1:C:2211:GLU:OE2	1:C:2211:GLU:N	2.42	0.48
1:D:3233:PRO:N	1:D:3234:PRO:HD2	2.28	0.48
1:A:82:GLU:OE1	1:B:1040:LYS:HE3	2.12	0.48
1:B:1209:ILE:HG21	1:B:1314:LEU:HG	1.95	0.48
1:B:1005:ILE:HD11	1:B:1303:ILE:HD13	1.96	0.48
1:D:3241:LEU:HD13	1:D:3269:LEU:HD23	1.96	0.47
1:C:2118:ILE:O	1:C:2122:ARG:HG2	2.13	0.47
1:D:3049:ILE:HG22	1:D:3058:LEU:HD23	1.95	0.47
1:B:1307:LYS:O	1:B:1311:ILE:HG13	2.14	0.47
1:A:167:GLY:HA2	1:A:199:ILE:HG23	1.96	0.47
1:A:75:SER:HB2	1:B:1037:TYR:O	2.14	0.47
1:D:3186:LYS:O	1:D:3190:GLU:HG3	2.15	0.47
1:D:3009:PRO:HB2	1:D:3040:LYS:HB2	1.98	0.46
1:A:198:ASP:C	1:A:199:ILE:HD12	2.35	0.46
1:D:3287:GLU:O	1:D:3291:GLU:HG3	2.15	0.46
1:B:1179:GLU:HA	1:B:1292:MET:HE2	1.97	0.46
1:C:2097:LYS:HB2	1:C:2107:TRP:CE3	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:PRO:HB3	1:A:157:MET:HE3	1.97	0.46
1:A:173:SER:HB3	1:A:275:VAL:HG23	1.98	0.46
1:C:2242:PRO:HG2	1:C:2245:THR:HG1	1.80	0.46
1:D:3270:MET:CE	1:D:3276:VAL:HG21	2.45	0.46
1:A:257:ASP:OD2	1:A:260:GLY:HA3	2.16	0.46
1:C:2302:PRO:O	1:C:2303:ILE:HB	2.16	0.46
1:B:1106:GLU:CG	1:B:1108:VAL:HG13	2.33	0.45
1:B:1159:LYS:HZ1	1:B:1184:LEU:HD22	1.82	0.45
1:D:3304:GLY:HA3	1:D:3310:SER:OG	2.17	0.45
1:D:3232:PRO:HG2	1:D:3235:VAL:HG23	1.98	0.45
1:D:3217:ALA:CA	1:D:3276:VAL:HG11	2.44	0.45
1:D:3209:ILE:HG21	1:D:3314:LEU:HG	1.99	0.45
1:D:3233:PRO:HG2	1:D:3234:PRO:CD	2.47	0.45
1:D:3159:LYS:O	1:D:3163:GLU:HG3	2.18	0.44
1:C:2136:LEU:O	1:C:2137:MET:HE3	2.16	0.44
1:B:1186:LYS:O	1:B:1190:GLU:HG3	2.17	0.44
1:D:3244:ASP:O	1:D:3248:LYS:HG2	2.17	0.44
1:B:1302:PRO:O	1:B:1303:ILE:HB	2.17	0.44
1:D:3276:VAL:HG12	1:D:3277:GLY:N	2.33	0.44
1:A:245:THR:O	1:A:248:LYS:HB3	2.17	0.44
1:B:1232:PRO:HG2	1:B:1235:VAL:HG23	1.99	0.44
1:A:302:PRO:O	1:A:303:ILE:HB	2.18	0.44
1:D:3011:GLU:OE1	1:D:3015:LYS:HD3	2.17	0.44
1:A:94:PRO:HB3	1:A:157:MET:HE1	1.98	0.44
1:D:3283:ILE:O	1:D:3287:GLU:HG3	2.17	0.44
1:B:1064:ASN:HB2	1:B:1065:PRO:HD2	1.98	0.43
1:A:72:ILE:HG13	1:B:1067:VAL:HB	2.00	0.43
1:B:1302:PRO:C	1:B:1304:GLY:H	2.21	0.43
1:A:199:ILE:HD12	1:A:199:ILE:N	2.34	0.43
1:B:1251:GLU:O	1:B:1255:LYS:HG3	2.18	0.43
1:D:3236:PHE:CE2	1:D:3245:THR:HB	2.53	0.43
1:B:1013:ILE:HG21	1:B:1048:LEU:HD12	2.00	0.43
1:D:3143:GLN:HE22	1:D:3147:PRO:HD3	1.83	0.43
1:B:1058:LEU:HD12	1:B:1058:LEU:N	2.34	0.43
1:C:2233:PRO:HG2	1:C:2234:PRO:CD	2.48	0.43
1:D:3242:PRO:HD2	1:D:3245:THR:OG1	2.18	0.43
1:A:208:SER:HB3	1:A:276:VAL:HG12	2.00	0.43
1:D:3207:CYS:O	1:D:3303:ILE:N	2.52	0.42
1:B:1029:GLU:HG3	5:B:792:HOH:O	2.19	0.42
1:A:37:TYR:CD1	1:A:37:TYR:C	2.91	0.42
1:C:2006:GLU:HB3	1:C:2300:GLY:HA2	2.01	0.42
1:C:2009:PRO:HB2	1:C:2040:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2067:VAL:HB	1:D:3072:ILE:HG13	2.00	0.42
1:D:3208:SER:O	1:D:3276:VAL:HA	2.19	0.42
1:A:108:VAL:O	1:A:109:LYS:C	2.58	0.42
1:A:137:MET:CE	1:A:137:MET:HA	2.49	0.42
1:A:204:TYR:CE1	1:A:298:VAL:HG11	2.54	0.42
1:C:2137:MET:HA	1:C:2137:MET:CE	2.49	0.42
1:C:2131:GLU:HG3	5:C:673:HOH:O	2.19	0.42
1:A:171:ASN:HD21	3:A:331:MPO:H31	1.85	0.42
1:C:2302:PRO:C	1:C:2304:GLY:H	2.22	0.42
1:C:2232:PRO:HG2	1:C:2235:VAL:HG23	2.02	0.42
1:C:2010:ASN:H	1:C:2010:ASN:HD21	1.68	0.42
1:B:1006:GLU:HB3	1:B:1300:GLY:HA2	2.02	0.42
1:A:140:LYS:HE2	5:A:417:HOH:O	2.19	0.42
1:D:3211:GLU:CG	5:D:934:HOH:O	2.66	0.42
1:B:1111:VAL:HG11	1:B:1156:MET:HE2	2.01	0.42
1:D:3169:LEU:HD23	1:D:3202:ALA:HB3	2.01	0.42
1:D:3224:VAL:HG13	1:D:3273:PHE:HB2	2.02	0.41
1:C:2021:LYS:HE2	1:C:2025:ASP:OD1	2.20	0.41
1:D:3064:ASN:ND2	1:D:3067:VAL:H	2.15	0.41
1:B:1210:ASP:OD1	1:B:1211:GLU:N	2.53	0.41
1:B:1209:ILE:HD11	1:B:1279:PRO:HG3	2.02	0.41
1:B:1081:ASP:OD2	1:B:1086:GLY:HA2	2.20	0.41
1:C:2058:LEU:HD23	1:C:2058:LEU:N	2.34	0.41
1:C:2111:VAL:HA	1:C:2157:MET:HE1	2.02	0.41
1:A:171:ASN:HD21	3:A:331:MPO:H12	1.85	0.41
1:C:2058:LEU:HD23	1:C:2058:LEU:H	1.85	0.41
1:C:2030:TYR:CE2	1:C:2057:LYS:HD2	2.56	0.41
1:B:1208:SER:HB2	1:B:1220:ALA:HB2	2.03	0.41
1:B:1143:GLN:NE2	1:B:1147:PRO:HD3	2.36	0.41
1:D:3209:ILE:HB	1:D:3282:PHE:CZ	2.56	0.40
1:C:2010:ASN:N	1:C:2010:ASN:HD21	2.19	0.40
1:A:146:ILE:HA	1:A:147:PRO:HD3	1.93	0.40
1:A:171:ASN:HD22	3:A:331:MPO:H41	1.86	0.40
1:C:2158:LEU:HD11	4:C:337:MPD:H32	2.02	0.40
1:D:3078:ALA:O	1:D:3082:GLU:HG3	2.21	0.40
1:A:233:PRO:N	1:A:234:PRO:HD2	2.36	0.40
1:B:1222:ILE:HG23	1:B:1223:VAL:N	2.37	0.40
1:A:169:LEU:HD23	1:A:202:ALA:HB3	2.03	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	319/321 (99%)	313 (98%)	6 (2%)	0	100	100
1	B	319/321 (99%)	313 (98%)	5 (2%)	1 (0%)	50	44
1	C	319/321 (99%)	312 (98%)	6 (2%)	1 (0%)	50	44
1	D	319/321 (99%)	310 (97%)	8 (2%)	1 (0%)	50	44
All	All	1276/1284 (99%)	1248 (98%)	25 (2%)	3 (0%)	56	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1303	ILE
1	D	3109	LYS
1	C	2303	ILE

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	241/241 (100%)	236 (98%)	5 (2%)	66	67
1	B	241/241 (100%)	235 (98%)	6 (2%)	60	59
1	C	241/241 (100%)	235 (98%)	6 (2%)	60	59
1	D	241/241 (100%)	235 (98%)	6 (2%)	60	59
All	All	964/964 (100%)	941 (98%)	23 (2%)	61	61

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	58	LEU
1	A	109	LYS
1	A	204	TYR
1	A	302	PRO
1	B	1058	LEU
1	B	1065	PRO
1	B	1085	ASN
1	B	1204	TYR
1	B	1244	ASP
1	B	1302	PRO
1	C	2010	ASN
1	C	2014	GLU
1	C	2085	ASN
1	C	2204	TYR
1	C	2267	ASP
1	C	2302	PRO
1	D	3014	GLU
1	D	3058	LEU
1	D	3065	PRO
1	D	3204	TYR
1	D	3280	ASP
1	D	3302	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	135	GLN
1	A	143	GLN
1	A	171	ASN
1	B	1036	HIS
1	B	1064	ASN
1	B	1085	ASN
1	B	1143	GLN
1	B	1218	ASN
1	C	2010	ASN
1	C	2036	HIS
1	C	2064	ASN
1	C	2085	ASN
1	C	2135	GLN
1	C	2143	GLN
1	C	2153	GLN

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Mol	Chain	Res	Type
1	D	3064	ASN
1	D	3135	GLN
1	D	3143	GLN
1	D	3171	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
3	MPO	A	331	-	13,13,13	0.82	1 (7%)	17,17,17	1.18	2 (11%)
4	MPD	A	335	-	7,7,7	1.07	1 (14%)	10,10,10	2.75	4 (40%)
3	MPO	B	332	-	13,13,13	0.88	1 (7%)	17,17,17	1.02	1 (5%)
4	MPD	B	336	-	7,7,7	1.09	1 (14%)	10,10,10	2.84	4 (40%)
3	MPO	C	333	-	13,13,13	0.94	0	17,17,17	0.85	0
4	MPD	C	337	-	7,7,7	1.11	1 (14%)	10,10,10	2.72	3 (30%)
3	MPO	D	334	-	13,13,13	0.93	1 (7%)	17,17,17	0.80	1 (5%)
4	MPD	D	338	-	7,7,7	0.97	0	10,10,10	2.82	4 (40%)

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
3	MPO	A	331	-	-	0/7/15/15	0/1/1/1
4	MPD	A	335	-	1/1/2/2	0/5/5/5	0/0/0/0
3	MPO	B	332	-	-	0/7/15/15	0/1/1/1
4	MPD	B	336	-	1/1/2/2	0/5/5/5	0/0/0/0
3	MPO	C	333	-	-	0/7/15/15	0/1/1/1
4	MPD	C	337	-	1/1/2/2	0/5/5/5	0/0/0/0
3	MPO	D	334	-	-	0/7/15/15	0/1/1/1
4	MPD	D	338	-	1/1/2/2	0/5/5/5	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	337	MPD	O2-C2	2.36	1.51	1.44
4	B	336	MPD	O2-C2	2.35	1.51	1.44
4	A	335	MPD	O2-C2	2.17	1.50	1.44
3	D	334	MPO	C7-N1	2.12	1.52	1.47
3	A	331	MPO	C4-N1	2.04	1.52	1.47
3	B	332	MPO	C4-N1	2.03	1.52	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	336	MPD	CM-C2-C1	7.95	127.72	110.11
4	D	338	MPD	CM-C2-C1	7.93	127.69	110.11
4	A	335	MPD	CM-C2-C1	7.77	127.32	110.11
4	C	337	MPD	CM-C2-C1	7.74	127.26	110.11
3	A	331	MPO	C2-C1-S1	2.84	116.90	113.24
4	D	338	MPD	O2-C2-CM	-2.57	98.28	107.98
4	B	336	MPD	O2-C2-CM	-2.36	99.08	107.98
4	C	337	MPD	O2-C2-CM	-2.34	99.13	107.98
4	A	335	MPD	O2-C2-CM	-2.33	99.17	107.98
4	B	336	MPD	O2-C2-C1	-2.31	99.25	107.98
3	A	331	MPO	O1-S1-C1	-2.23	104.89	106.81
4	D	338	MPD	O2-C2-C1	-2.22	99.60	107.98
4	B	336	MPD	O4-C4-C3	2.16	120.93	111.04
4	A	335	MPD	O2-C2-C1	-2.15	99.85	107.98
4	C	337	MPD	O2-C2-C1	-2.05	100.22	107.98
3	B	332	MPO	C2-C3-N1	-2.04	108.60	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	334	MPO	C7-N1-C4	2.03	113.92	108.86
4	A	335	MPD	O4-C4-C3	2.00	120.20	111.04
4	D	338	MPD	O4-C4-C3	2.00	120.20	111.04

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	335	MPD	C4
4	D	338	MPD	C4
4	B	336	MPD	C4
4	C	337	MPD	C4

There are no torsion outliers.

There are no ring outliers.

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	321/321 (100%)	-0.20	5 (1%) 68 69	17, 31, 51, 61	0
1	B	321/321 (100%)	0.14	11 (3%) 43 43	18, 38, 64, 73	0
1	C	321/321 (100%)	-0.28	3 (0%) 81 82	18, 30, 46, 53	0
1	D	321/321 (100%)	-0.08	8 (2%) 54 54	20, 34, 54, 66	0
All	All	1284/1284 (100%)	-0.11	27 (2%) 60 61	17, 33, 55, 73	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1247	LYS	4.9
1	B	1244	ASP	4.9
1	D	3251	GLU	4.0
1	B	1255	LYS	3.7
1	B	1251	GLU	3.0
1	B	1131	GLU	2.9
1	D	3254	GLY	2.9
1	A	131	GLU	2.8
1	A	233	PRO	2.8
1	B	1233	PRO	2.8
1	D	3131	GLU	2.8
1	B	1321	PHE	2.7
1	A	321	PHE	2.6
1	D	3280	ASP	2.6
1	B	1189	ALA	2.5
1	A	237	GLU	2.4
1	C	2247	LYS	2.4
1	D	3237	GLU	2.4
1	C	2267	ASP	2.4
1	C	2237	GLU	2.2
1	D	3255	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1014	GLU	2.1
1	D	3189	ALA	2.1
1	B	1128	GLU	2.1
1	D	3309	LYS	2.1
1	A	251	GLU	2.0
1	B	1237	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MPO	A	331	13/13	0.18	3.65	38,40,43,44	13
3	MPO	B	332	13/13	0.11	1.91	33,34,35,36	13
3	MPO	D	334	13/13	0.11	0.61	35,38,39,39	13
3	MPO	C	333	13/13	0.10	0.52	32,34,38,39	13
4	MPD	D	338	8/8	0.13	0.28	68,70,71,72	0
4	MPD	B	336	8/8	0.12	-0.19	48,50,50,51	0
4	MPD	A	335	8/8	0.08	-0.77	40,41,41,41	0
4	MPD	C	337	8/8	0.07	-0.92	37,39,39,39	0
2	CL	C	323	1/1	0.06	-1.71	30,30,30,30	0
2	CL	B	324	1/1	0.05	-1.84	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.