



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:07 PM UTC

PDB ID : 4IOJ / pdb_00004ioj
Title : N10-formyltetrahydrofolate synthetase from Moorella thermoacetica with sulfate
Authors : Stec, B.
Deposited on : 2013-01-08
Resolution : 2.20 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

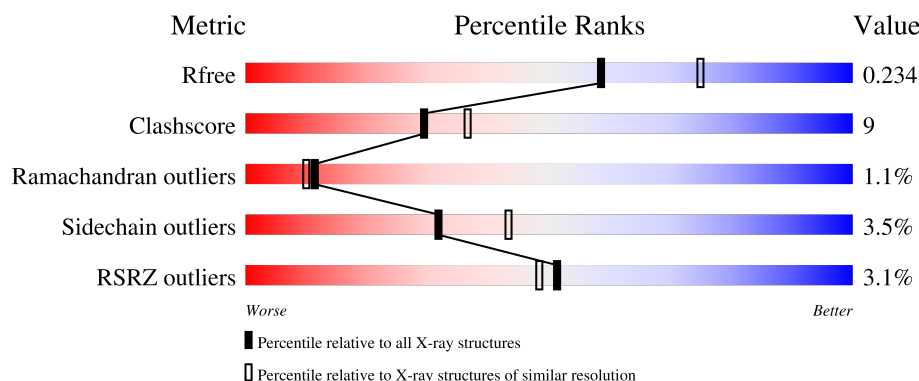
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	559	 87% 12% .
1	B	559	 6% 70% 26% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8915 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 Formate--tetrahydrofolate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4195	2661	721	792	21			
1	B	557	Total	C	N	O	S	0	0	0
			4195	2661	721	792	21			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



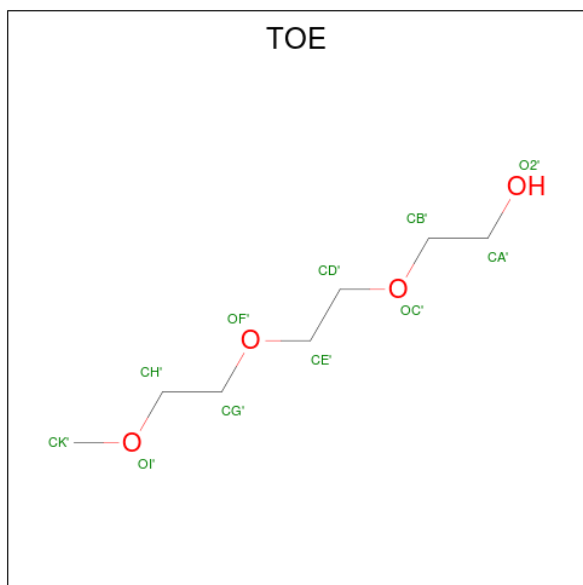
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (CCD ID: TOE) (formula: C₇H₁₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	7	4		
3	A	1	Total	C	O	0	0
			11	7	4		
3	B	1	Total	C	O	0	0
			11	7	4		
3	B	1	Total	C	O	0	0
			11	7	4		

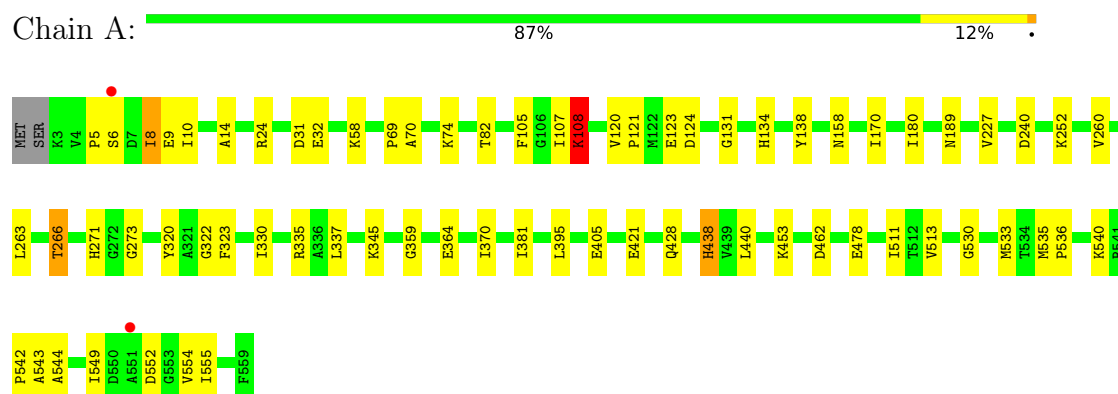
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	331	Total	O	0	0
			331	331		
4	B	125	Total	O	0	0
			125	125		

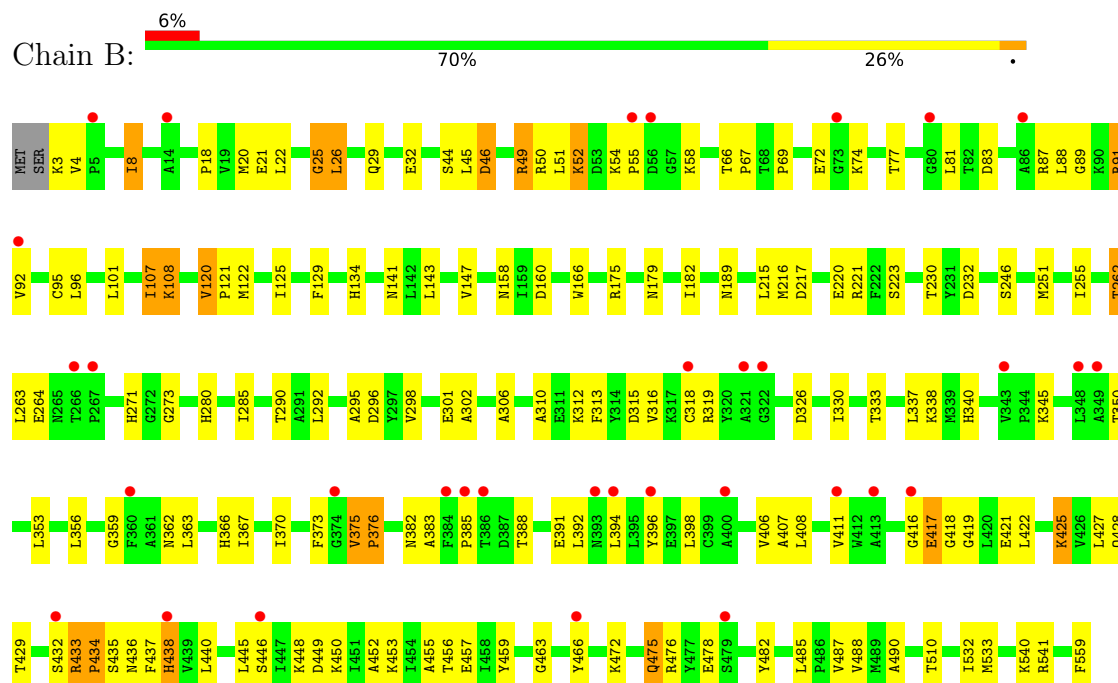
3 Residue-property plots

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: Formate--tetrahydrofolate ligase



• Molecule 1: Formate--tetrahydrofolate ligase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	161.20Å 161.20Å 256.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	122.67 – 2.20 122.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (122.67-2.20) 95.2 (122.67-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.178 , 0.233 0.178 , 0.234	Depositor DCC
R_{free} test set	3292 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8915	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: TOE, SO4

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	1.34	14/4266 (0.3%)	1.25	13/5778 (0.2%)
1	B	1.12	4/4266 (0.1%)	1.21	14/5778 (0.2%)
All	All	1.23	18/8532 (0.2%)	1.23	27/11556 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	HIS	CG-ND1	-6.82	1.30	1.38
1	A	364	GLU	C-O	-6.55	1.16	1.24
1	A	134	HIS	CG-CD2	6.29	1.42	1.35
1	A	227	VAL	C-O	-6.18	1.18	1.24
1	B	375	VAL	CA-CB	6.06	1.59	1.54
1	A	320	TYR	C-O	-6.04	1.17	1.24
1	A	271	HIS	ND1-CE1	5.74	1.38	1.32
1	A	438	HIS	ND1-CE1	5.70	1.38	1.32
1	A	134	HIS	CG-ND1	-5.63	1.32	1.38
1	A	438	HIS	CG-CD2	5.57	1.42	1.35
1	A	252	LYS	C-O	-5.47	1.17	1.24
1	A	271	HIS	CG-CD2	5.29	1.41	1.35
1	A	513	VAL	C-O	5.26	1.29	1.24
1	B	134	HIS	CG-CD2	5.24	1.41	1.35
1	B	175	ARG	CZ-NH1	5.23	1.40	1.32
1	A	323	PHE	N-CA	5.23	1.52	1.45
1	A	421	GLU	CA-C	5.17	1.59	1.52
1	A	134	HIS	ND1-CE1	5.09	1.37	1.32

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	LEU	N-CA-C	-6.76	104.66	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	GLY	N-CA-C	-6.69	106.00	115.43
1	B	160	ASP	CA-C-N	6.47	126.40	119.28
1	B	160	ASP	C-N-CA	6.47	126.40	119.28
1	B	25	GLY	N-CA-C	6.42	121.52	114.40
1	B	92	VAL	N-CA-C	6.39	117.50	108.17
1	B	46	ASP	N-CA-C	-6.32	104.63	112.90
1	B	541	ARG	CA-C-N	6.30	126.25	119.76
1	B	541	ARG	C-N-CA	6.30	126.25	119.76
1	A	266	THR	CA-C-N	-6.14	113.65	119.85
1	A	266	THR	C-N-CA	-6.14	113.65	119.85
1	B	189	ASN	N-CA-C	6.10	120.04	112.59
1	A	530	GLY	N-CA-C	-5.98	105.61	112.79
1	A	32	GLU	N-CA-C	-5.96	105.66	113.17
1	A	74	LYS	N-CA-C	5.93	117.54	111.14
1	B	478	GLU	N-CA-C	-5.64	104.34	111.11
1	A	24	ARG	N-CA-C	-5.55	105.31	111.36
1	B	301	GLU	N-CA-C	5.51	117.35	109.14
1	A	138	TYR	N-CA-C	5.40	117.25	111.36
1	B	120	VAL	N-CA-C	-5.39	102.92	109.01
1	B	290	THR	N-CA-C	-5.36	104.87	111.40
1	A	335	ARG	CG-CD-NE	-5.35	100.24	112.00
1	A	70	ALA	N-CA-C	5.34	117.85	111.71
1	A	240	ASP	N-CA-C	-5.34	106.03	112.54
1	A	478	GLU	CA-CB-CG	-5.24	103.62	114.10
1	A	131	GLY	N-CA-C	5.17	122.48	115.30
1	B	432	SER	N-CA-C	5.01	119.42	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4195	0	4278	33	1
1	B	4195	0	4278	119	0
2	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
3	A	22	0	32	1	0
3	B	22	0	32	1	0
4	A	331	0	0	7	0
4	B	125	0	0	5	0
All	All	8915	0	8620	147	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 9.

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:B:330:ILE:HD11	1:B:370:ILE:HD13	1.26	1.13
1:B:330:ILE:HD11	1:B:370:ILE:CD1	1.85	1.06
1:B:49:ARG:HH11	1:B:49:ARG:HG2	1.23	0.98
1:B:394:LEU:O	1:B:398:LEU:HG	1.63	0.98
1:B:262:THR:HG22	1:B:264:GLU:H	1.30	0.94
1:B:26:LEU:HG	4:B:806:HOH:O	1.70	0.90
1:B:383:ALA:HB2	1:B:408:LEU:HD11	1.54	0.88
1:B:429:THR:HG23	1:B:433:ARG:HD3	1.55	0.85
1:B:490:ALA:HB1	1:B:532:ILE:HD12	1.56	0.85
1:A:107:ILE:O	1:A:108:LYS:HB2	1.75	0.83
1:B:452:ALA:O	1:B:456:THR:HG22	1.81	0.80
1:B:330:ILE:CD1	1:B:370:ILE:HD13	2.08	0.80
1:B:326:ASP:O	1:B:376:PRO:HG2	1.83	0.76
1:B:262:THR:HG22	1:B:264:GLU:N	2.00	0.76
1:B:312:LYS:O	1:B:316:VAL:HG12	1.85	0.76
1:B:472:LYS:HD2	1:B:475:GLN:HE22	1.52	0.74
1:B:330:ILE:CD1	1:B:370:ILE:CD1	2.63	0.74
1:B:49:ARG:HH11	1:B:49:ARG:CG	2.00	0.73
1:B:262:THR:CG2	1:B:264:GLU:H	2.01	0.73
1:B:49:ARG:HG2	1:B:49:ARG:NH1	2.00	0.73
1:B:292:LEU:HD23	1:B:298:VAL:CG2	2.19	0.73
1:B:83:ASP:OD2	1:B:262:THR:HG21	1.89	0.72
1:A:330:ILE:HD11	1:A:370:ILE:CD1	2.22	0.70
1:B:476:ARG:HD3	4:B:824:HOH:O	1.92	0.70
1:B:58:LYS:N	1:B:296:ASP:O	2.20	0.67
1:B:125:ILE:HD13	1:B:129:PHE:CE1	2.29	0.67
1:B:394:LEU:HG	1:B:398:LEU:HD11	1.77	0.67
1:B:29:GLN:HG3	1:B:32:GLU:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ALA:HB1	1:B:532:ILE:CD1	2.25	0.65
1:B:312:LYS:HE2	1:B:488:VAL:HG13	1.78	0.64
1:B:83:ASP:HB3	1:B:416:GLY:HA3	1.80	0.64
1:B:292:LEU:HD23	1:B:298:VAL:HG21	1.81	0.63
1:A:189:ASN:HD22	1:B:179:ASN:HD22	1.45	0.63
1:A:330:ILE:HD11	1:A:370:ILE:HD12	1.79	0.62
1:B:315:ASP:O	1:B:319:ARG:HD2	1.99	0.62
1:B:66:THR:H	1:B:362:ASN:HD21	1.47	0.62
1:A:5:PRO:HB2	1:A:10:ILE:HG13	1.83	0.61
1:A:381:ILE:HD12	1:A:395:LEU:HD21	1.84	0.60
1:B:425:LYS:O	1:B:428:GLN:HB2	2.03	0.59
1:B:87:ARG:C	1:B:89:GLY:H	2.11	0.59
1:B:215:LEU:HA	1:B:255:ILE:HD13	1.85	0.59
1:B:449:ASP:O	1:B:452:ALA:HB3	2.03	0.59
1:A:552:ASP:HB2	1:A:554:VAL:HG23	1.85	0.59
1:A:189:ASN:HD22	1:B:179:ASN:ND2	2.01	0.58
1:B:463:GLY:O	1:B:510:THR:HB	2.03	0.58
1:B:8:ILE:HG22	4:B:722:HOH:O	2.04	0.58
1:B:333:THR:HG22	1:B:382:ASN:HB3	1.86	0.57
1:B:383:ALA:HB2	1:B:408:LEU:CD1	2.32	0.57
1:B:49:ARG:O	1:B:52:LYS:HD3	2.05	0.56
1:B:453:LYS:HG2	1:B:457:GLU:OE1	2.04	0.56
1:B:306:ALA:O	1:B:310:ALA:HB3	2.06	0.56
1:A:170:ILE:HD11	1:B:141:ASN:HD22	1.71	0.56
1:A:189:ASN:ND2	1:B:179:ASN:ND2	2.52	0.56
1:B:8:ILE:HA	1:B:122:MET:HE1	1.88	0.56
1:B:74:LYS:NZ	1:B:302:ALA:O	2.36	0.56
1:B:54:LYS:HG3	1:B:55:PRO:HD2	1.88	0.55
1:B:107:ILE:O	1:B:108:LYS:HB2	2.07	0.55
1:B:330:ILE:HD11	1:B:370:ILE:HD12	1.84	0.55
1:B:392:LEU:O	1:B:396:TYR:HB2	2.07	0.55
1:B:337:LEU:O	1:B:359:GLY:HA3	2.06	0.55
1:B:422:LEU:O	1:B:425:LYS:HB2	2.07	0.55
1:A:69:PRO:HB2	1:A:345:LYS:HD2	1.89	0.54
1:B:220:GLU:O	1:B:223:SER:OG	2.23	0.54
1:A:31:ASP:OD2	1:A:31:ASP:N	2.41	0.52
1:B:50:ARG:C	1:B:52:LYS:H	2.17	0.52
1:A:438:HIS:CD2	4:A:875:HOH:O	2.63	0.51
1:B:121:PRO:O	1:B:125:ILE:HG12	2.10	0.51
1:B:407:ALA:HB2	1:B:425:LYS:HG3	1.91	0.51
1:A:540:LYS:HG3	4:A:1025:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASP:O	1:B:221:ARG:HG3	2.12	0.50
1:B:91:ARG:O	1:B:295:ALA:HB1	2.11	0.50
1:B:466:TYR:N	1:B:466:TYR:CD1	2.80	0.50
1:B:356:LEU:HD23	1:B:394:LEU:HD23	1.94	0.49
1:A:337:LEU:O	1:A:359:GLY:HA3	2.12	0.49
1:B:417:GLU:C	1:B:419:GLY:H	2.21	0.49
1:B:376:PRO:HG3	1:B:434:PRO:O	2.14	0.48
1:A:105:PHE:CE2	1:B:246:SER:HB3	2.49	0.48
1:A:120:VAL:HB	1:A:121:PRO:HA	1.96	0.48
1:A:440:LEU:O	1:A:453:LYS:HE2	2.14	0.48
1:B:77:THR:HG23	1:B:382:ASN:HD22	1.78	0.48
1:B:373:PHE:O	1:B:437:PHE:HA	2.14	0.47
1:A:5:PRO:HB3	1:A:9:GLU:HG3	1.96	0.47
1:B:67:PRO:HA	1:B:72:GLU:OE1	2.15	0.47
1:B:101:LEU:C	1:B:101:LEU:HD23	2.40	0.47
1:B:158:ASN:O	1:B:230:THR:HA	2.15	0.46
3:A:604:TOE:H7	4:A:917:HOH:O	2.15	0.46
1:B:122:MET:HE3	1:B:559:PHE:CE2	2.50	0.46
1:B:353:LEU:CD2	1:B:391:GLU:HA	2.46	0.46
1:B:373:PHE:CE2	1:B:440:LEU:HB2	2.50	0.46
1:B:66:THR:HB	1:B:340:HIS:CE1	2.51	0.46
1:B:143:LEU:HD23	1:B:166:TRP:CE2	2.51	0.45
1:B:107:ILE:HD12	1:B:107:ILE:H	1.80	0.45
1:B:333:THR:CG2	1:B:382:ASN:HB3	2.46	0.45
1:A:330:ILE:CD1	1:A:370:ILE:CD1	2.94	0.45
1:B:26:LEU:HA	1:B:91:ARG:HH12	1.80	0.45
1:B:49:ARG:CG	1:B:49:ARG:NH1	2.69	0.45
1:A:123:GLU:OE2	1:A:555:ILE:HD12	2.17	0.45
1:B:425:LYS:HB3	1:B:425:LYS:HE3	1.75	0.45
1:A:542:PRO:C	1:A:544:ALA:N	2.74	0.45
1:B:77:THR:HA	1:B:411:VAL:HG21	1.99	0.45
1:B:292:LEU:HD23	1:B:298:VAL:HG23	1.96	0.44
1:B:44:SER:C	1:B:46:ASP:H	2.26	0.44
1:B:388:THR:OG1	1:B:391:GLU:HG3	2.18	0.44
1:B:25:GLY:C	4:B:806:HOH:O	2.60	0.44
1:B:330:ILE:CG1	1:B:370:ILE:HD13	2.47	0.44
1:A:180:ILE:HG22	1:B:182:ILE:HA	1.99	0.43
1:B:445:LEU:O	1:B:450:LYS:HE3	2.18	0.43
1:B:95:CYS:O	1:B:96:LEU:HD23	2.18	0.43
1:B:440:LEU:O	1:B:440:LEU:HG	2.19	0.43
1:B:485:LEU:HA	1:B:485:LEU:HD23	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:PRO:HB2	1:B:345:LYS:HD3	2.01	0.43
1:B:330:ILE:CG1	1:B:370:ILE:CD1	2.97	0.43
1:B:143:LEU:O	1:B:147:VAL:HG23	2.19	0.43
1:B:87:ARG:C	1:B:89:GLY:N	2.76	0.43
1:B:280:HIS:HA	1:B:312:LYS:HD3	2.01	0.42
1:B:22:LEU:O	1:B:26:LEU:HD12	2.19	0.42
1:B:394:LEU:HG	1:B:398:LEU:CD1	2.48	0.42
1:B:446:SER:O	1:B:450:LYS:HG3	2.19	0.42
1:A:405:GLU:HG3	4:A:1024:HOH:O	2.18	0.42
1:B:26:LEU:N	4:B:806:HOH:O	2.52	0.42
1:B:448:LYS:HG2	1:B:466:TYR:CZ	2.54	0.42
1:B:455:ALA:HA	1:B:459:TYR:CD2	2.54	0.42
1:B:122:MET:HE2	1:B:122:MET:HB3	1.80	0.42
1:B:216:MET:HA	1:B:216:MET:HE2	2.01	0.42
1:A:549:ILE:HA	1:A:554:VAL:O	2.20	0.42
1:B:437:PHE:CD1	1:B:437:PHE:C	2.97	0.42
1:A:428:GLN:HG2	4:A:956:HOH:O	2.19	0.41
1:B:81:LEU:HD13	1:B:422:LEU:HG	2.02	0.41
1:B:251:MET:HE3	1:B:251:MET:HB3	1.88	0.41
1:A:123:GLU:HB2	4:A:944:HOH:O	2.19	0.41
1:B:262:THR:CG2	1:B:263:LEU:N	2.81	0.41
1:B:306:ALA:HB3	1:B:366:HIS:ND1	2.34	0.41
1:A:58:LYS:NZ	4:A:899:HOH:O	2.53	0.41
1:A:535:MET:O	1:A:535:MET:HG3	2.19	0.41
1:B:313:PHE:CE2	1:B:318:CYS:SG	3.14	0.41
1:B:482:TYR:CE2	3:B:604:TOE:H5	2.56	0.41
1:B:421:GLU:O	1:B:425:LYS:HG2	2.21	0.41
1:B:438:HIS:ND1	1:B:438:HIS:N	2.69	0.41
1:A:14:ALA:HB2	1:A:263:LEU:HD22	2.02	0.41
1:A:533:MET:SD	1:A:536:PRO:HA	2.61	0.40
1:B:375:VAL:HA	1:B:376:PRO:HD2	1.81	0.40
1:A:82:THR:HG22	1:A:266:THR:HG21	2.02	0.40
1:A:6:SER:OG	1:A:8:ILE:HG22	2.20	0.40
1:B:427:LEU:O	1:B:428:GLN:C	2.64	0.40
1:B:18:PRO:C	1:B:20:MET:N	2.77	0.40
1:B:125:ILE:CD1	1:B:129:PHE:CE1	3.01	0.40
1:B:363:LEU:O	1:B:367:ILE:HG13	2.21	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)
1:A:462:ASP:O	1:A:462:ASP:O[16_545]	2.01	0.19

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	555/559 (99%)	532 (96%)	19 (3%)	4 (1%)	18	19
1	B	555/559 (99%)	511 (92%)	36 (6%)	8 (1%)	9	7
All	All	1110/1118 (99%)	1043 (94%)	55 (5%)	12 (1%)	11	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	434	PRO
1	A	108	LYS
1	B	88	LEU
1	A	543	ALA
1	B	108	LYS
1	B	51	LEU
1	B	385	PRO
1	B	376	PRO
1	B	418	GLY
1	A	273	GLY
1	B	273	GLY
1	A	260	VAL

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	439/441 (100%)	434 (99%)	5 (1%)	65	79
1	B	439/441 (100%)	413 (94%)	26 (6%)	18	22
All	All	878/882 (100%)	847 (96%)	31 (4%)	32	43

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	108	LYS
1	A	124	ASP
1	A	158	ASN
1	A	511	ILE
1	B	3	LYS
1	B	4	VAL
1	B	8	ILE
1	B	21	GLU
1	B	45	LEU
1	B	49	ARG
1	B	52	LYS
1	B	91	ARG
1	B	107	ILE
1	B	120	VAL
1	B	232	ASP
1	B	262	THR
1	B	285	ILE
1	B	338	LYS
1	B	350	THR
1	B	406	VAL
1	B	417	GLU
1	B	425	LYS
1	B	433	ARG
1	B	435	SER
1	B	436	ASN
1	B	438	HIS
1	B	475	GLN
1	B	487	VAL
1	B	533	MET
1	B	540	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	173	ASN
1	A	283	ASN
1	A	465	ASN
1	B	126	ASN
1	B	179	ASN
1	B	362	ASN
1	B	382	ASN
1	B	428	GLN
1	B	465	ASN
1	B	475	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 ⓘ

9 ligands 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	$\# Z > 2$
3	TOE	A	604	-	10,10,10	0.93	0	9,9,9	1.15	0
2	SO4	A	602	-	4,4,4	0.56	0	6,6,6	0.77	0
2	SO4	B	602	-	4,4,4	0.37	0	6,6,6	0.88	0
3	TOE	B	604	-	10,10,10	0.70	0	9,9,9	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TOE	A	605	-	10,10,10	0.63	0	9,9,9	0.88	0
2	SO4	A	603	-	4,4,4	0.74	0	6,6,6	0.46	0
2	SO4	A	601	-	4,4,4	0.30	0	6,6,6	0.63	0
3	TOE	B	603	-	10,10,10	0.66	0	9,9,9	0.59	0
2	SO4	B	601	-	4,4,4	0.43	0	6,6,6	1.23	1 (16%)

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	TOE	B	604	-	-	5/8/8/8	-
3	TOE	A	605	-	-	4/8/8/8	-
3	TOE	B	603	-	-	2/8/8/8	-
3	TOE	A	604	-	-	7/8/8/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	SO4	O4-S-O2	-2.07	98.76	109.56

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	TOE	CH'-CG'-OF'-CE'
3	B	604	TOE	OF'-CG'-CH'-OI'
3	A	605	TOE	O2'-CA'-CB'-OC'
3	B	603	TOE	O2'-CA'-CB'-OC'
3	A	605	TOE	OF'-CG'-CH'-OI'
3	A	604	TOE	OC'-CD'-CE'-OF'
3	B	604	TOE	CD'-CE'-OF'-CG'
3	A	605	TOE	CE'-CD'-OC'-CB'
3	A	605	TOE	CH'-CG'-OF'-CE'
3	B	604	TOE	O2'-CA'-CB'-OC'
3	B	604	TOE	CH'-CG'-OF'-CE'
3	A	604	TOE	CE'-CD'-OC'-CB'
3	A	604	TOE	OF'-CG'-CH'-OI'

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Mol	Chain	Res	Type	Atoms
3	B	603	TOE	CE'-CD'-OC'-CB'
3	B	604	TOE	CA'-CB'-OC'-CD'
3	A	604	TOE	CG'-CH'-OI'-CK'
3	A	604	TOE	CD'-CE'-OF'-CG'
3	A	604	TOE	O2'-CA'-CB'-OC'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	TOE	1	0
3	B	604	TOE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/559 (99%)	-0.54	2 (0%) 88 87	17, 27, 54, 85	0
1	B	557/559 (99%)	0.48	33 (5%) 28 25	18, 52, 87, 114	0
All	All	1114/1118 (99%)	-0.03	35 (3%) 51 48	17, 37, 77, 114	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	SER	3.7
1	B	432	SER	3.1
1	B	86	ALA	3.0
1	B	92	VAL	3.0
1	B	267	PRO	3.0
1	B	396	TYR	2.9
1	B	80	GLY	2.9
1	B	343	VAL	2.9
1	B	73	GLY	2.9
1	B	413	ALA	2.7
1	B	400	ALA	2.7
1	B	438	HIS	2.6
1	B	394	LEU	2.6
1	B	322	GLY	2.5
1	B	479	SER	2.5
1	B	393	ASN	2.5
1	B	416	GLY	2.5
1	A	551	ALA	2.4
1	B	55	PRO	2.4
1	B	349	ALA	2.4
1	B	14	ALA	2.4
1	B	374	GLY	2.4
1	A	6	SER	2.3
1	B	411	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	348	LEU	2.2
1	B	56	ASP	2.2
1	B	318	CYS	2.1
1	B	385	PRO	2.1
1	B	386	THR	2.1
1	B	466	TYR	2.1
1	B	360	PHE	2.1
1	B	384	PHE	2.1
1	B	266	THR	2.0
1	B	321	ALA	2.0
1	B	5	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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
3	TOE	B	604	11/11	0.80	0.14	57,67,82,86	0
3	TOE	A	605	11/11	0.87	0.12	37,47,71,72	0
3	TOE	B	603	11/11	0.89	0.11	43,47,51,61	0
3	TOE	A	604	11/11	0.90	0.12	34,41,54,56	0
2	SO4	A	602	5/5	0.92	0.09	56,58,61,66	0
2	SO4	B	602	5/5	0.93	0.09	54,63,64,71	0
2	SO4	B	601	5/5	0.94	0.10	49,55,61,66	0
2	SO4	A	603	5/5	0.94	0.12	55,56,67,70	0
2	SO4	A	601	5/5	0.97	0.06	32,36,38,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.