



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:23 AM UTC

PDB ID : 4JIM / pdb_00004jim
Title : Native Crystal Structure of N10-Formyltetrahydrofolate Synthetase
Authors : Celeste, L.R.; Lovelace, L.L.; Lebioda, L.
Deposited on : 2013-03-06
Resolution : 2.10 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

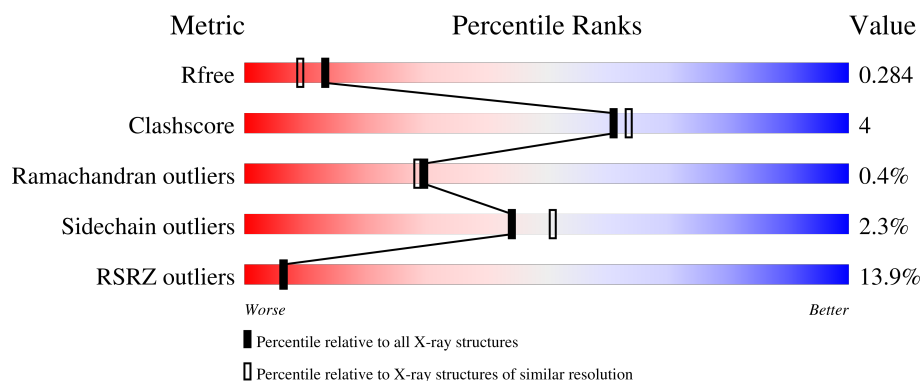
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	8% 91% 8% .
1	B	559	20% 87% 11% ..

2 Entry composition [i](#)

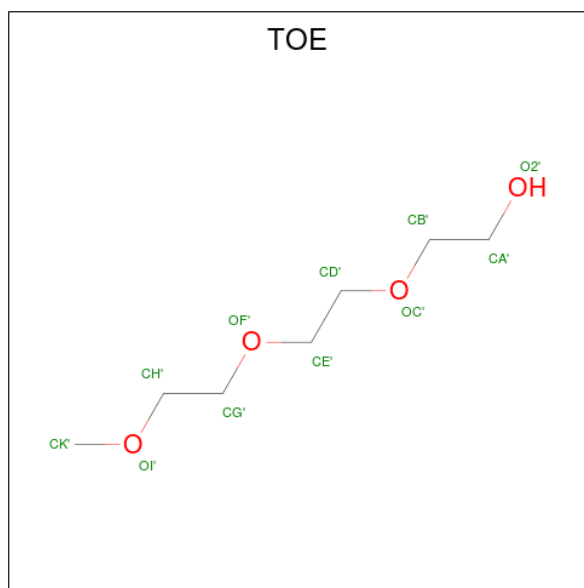
There are 4 unique types of molecules in this entry. The entry contains 8890 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

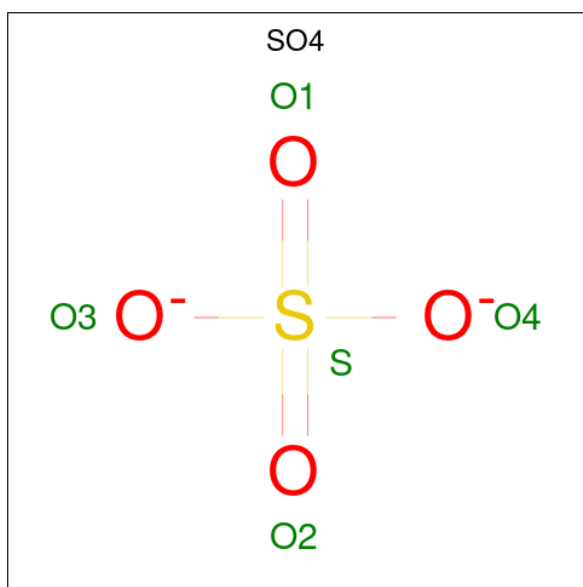
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	20	3	0
			4174	2652	716	784	22			
1	B	555	Total	C	N	O	S	8	2	0
			4091	2595	700	775	21			

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



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

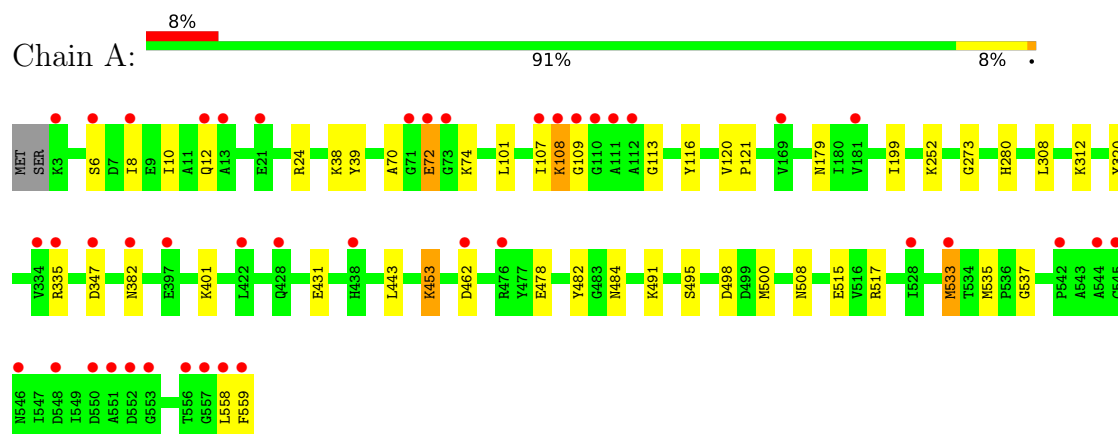
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	399	Total	O	0	0
			399	399		
4	B	153	Total	O	0	0
			153	153		

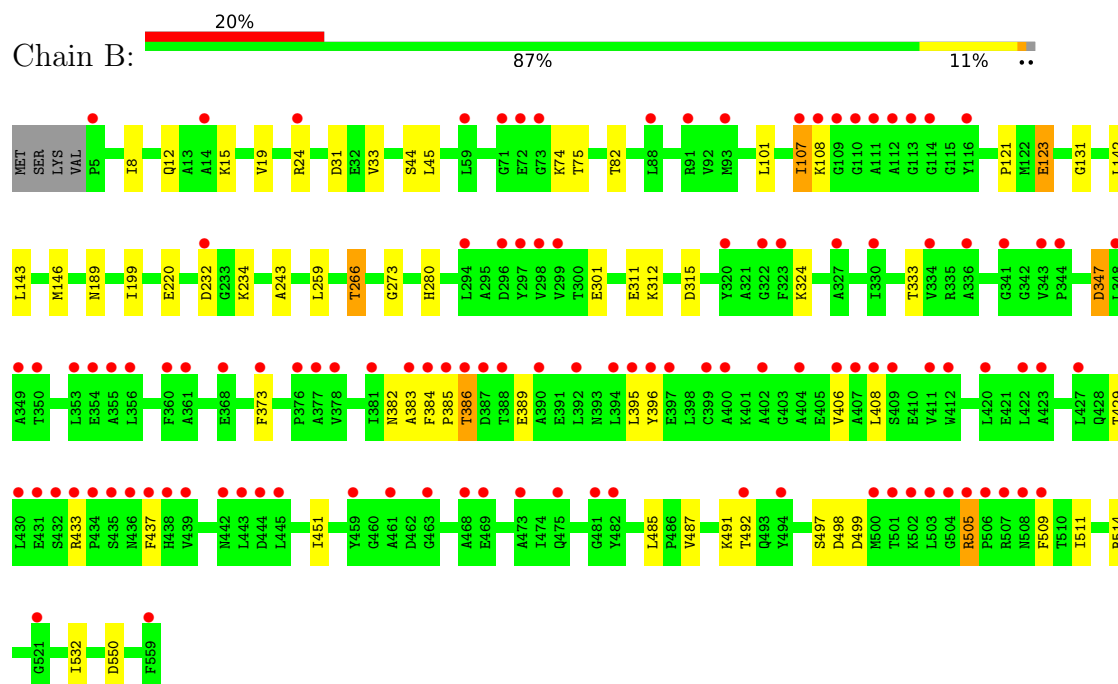
3 Residue-property plots

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	161.19Å 161.19Å 256.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.92 – 2.10 40.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.92-2.10) 99.9 (40.92-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.234 , 0.274 0.243 , 0.284	Depositor DCC
R_{free} test set	3753 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8890	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: SO4, TOE

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	1.21	5/4255 (0.1%)	1.09	4/5771 (0.1%)
1	B	1.09	2/4168 (0.0%)	1.09	13/5669 (0.2%)
All	All	1.15	7/8423 (0.1%)	1.09	17/11440 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	509	PHE	C-O	11.04	1.38	1.23
1	A	320	TYR	C-O	-6.00	1.17	1.24
1	A	537	GLY	C-O	-5.74	1.15	1.23
1	A	308	LEU	CA-C	5.57	1.56	1.52
1	A	453	LYS	C-O	-5.55	1.17	1.24
1	A	443	LEU	C-O	-5.13	1.17	1.24
1	B	532	ILE	N-CA	-5.09	1.40	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	LYS	N-CA-C	7.62	119.27	110.97
1	B	131	GLY	N-CA-C	6.63	124.51	115.30
1	B	189	ASN	N-CA-C	6.52	120.88	112.41
1	B	123	GLU	N-CA-C	6.38	117.89	111.07
1	B	234	LYS	CA-C-N	5.58	125.51	119.76
1	B	234	LYS	C-N-CA	5.58	125.51	119.76
1	A	70	ALA	N-CA-C	5.28	117.95	111.82
1	B	266	THR	CA-C-N	-5.20	114.62	120.14
1	B	266	THR	C-N-CA	-5.20	114.62	120.14
1	B	324	LYS	CA-C-N	5.16	125.16	119.90
1	B	324	LYS	C-N-CA	5.16	125.16	119.90
1	A	478	GLU	CB-CG-CD	5.08	121.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	VAL	CB-CA-C	-5.07	103.12	110.63
1	A	113	GLY	N-CA-C	-5.06	105.95	111.21
1	B	15	LYS	N-CA-C	-5.05	98.36	107.75
1	B	485	LEU	CA-C-N	5.01	124.92	119.76
1	B	485	LEU	C-N-CA	5.01	124.92	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4174	0	4231	30	1
1	B	4091	0	4067	39	0
2	A	22	0	32	1	0
2	B	11	0	16	1	0
3	A	25	0	0	0	0
3	B	15	0	0	2	0
4	A	399	0	0	10	0
4	B	153	0	0	7	0
All	All	8890	0	8346	69	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 4.

All (69) 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:505[A]:ARG:HG2	1:B:505[A]:ARG:HH21	1.17	1.09
1:B:505[A]:ARG:HH21	1:B:505[A]:ARG:CG	1.73	0.99
1:A:108:LYS:CB	1:A:109:GLY:HA2	2.03	0.89
1:A:533[B]:MET:SD	4:A:1174:HOH:O	2.32	0.86
1:A:72:GLU:HG3	4:A:875:HOH:O	1.79	0.82
1:B:429:THR:HG23	1:B:433:ARG:HD3	1.66	0.77
1:B:491:LYS:NZ	1:B:497:SER:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:MET:CE	4:A:1180:HOH:O	2.35	0.73
1:A:8:ILE:O	1:A:12:GLN:HG2	1.89	0.73
1:B:505[A]:ARG:HG2	1:B:505[A]:ARG:NH2	1.96	0.71
1:B:142:LEU:HG	1:B:146:MET:HE2	1.78	0.66
1:A:491:LYS:NZ	1:A:495:SER:O	2.30	0.65
1:A:108:LYS:CB	1:A:109:GLY:CA	2.76	0.65
1:B:107:ILE:HD12	1:B:108:LYS:CB	2.28	0.63
1:B:146:MET:HE1	1:B:243:ALA:HB1	1.79	0.62
1:A:515:GLU:OE1	1:A:517:ARG:CZ	2.48	0.61
1:B:383:ALA:HB2	1:B:408:LEU:HD11	1.84	0.60
1:B:505[A]:ARG:NH1	4:B:786:HOH:O	2.35	0.60
1:A:515:GLU:OE1	1:A:517:ARG:NH1	2.35	0.59
1:A:500:MET:HE3	4:A:1180:HOH:O	1.99	0.58
1:A:484:ASN:OD1	4:A:1084:HOH:O	2.17	0.57
1:A:252:LYS:HE2	1:B:123:GLU:OE1	2.04	0.57
1:B:347:ASP:OD1	1:B:347:ASP:N	2.38	0.57
1:B:8:ILE:O	1:B:12:GLN:HG2	2.07	0.55
1:B:333:THR:HG22	1:B:382:ASN:HB3	1.89	0.55
1:B:499:ASP:C	1:B:499:ASP:OD1	2.50	0.54
1:B:101:LEU:C	1:B:101:LEU:HD23	2.33	0.54
1:B:384:PHE:O	1:B:386:THR:N	2.41	0.53
1:A:6:SER:O	1:A:10:ILE:HG12	2.08	0.53
1:A:179:ASN:ND2	4:A:1090:HOH:O	2.43	0.52
1:A:558:LEU:HD23	1:A:559:PHE:CE2	2.45	0.52
1:B:44:SER:HB2	3:B:604:SO4:O3	2.11	0.51
1:B:45:LEU:HA	4:B:768:HOH:O	2.09	0.51
1:B:505[A]:ARG:CG	1:B:505[A]:ARG:NH2	2.45	0.51
1:B:514:ARG:NH2	4:B:734:HOH:O	2.43	0.51
1:B:498:ASP:OD2	1:B:511:ILE:HA	2.11	0.50
1:A:462:ASP:C	4:A:901:HOH:O	2.55	0.50
1:B:280:HIS:HA	1:B:312:LYS:HD3	1.94	0.50
1:A:10:ILE:HD12	1:A:116:TYR:CE2	2.49	0.48
1:B:143:LEU:HA	1:B:146:MET:HE3	1.95	0.48
1:B:146:MET:HE1	1:B:243:ALA:CB	2.44	0.47
1:B:395:LEU:O	1:B:396:TYR:C	2.57	0.47
1:B:74:LYS:NZ	3:B:603:SO4:O4	2.47	0.47
1:A:10:ILE:HD12	1:A:116:TYR:CZ	2.49	0.47
1:A:120:VAL:HB	1:A:121:PRO:HA	1.98	0.46
1:A:38:LYS:HG3	1:A:39:TYR:CZ	2.52	0.45
1:B:82:THR:HG22	1:B:266:THR:HG21	1.98	0.45
1:B:121:PRO:HA	4:B:805:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LYS:HB3	4:B:803:HOH:O	2.16	0.45
2:B:601:TOE:H12	4:B:836:HOH:O	2.16	0.44
1:B:373:PHE:O	1:B:437:PHE:HA	2.17	0.44
1:A:500:MET:HE2	4:A:1180:HOH:O	2.13	0.44
1:A:482:TYR:CE1	2:A:702:TOE:H7	2.53	0.44
1:B:75:THR:HA	1:B:301:GLU:OE1	2.17	0.44
1:B:505[A]:ARG:HH21	1:B:505[A]:ARG:HG3	1.73	0.44
1:B:19:VAL:HG13	1:B:259:LEU:HD23	2.00	0.44
1:A:347:ASP:HB3	4:A:913:HOH:O	2.18	0.43
1:A:498:ASP:OD1	1:A:498:ASP:C	2.62	0.43
1:A:558:LEU:HG	1:A:559:PHE:CZ	2.54	0.43
1:B:492:THR:HG22	4:B:779:HOH:O	2.18	0.42
4:A:1186:HOH:O	1:B:31:ASP:HA	2.19	0.42
1:A:535:MET:O	1:A:535:MET:HG3	2.19	0.41
1:A:101:LEU:C	1:A:101:LEU:HD23	2.45	0.41
1:B:550:ASP:C	1:B:550:ASP:OD1	2.64	0.41
1:A:280:HIS:HA	1:A:312:LYS:HD3	2.01	0.41
1:B:451:ILE:HG12	1:B:487:VAL:HG11	2.03	0.40
1:A:335[B]:ARG:HH11	1:A:335[B]:ARG:HD2	1.77	0.40
1:A:462:ASP:OD2	1:A:508:ASN:HA	2.22	0.40
1:B:311:GLU:OE2	1:B:315:ASP:OD2	2.38	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[17_554]	2.02	0.18

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	558/559 (100%)	537 (96%)	19 (3%)	2 (0%)	30	28
1	B	555/559 (99%)	521 (94%)	32 (6%)	2 (0%)	30	28
All	All	1113/1118 (100%)	1058 (95%)	51 (5%)	4 (0%)	30	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	385	PRO
1	A	108	LYS
1	B	273	GLY
1	A	273	GLY

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	432/441 (98%)	422 (98%)	10 (2%)	44	51
1	B	414/441 (94%)	402 (97%)	12 (3%)	37	42
All	All	846/882 (96%)	824 (97%)	22 (3%)	44	46

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	72	GLU
1	A	107	ILE
1	A	199	ILE
1	A	382	ASN
1	A	401	LYS
1	A	431	GLU
1	A	453	LYS
1	A	533[A]	MET
1	A	533[B]	MET
1	B	24[A]	ARG
1	B	24[B]	ARG

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Mol	Chain	Res	Type
1	B	107	ILE
1	B	199	ILE
1	B	220	GLU
1	B	232	ASP
1	B	347	ASP
1	B	386	THR
1	B	389	GLU
1	B	406	VAL
1	B	505[A]	ARG
1	B	505[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	382	ASN
1	B	283	ASN
1	B	382	ASN
1	B	428	GLN
1	B	442	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
2	TOE	A	702	-	10,10,10	0.77	0	9,9,9	0.82	0
3	SO4	B	603	-	4,4,4	0.76	0	6,6,6	1.08	0
2	TOE	B	601	-	10,10,10	0.67	0	9,9,9	0.52	0
3	SO4	A	704	-	4,4,4	0.97	0	6,6,6	1.12	0
3	SO4	A	703	-	4,4,4	0.78	0	6,6,6	0.44	0
2	TOE	A	701	-	10,10,10	1.24	0	9,9,9	1.66	3 (33%)
3	SO4	A	705	-	4,4,4	1.00	0	6,6,6	0.62	0
3	SO4	B	602	-	4,4,4	0.77	0	6,6,6	0.83	0
3	SO4	B	604	-	4,4,4	0.53	0	6,6,6	0.22	0
3	SO4	A	707	-	4,4,4	0.59	0	6,6,6	0.36	0
3	SO4	A	706	-	4,4,4	0.61	0	6,6,6	0.34	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	TOE	A	701	-	-	5/8/8/8	-
2	TOE	A	702	-	-	7/8/8/8	-
2	TOE	B	601	-	-	3/8/8/8	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	TOE	CG'-OF'-CE'	3.19	127.21	113.26
2	A	701	TOE	OF'-CG'-CH'	2.78	123.04	110.35
2	A	701	TOE	OC'-CD'-CE'	2.01	119.54	110.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	TOE	OF'-CG'-CH'-OI'
2	A	702	TOE	OC'-CD'-CE'-OF'
2	A	701	TOE	CH'-CG'-OF'-CE'
2	B	601	TOE	O2'-CA'-CB'-OC'
2	A	701	TOE	O2'-CA'-CB'-OC'
2	A	702	TOE	CE'-CD'-OC'-CB'
2	B	601	TOE	CD'-CE'-OF'-CG'
2	A	702	TOE	CG'-CH'-OI'-CK'
2	A	701	TOE	OC'-CD'-CE'-OF'
2	A	702	TOE	OF'-CG'-CH'-OI'
2	A	702	TOE	O2'-CA'-CB'-OC'
2	A	702	TOE	CA'-CB'-OC'-CD'
2	A	701	TOE	CE'-CD'-OC'-CB'
2	A	701	TOE	OF'-CG'-CH'-OI'
2	A	702	TOE	CD'-CE'-OF'-CG'

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	TOE	1	0
3	B	603	SO4	1	0
2	B	601	TOE	1	0
3	B	604	SO4	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%)	1.12	42 (7%)	20 21	12, 43, 47, 64	3 (0%)
1	B	555/559 (99%)	1.29	113 (20%)	3 3	17, 54, 107, 143	2 (0%)
All	All	1112/1118 (99%)	1.20	155 (13%)	6 6	12, 44, 97, 143	5 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	438[A]	HIS	8.1
1	A	335[A]	ARG	7.0
1	A	559	PHE	5.8
1	A	73	GLY	5.3
1	A	533[A]	MET	5.1
1	A	72	GLU	5.1
1	B	468	ALA	4.5
1	B	353	LEU	4.2
1	B	355	ALA	4.1
1	B	73	GLY	4.0
1	B	396	TYR	3.9
1	B	432	SER	3.9
1	A	551	ALA	3.7
1	A	109	GLY	3.7
1	A	557	GLY	3.6
1	B	427	LEU	3.5
1	B	110	GLY	3.5
1	B	349	ALA	3.4
1	B	408	LEU	3.4
1	B	433	ARG	3.4
1	B	385	PRO	3.4
1	A	71	GLY	3.3
1	B	559	PHE	3.3
1	B	392	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	3.2
1	B	384	PHE	3.2
1	A	3	LYS	3.2
1	A	550	ASP	3.1
1	A	558	LEU	3.1
1	B	409	SER	3.1
1	B	109	GLY	3.1
1	B	431	GLU	3.1
1	B	420	LEU	3.1
1	B	356	LEU	3.0
1	B	381	ILE	3.0
1	B	113	GLY	3.0
1	B	378	VAL	3.0
1	B	423	ALA	3.0
1	B	505[A]	ARG	3.0
1	B	348	LEU	3.0
1	B	445	LEU	3.0
1	A	546	ASN	3.0
1	B	107	ILE	3.0
1	A	545	CYS	2.9
1	B	373	PHE	2.9
1	B	435	SER	2.9
1	B	430	LEU	2.9
1	B	434	PRO	2.9
1	B	322	GLY	2.8
1	B	72	GLU	2.8
1	B	503	LEU	2.8
1	B	388	THR	2.8
1	A	12	GLN	2.8
1	B	438	HIS	2.8
1	B	116	TYR	2.8
1	B	343	VAL	2.8
1	A	553	GLY	2.7
1	B	323	PHE	2.7
1	B	507	ARG	2.7
1	B	504	GLY	2.7
1	B	402	ALA	2.7
1	B	394	LEU	2.7
1	B	411	VAL	2.7
1	B	399	CYS	2.7
1	B	336	ALA	2.7
1	B	88	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	344	PRO	2.6
1	B	436	ASN	2.6
1	B	412	TRP	2.6
1	A	111	ALA	2.6
1	A	112	ALA	2.6
1	B	390	ALA	2.6
1	B	407	ALA	2.6
1	A	556	THR	2.6
1	B	24[A]	ARG	2.6
1	B	91	ARG	2.6
1	B	320	TYR	2.6
1	B	439	VAL	2.6
1	B	386	THR	2.6
1	B	395	LEU	2.6
1	B	444	ASP	2.6
1	A	108	LYS	2.6
1	B	112	ALA	2.6
1	B	509	PHE	2.5
1	B	354	GLU	2.5
1	B	299	VAL	2.5
1	B	521	GLY	2.5
1	B	361	ALA	2.5
1	B	461	ALA	2.5
1	B	422	LEU	2.5
1	A	6	SER	2.5
1	A	542	PRO	2.5
1	B	330	ILE	2.5
1	B	297	TYR	2.5
1	B	114	GLY	2.5
1	A	347	ASP	2.4
1	B	5	PRO	2.4
1	B	443	LEU	2.4
1	A	110	GLY	2.4
1	B	469	GLU	2.4
1	B	334	VAL	2.4
1	A	476	ARG	2.4
1	B	111	ALA	2.4
1	B	406	VAL	2.4
1	B	501	THR	2.4
1	B	400	ALA	2.3
1	B	14	ALA	2.3
1	B	387	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	475	GLN	2.3
1	B	327	ALA	2.3
1	B	404	ALA	2.3
1	B	459	TYR	2.3
1	B	482	TYR	2.3
1	A	21	GLU	2.3
1	B	481	GLY	2.3
1	B	93	MET	2.3
1	B	492	THR	2.2
1	B	296	ASP	2.2
1	B	437	PHE	2.2
1	A	107	ILE	2.2
1	A	528	ILE	2.2
1	A	181	VAL	2.2
1	B	108	LYS	2.2
1	B	350	THR	2.2
1	B	360	PHE	2.2
1	B	463	GLY	2.2
1	A	382	ASN	2.2
1	B	442	ASN	2.2
1	A	462	ASP	2.2
1	A	548	ASP	2.2
1	B	376	PRO	2.1
1	A	8	ILE	2.1
1	B	368	GLU	2.1
1	A	428	GLN	2.1
1	A	552	ASP	2.1
1	B	397	GLU	2.1
1	B	506	PRO	2.1
1	B	341	GLY	2.1
1	B	232	ASP	2.1
1	B	298	VAL	2.1
1	B	377	ALA	2.1
1	B	383	ALA	2.1
1	B	508	ASN	2.1
1	A	169	VAL	2.1
1	A	397	GLU	2.0
1	A	544	ALA	2.1
1	B	473	ALA	2.1
1	B	500	MET	2.0
1	A	422	LEU	2.0
1	B	59	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	294	LEU	2.0
1	B	494	TYR	2.0
1	B	502	LYS	2.0
1	A	334	VAL	2.0
1	A	13	ALA	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($\text{\AA}^2$)	Q<0.9
3	SO4	A	706	5/5	0.68	0.12	67,72,83,101	0
3	SO4	B	604	5/5	0.71	0.12	80,86,102,113	0
3	SO4	A	707	5/5	0.73	0.15	59,77,92,98	0
3	SO4	A	704	5/5	0.85	0.13	42,43,50,61	0
2	TOE	B	601	11/11	0.85	0.14	33,38,46,48	0
2	TOE	A	702	11/11	0.87	0.13	33,39,59,60	0
3	SO4	B	603	5/5	0.89	0.13	41,55,63,64	0
2	TOE	A	701	11/11	0.89	0.13	23,34,47,47	0
3	SO4	B	602	5/5	0.93	0.11	37,38,47,49	0
3	SO4	A	705	5/5	0.95	0.20	34,38,51,60	0
3	SO4	A	703	5/5	0.97	0.14	21,25,26,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.