



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:09 PM GMT

PDB ID : 1RD7
Title : DIHYDROFOLATE REDUCTASE COMPLEXED WITH FOLATE
Authors : Sawaya, M.R.; Kraut, J.
Deposited on : 1996-11-01
Resolution : 2.60 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>

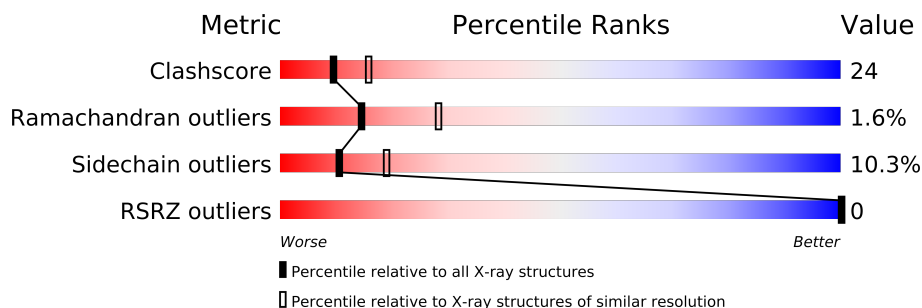
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	159	<div><div></div><div></div><div></div><div></div></div>
1	B	159	<div><div></div><div></div><div></div><div></div></div>

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

Mol	Type	Chain	Res	Geometry	Electron density
2	FOL	A	161	X	-
3	BME	A	162	-	X
3	BME	B	362	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2644 atoms, of which 0 are hydrogen 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.

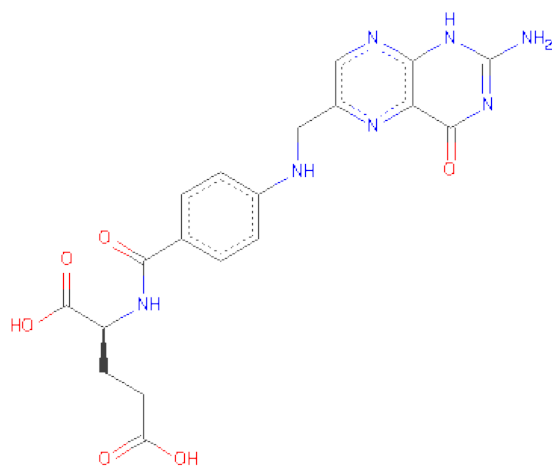
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	6	0	0
			1268	805	216	240	7			
1	B	159	Total	C	N	O	S	3	0	0
			1268	805	216	240	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASP	ASN	CONFLICT	UNP P0ABQ4
B	37	ASP	ASN	CONFLICT	UNP P0ABQ4

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: C₁₉H₁₉N₇O₆).



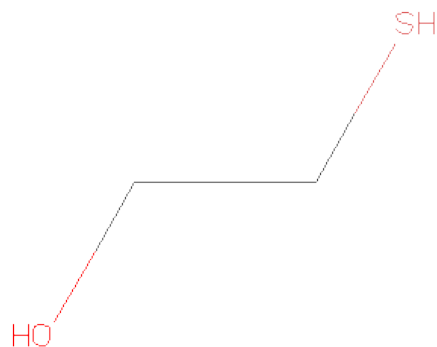
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	19	7	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			32	19	7	6		

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	S		0	0
			1	1			
3	B	1	Total	C	S	0	0
			2	1	1		

- Molecule 4 is water.

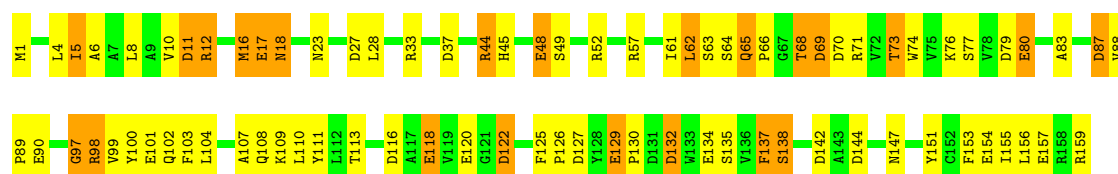
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	17	Total	O	0	0
			17	17		

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.

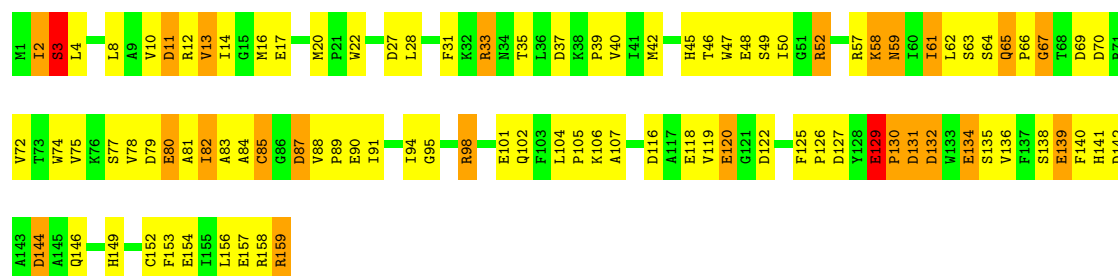
• Molecule 1: DIHYDROFOLATE REDUCTASE

Chain A:



• Molecule 1: DIHYDROFOLATE REDUCTASE

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.23Å 65.66Å 116.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 45.37 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.60) 87.9 (45.37-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.20Å)	Xtriage
Refinement program	TNT V. 5-D	Depositor
R, R_{free}	0.163 , (Not available) 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 17388 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2644	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: FOL, BME

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	1.27	10/1302 (0.8%)	1.74	33/1770 (1.9%)
1	B	1.29	11/1302 (0.8%)	1.71	38/1770 (2.1%)
All	All	1.28	21/2604 (0.8%)	1.72	71/3540 (2.0%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	154	GLU	CD-OE2	8.99	1.35	1.25
1	B	118	GLU	CD-OE2	8.76	1.35	1.25
1	A	157	GLU	CD-OE2	8.54	1.35	1.25
1	B	139	GLU	CD-OE2	7.57	1.33	1.25
1	B	48	GLU	CD-OE2	7.56	1.33	1.25
1	A	101	GLU	CD-OE2	7.44	1.33	1.25
1	B	134	GLU	CD-OE2	7.39	1.33	1.25
1	A	90	GLU	CD-OE2	7.31	1.33	1.25
1	B	101	GLU	CD-OE2	7.00	1.33	1.25
1	B	80	GLU	CD-OE1	6.83	1.33	1.25
1	B	120	GLU	CD-OE2	6.67	1.32	1.25
1	B	17	GLU	CD-OE2	6.59	1.32	1.25
1	A	120	GLU	CD-OE2	6.55	1.32	1.25
1	B	90	GLU	CD-OE2	6.46	1.32	1.25
1	A	48	GLU	CD-OE2	6.07	1.32	1.25
1	A	154	GLU	CD-OE2	6.03	1.32	1.25
1	A	134	GLU	CD-OE2	5.96	1.32	1.25
1	A	80	GLU	CD-OE2	5.93	1.32	1.25
1	A	17	GLU	CD-OE2	5.84	1.32	1.25
1	B	157	GLU	CD-OE2	5.74	1.31	1.25
1	A	118	GLU	CD-OE2	5.25	1.31	1.25

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ASP	CB-CG-OD2	-10.62	108.74	118.30
1	B	69	ASP	CB-CG-OD2	-9.40	109.84	118.30
1	A	27	ASP	CB-CG-OD2	-8.97	110.22	118.30
1	B	27	ASP	CB-CG-OD2	-8.92	110.27	118.30
1	A	27	ASP	CB-CG-OD1	8.86	126.27	118.30
1	B	87	ASP	CB-CA-C	-8.68	93.04	110.40
1	A	116	ASP	CB-CG-OD1	-8.43	110.72	118.30
1	B	144	ASP	CB-CG-OD1	8.23	125.71	118.30
1	B	11	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	B	27	ASP	CB-CG-OD1	7.86	125.37	118.30
1	B	142	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	B	37	ASP	CB-CG-OD1	7.80	125.32	118.30
1	B	87	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	A	79	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	A	129	GLU	C-N-CD	-7.49	104.11	120.60
1	B	127	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	37	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	52	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	142	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	11	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	B	131	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	69	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	B	132	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	116	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	A	122	ASP	CB-CG-OD1	-6.82	112.17	118.30
1	A	127	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	127	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	132	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	11	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	70	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	B	131	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	A	87	ASP	CB-CG-OD1	-6.42	112.53	118.30
1	A	44	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	58	LYS	CA-CB-CG	-6.33	99.48	113.40
1	B	79	ASP	CB-CG-OD2	-6.27	112.65	118.30
1	B	69	ASP	N-CA-CB	-6.23	99.38	110.60
1	A	137	PHE	CB-CA-C	6.21	122.83	110.40
1	B	98	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	B	37	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	159	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	B	144	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	66	PRO	C-N-CA	-6.01	109.68	122.30
1	A	11	ASP	CB-CG-OD1	5.92	123.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	CYS	CA-CB-SG	-5.92	103.34	114.00
1	B	116	ASP	CB-CG-OD1	5.92	123.62	118.30
1	B	8	LEU	CB-CA-C	-5.90	98.99	110.20
1	A	79	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	70	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	159	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	116	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	73	THR	CB-CA-C	-5.66	96.32	111.60
1	A	144	ASP	CB-CG-OD1	5.65	123.38	118.30
1	B	70	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	B	61	ILE	CB-CA-C	-5.42	100.75	111.60
1	A	73	THR	CA-CB-CG2	-5.36	104.89	112.40
1	A	108	GLN	CB-CA-C	-5.36	99.69	110.40
1	B	129	GLU	C-N-CD	-5.35	108.83	120.60
1	A	68	THR	N-CA-CB	5.34	120.45	110.30
1	A	113	THR	N-CA-CB	5.28	120.33	110.30
1	A	122	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	142	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	18	ASN	CA-CB-CG	-5.18	102.01	113.40
1	B	13	VAL	CA-CB-CG2	-5.15	103.18	110.90
1	B	132	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	79	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	127	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	70	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	94	ILE	N-CA-C	5.04	124.61	111.00
1	B	3	SER	CA-C-N	-5.03	106.13	117.20
1	B	33	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	12	ARG	CD-NE-CZ	5.02	130.63	123.60

There are no chirality outliers.

There are no planarity outliers.

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	1268	0	1220	47	0
1	B	1268	0	1220	77	0
2	A	32	0	18	1	0
2	B	32	0	17	1	0
3	A	1	0	0	0	0
3	B	2	0	0	1	0
4	A	24	0	0	1	0
4	B	17	0	0	3	0
All	All	2644	0	2475	124	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 24.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:362:BME:C2	3:B:362:BME:S2	2.10	1.39
1:B:135:SER:HA	1:B:156:LEU:HD23	1.32	1.09
1:A:98:ARG:HB3	1:A:98:ARG:HH11	1.34	0.91
1:A:125:PHE:CD1	1:A:126:PRO:HD2	2.07	0.90
1:A:98:ARG:NH1	1:A:98:ARG:HB3	1.88	0.87
1:A:125:PHE:CG	1:A:126:PRO:HD2	2.15	0.82
1:B:139:GLU:HG2	1:B:141:HIS:HE2	1.48	0.78
1:A:129:GLU:CG	1:A:130:PRO:HD2	2.15	0.77
1:A:77:SER:OG	1:A:80:GLU:HG3	1.87	0.75
1:A:129:GLU:HG2	1:A:130:PRO:HD2	1.68	0.74
1:B:13:VAL:HG11	1:B:119:VAL:HG23	1.70	0.73
1:B:139:GLU:HG2	1:B:141:HIS:NE2	2.05	0.70
1:B:135:SER:CA	1:B:156:LEU:HD23	2.18	0.70
1:A:64:SER:HB2	1:A:65:GLN:NE2	2.08	0.68
1:B:65:GLN:N	1:B:65:GLN:HE21	1.94	0.66
1:B:67:GLY:HA2	1:B:74:TRP:CE2	2.31	0.66
1:B:65:GLN:NE2	1:B:65:GLN:N	2.44	0.66
1:B:59:ASN:HD22	1:B:59:ASN:N	1.94	0.65
1:A:61:ILE:HD12	1:A:61:ILE:N	2.12	0.64
1:B:140:PHE:HD1	1:B:152:CYS:HB2	1.62	0.64
1:B:42:MET:SD	1:B:47:TRP:HB2	2.37	0.64
1:A:80:GLU:O	1:A:83:ALA:HB3	1.97	0.63
1:B:104:LEU:N	1:B:105:PRO:HD2	2.11	0.63
1:B:88:VAL:HB	1:B:89:PRO:HD2	1.81	0.63
1:B:95:GLY:HA3	4:B:429:HOH:O	1.98	0.62
1:A:62:LEU:HD12	1:A:63:SER:N	2.14	0.62
1:B:20:MET:HE2	1:B:22:TRP:CH2	2.35	0.62
1:B:144:ASP:OD1	1:B:146:GLN:N	2.31	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:SER:O	1:A:76:LYS:HA	2.00	0.61
1:B:104:LEU:HD22	1:B:126:PRO:HB2	1.81	0.61
1:B:3:SER:C	1:B:4:LEU:HD12	2.21	0.61
1:A:138:SER:HA	1:A:153:PHE:O	2.01	0.61
1:B:85:CYS:CB	1:B:91:ILE:HD13	2.31	0.61
1:A:44:ARG:O	1:A:48:GLU:HG3	2.00	0.60
1:B:42:MET:CG	1:B:61:ILE:HD12	2.32	0.60
1:A:98:ARG:O	1:A:102:GLN:HG3	2.01	0.59
1:B:65:GLN:HB3	1:B:66:PRO:CD	2.33	0.58
1:B:45:HIS:CD2	1:B:45:HIS:H	2.20	0.58
1:B:64:SER:HB2	1:B:65:GLN:HE22	1.68	0.58
1:A:4:LEU:N	1:A:4:LEU:HD12	2.18	0.58
1:B:4:LEU:N	1:B:4:LEU:HD12	2.19	0.57
1:A:99:VAL:O	1:A:103:PHE:HD1	1.87	0.57
1:A:64:SER:HA	1:A:76:LYS:HD3	1.88	0.55
1:A:64:SER:HB2	1:A:65:GLN:HE22	1.71	0.54
1:A:62:LEU:HD12	1:A:62:LEU:C	2.28	0.54
1:A:129:GLU:O	1:A:132:ASP:HB2	2.07	0.54
1:A:57:ARG:NH1	2:A:161:FOL:O1	2.39	0.54
1:B:67:GLY:HA2	1:B:74:TRP:CD2	2.43	0.53
1:B:98:ARG:O	1:B:102:GLN:HG3	2.08	0.53
1:B:129:GLU:O	1:B:132:ASP:N	2.35	0.53
1:B:40:VAL:O	1:B:40:VAL:HG23	2.09	0.52
1:B:64:SER:C	1:B:65:GLN:HE21	2.12	0.52
1:B:75:VAL:HG21	1:B:81:ALA:CA	2.39	0.52
1:B:62:LEU:HD12	1:B:63:SER:N	2.24	0.52
1:B:138:SER:HA	1:B:153:PHE:O	2.09	0.52
1:B:12:ARG:NH1	1:B:125:PHE:O	2.42	0.52
1:A:110:LEU:HD12	1:A:156:LEU:HD12	1.91	0.51
1:B:46:THR:HG22	1:B:50:ILE:CD1	2.41	0.51
1:A:97:GLY:O	1:A:100:TYR:HB2	2.11	0.51
1:B:82:ILE:HG22	1:B:83:ALA:N	2.26	0.51
1:B:66:PRO:O	1:B:67:GLY:O	2.29	0.50
1:B:134:GLU:O	1:B:136:VAL:HG13	2.11	0.50
1:A:16:MET:HA	1:A:122:ASP:OD2	2.11	0.50
1:A:159:ARG:HA	4:A:430:HOH:O	2.12	0.50
1:A:10:VAL:O	1:A:11:ASP:HB2	2.12	0.50
1:A:5:ILE:HG13	1:A:6:ALA:N	2.27	0.50
1:B:149:HIS:HB3	4:B:417:HOH:O	2.11	0.50
1:A:110:LEU:O	1:A:155:ILE:HA	2.12	0.49
1:A:74:TRP:CD1	1:A:74:TRP:N	2.80	0.49
1:A:8:LEU:HD12	1:A:8:LEU:N	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:SER:HB2	1:B:65:GLN:NE2	2.28	0.49
1:B:75:VAL:HG21	1:B:81:ALA:HA	1.94	0.48
1:B:74:TRP:N	1:B:74:TRP:CD1	2.81	0.48
1:B:131:ASP:O	1:B:159:ARG:HD2	2.13	0.48
1:B:129:GLU:HG3	1:B:130:PRO:HD2	1.95	0.48
1:B:31:PHE:O	1:B:35:THR:HG23	2.14	0.48
1:B:75:VAL:HB	1:B:80:GLU:HB3	1.96	0.48
1:A:65:GLN:N	1:A:65:GLN:NE2	2.62	0.48
1:B:65:GLN:HB3	1:B:66:PRO:HD2	1.96	0.47
1:B:78:VAL:O	1:B:82:ILE:HD12	2.14	0.47
1:B:57:ARG:NH1	2:B:361:FOL:O1	2.31	0.47
1:B:16:MET:HG3	1:B:20:MET:HE1	1.95	0.47
1:B:22:TRP:HB3	1:B:149:HIS:CE1	2.49	0.47
1:B:45:HIS:N	1:B:45:HIS:CD2	2.83	0.47
1:B:64:SER:CB	1:B:65:GLN:NE2	2.78	0.46
1:A:135:SER:HA	1:A:156:LEU:HD23	1.98	0.46
1:A:69:ASP:CG	1:A:71:ARG:HE	2.19	0.46
1:B:42:MET:HG2	1:B:61:ILE:CD1	2.45	0.46
1:A:61:ILE:CD1	1:A:61:ILE:N	2.79	0.46
1:B:85:CYS:SG	1:B:91:ILE:HD13	2.56	0.46
1:A:88:VAL:HA	1:A:89:PRO:HD3	1.69	0.46
1:B:129:GLU:HA	1:B:130:PRO:HD3	1.73	0.45
1:B:78:VAL:O	1:B:82:ILE:HB	2.15	0.45
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.53	0.45
1:B:2:ILE:HG22	1:B:3:SER:N	2.32	0.45
1:B:12:ARG:O	1:B:14:ILE:HG23	2.17	0.44
1:A:45:HIS:CD2	1:A:45:HIS:H	2.34	0.44
1:A:23:ASN:O	1:A:147:ASN:HA	2.18	0.44
1:B:59:ASN:ND2	1:B:59:ASN:N	2.64	0.43
1:B:61:ILE:HD13	1:B:61:ILE:N	2.33	0.43
1:B:140:PHE:CD1	1:B:152:CYS:SG	3.11	0.43
1:A:11:ASP:O	1:A:12:ARG:HB2	2.17	0.43
1:A:18:ASN:OD1	1:B:144:ASP:HA	2.19	0.43
1:B:10:VAL:O	1:B:11:ASP:HB2	2.18	0.43
1:B:104:LEU:O	1:B:158:ARG:NH2	2.51	0.43
1:A:109:LYS:HA	1:A:156:LEU:O	2.19	0.43
1:B:129:GLU:O	1:B:131:ASP:N	2.52	0.43
1:B:42:MET:HG2	1:B:61:ILE:HD12	2.01	0.42
1:B:88:VAL:HB	1:B:89:PRO:CD	2.48	0.42
1:B:72:VAL:HG22	1:B:72:VAL:H	1.63	0.42
1:B:28:LEU:HD23	1:B:28:LEU:HA	1.81	0.42
1:B:11:ASP:O	1:B:12:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:39:PRO:HA	1:B:58:LYS:HB3	2.02	0.42
1:A:104:LEU:O	1:A:107:ALA:HB3	2.20	0.42
1:B:4:LEU:HD13	1:B:107:ALA:HB2	2.01	0.42
1:A:73:THR:HG22	1:A:74:TRP:N	2.25	0.42
1:A:63:SER:OG	1:A:64:SER:N	2.53	0.42
1:B:83:ALA:O	1:B:85:CYS:N	2.53	0.41
1:B:4:LEU:N	1:B:4:LEU:CD1	2.83	0.41
1:B:131:ASP:OD1	1:B:132:ASP:N	2.53	0.41
1:A:8:LEU:HD23	1:A:12:ARG:HA	2.03	0.41
1:B:52:ARG:NH2	4:B:441:HOH:O	2.29	0.40
1:B:139:GLU:OE2	1:B:141:HIS:NE2	2.55	0.40
1:A:151:TYR:CD1	1:A:151:TYR:N	2.89	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	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	33	63
1	B	157/159 (99%)	146 (93%)	7 (4%)	4 (2%)	9	14
All	All	314/318 (99%)	295 (94%)	14 (4%)	5 (2%)	14	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	GLY
1	B	129	GLU
1	B	84	ALA
1	A	97	GLY
1	B	130	PRO

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	136/136 (100%)	121 (89%)	15 (11%)	9	16
1	B	136/136 (100%)	123 (90%)	13 (10%)	12	22
All	All	272/272 (100%)	244 (90%)	28 (10%)	10	19

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	ILE
1	A	16	MET
1	A	17	GLU
1	A	33	ARG
1	A	49	SER
1	A	62	LEU
1	A	65	GLN
1	A	68	THR
1	A	87	ASP
1	A	98	ARG
1	A	111	TYR
1	A	118	GLU
1	A	137	PHE
1	A	138	SER
1	B	2	ILE
1	B	3	SER
1	B	33	ARG
1	B	49	SER
1	B	52	ARG
1	B	59	ASN
1	B	65	GLN
1	B	77	SER
1	B	82	ILE
1	B	87	ASP
1	B	106	LYS
1	B	120	GLU
1	B	122	ASP

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

Mol	Chain	Res	Type
1	A	45	HIS
1	A	65	GLN
1	B	45	HIS
1	B	65	GLN
1	B	124	HIS
1	B	146	GLN

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 4 ligands modelled in this entry, 1 is modelled with single atom - leaving 3 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	FOL	A	161	-	34,34,34	3.64	24 (70%)	45,47,47	2.57	20 (44%)
2	FOL	B	361	-	34,34,34	4.37	19 (55%)	45,47,47	3.19	22 (48%)
3	BME	B	362	1	0,1,3	0.00	-	0,0,2	0.00	-

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	FOL	A	161	-	-	0/22/22/22	0/1/3/3
2	FOL	B	361	-	-	0/22/22/22	0/1/3/3
3	BME	B	362	1	-	0/0/0/1	0/0/0/0

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	361	FOL	C4A-C8A	-14.20	1.16	1.40
2	B	361	FOL	C13-C14	7.00	1.51	1.39
2	B	361	FOL	C4-C4A	6.90	1.52	1.41
2	A	161	FOL	C8A-N8	-6.90	1.25	1.34
2	A	161	FOL	C4A-C8A	-6.87	1.29	1.40
2	A	161	FOL	C7-N8	-6.72	1.19	1.31
2	B	361	FOL	C16-C15	6.12	1.50	1.38
2	A	161	FOL	C11-C	-6.08	1.37	1.50
2	B	361	FOL	C11-C	5.95	1.62	1.50
2	A	161	FOL	C13-C12	-5.92	1.27	1.38
2	B	361	FOL	C8A-N8	-5.90	1.27	1.34
2	B	361	FOL	C2-N3	-5.80	1.26	1.33
2	B	361	FOL	C8A-N1	5.47	1.44	1.37
2	B	361	FOL	C12-C11	5.27	1.48	1.39
2	A	161	FOL	C4-C4A	5.15	1.49	1.41
2	A	161	FOL	C2-N3	4.86	1.39	1.33
2	B	361	FOL	C7-C6	-4.82	1.31	1.39
2	B	361	FOL	CB-CA	-4.58	1.43	1.53
2	A	161	FOL	C4A-N5	4.40	1.45	1.36
2	B	361	FOL	C2-N1	-3.72	1.30	1.36
2	B	361	FOL	C13-C12	3.72	1.45	1.38
2	A	161	FOL	C9-N10	3.69	1.54	1.45
2	A	161	FOL	C7-C6	3.66	1.45	1.39
2	B	361	FOL	C14-N10	3.65	1.48	1.38
2	A	161	FOL	O4-C4	3.64	1.31	1.24
2	A	161	FOL	C9-C6	3.57	1.58	1.51
2	A	161	FOL	C12-C11	-3.57	1.33	1.39
2	B	361	FOL	OE1-CD	3.57	1.35	1.22
2	A	161	FOL	CA-CT	3.48	1.62	1.52
2	B	361	FOL	CA-CT	-3.40	1.43	1.52
2	A	161	FOL	OE1-CD	3.37	1.34	1.22
2	A	161	FOL	C15-C14	-2.89	1.34	1.39
2	A	161	FOL	CG-CD	2.83	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	161	FOL	CA-N	2.80	1.52	1.45
2	A	161	FOL	C13-C14	2.73	1.43	1.39
2	A	161	FOL	C16-C11	2.70	1.44	1.39
2	B	361	FOL	C-N	2.61	1.39	1.34
2	A	161	FOL	O1-CT	2.54	1.30	1.22
2	A	161	FOL	C16-C15	-2.45	1.34	1.38
2	A	161	FOL	C14-N10	2.29	1.45	1.38
2	A	161	FOL	C8A-N1	-2.22	1.35	1.37
2	B	361	FOL	C6-N5	2.17	1.37	1.32
2	B	361	FOL	C9-C6	-2.01	1.46	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	FOL	NA2-C2-N1	9.09	127.86	117.86
2	B	361	FOL	C4-N3-C2	7.32	124.82	116.91
2	B	361	FOL	CG-CB-CA	-7.13	99.00	112.99
2	A	161	FOL	NA2-C2-N1	5.49	123.91	117.86
2	B	361	FOL	C7-C6-N5	-5.13	117.17	120.75
2	B	361	FOL	C6-C9-N10	-5.11	101.51	113.33
2	A	161	FOL	OE1-CD-CG	-5.00	105.84	123.03
2	B	361	FOL	N1-C2-N3	-4.89	114.95	121.75
2	A	161	FOL	C7-C6-N5	-4.86	117.36	120.75
2	A	161	FOL	C16-C15-C14	-4.68	114.84	120.27
2	B	361	FOL	OE1-CD-CG	-4.59	107.23	123.03
2	A	161	FOL	C6-C7-N8	4.51	127.92	123.16
2	A	161	FOL	C4-N3-C2	4.45	121.72	116.91
2	A	161	FOL	C4A-C8A-N1	4.42	124.69	118.78
2	B	361	FOL	C15-C16-C11	4.25	125.83	120.76
2	B	361	FOL	C16-C11-C12	-3.84	113.14	118.63
2	B	361	FOL	O-C-N	-3.83	115.52	122.44
2	A	161	FOL	C6-N5-C4A	-3.80	109.55	117.70
2	B	361	FOL	C2-N1-C8A	3.52	124.56	120.15
2	A	161	FOL	C8A-C4A-N5	3.41	124.60	120.45
2	A	161	FOL	C13-C14-N10	-3.40	114.07	121.02
2	B	361	FOL	O-C-C11	3.32	126.83	121.01
2	B	361	FOL	C9-C6-C7	3.21	127.12	121.41
2	A	161	FOL	CA-N-C	3.18	128.88	121.80
2	A	161	FOL	C15-C14-C13	3.04	123.37	119.10
2	A	161	FOL	CG-CB-CA	-3.02	107.06	112.99
2	B	361	FOL	CB-CA-N	-2.99	105.14	110.83
2	B	361	FOL	C12-C11-C	2.94	129.69	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	FOL	CT-CA-N	2.94	118.12	110.53
2	A	161	FOL	OE2-CD-CG	2.92	124.53	114.22
2	B	361	FOL	CA-N-C	2.91	128.28	121.80
2	B	361	FOL	OE2-CD-OE1	2.90	130.68	123.30
2	A	161	FOL	CB-CA-N	-2.72	105.65	110.83
2	A	161	FOL	N1-C8A-N8	-2.65	111.15	116.35
2	A	161	FOL	NA2-C2-N3	-2.58	116.80	120.30
2	B	361	FOL	C4A-C8A-N1	2.56	122.20	118.78
2	A	161	FOL	OE2-CD-OE1	2.46	129.56	123.30
2	B	361	FOL	C8A-C4A-N5	2.39	123.35	120.45
2	B	361	FOL	NA2-C2-N3	-2.29	117.19	120.30
2	B	361	FOL	OE2-CD-CG	2.23	122.09	114.22
2	A	161	FOL	C4-C4A-N5	-2.13	116.22	119.75
2	A	161	FOL	C11-C-N	2.12	120.42	116.89

There are no chirality outliers.

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	159/159 (100%)	-1.08	0 100 100	4, 21, 53, 83	2 (1%)
1	B	159/159 (100%)	-0.96	0 100 100	6, 23, 63, 89	1 (0%)
All	All	318/318 (100%)	-1.02	0 100 100	4, 22, 59, 89	3 (0%)

There are no RSRZ outliers to report.

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	BME	B	362	2/4	0.13	2.70	30,30,30,41	0
3	BME	A	162	1/4	0.11	2.37	36,36,36,36	0
2	FOL	A	161	32/32	0.12	1.29	10,20,70,73	0
2	FOL	B	361	32/32	0.11	0.54	11,22,72,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.