



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:38 AM UTC

PDB ID : 2UXQ / pdb_00002uxq
Title : Isocitrate dehydrogenase from the psychrophilic bacterium *Desulfotalea psychrophila*: biochemical properties and crystal structure analysis
Authors : Fedoy, A.-E.; Yang, N.; Martinez, A.; Leiros, H.-K.S.; Steen, I.H.
Deposited on : 2007-03-29
Resolution : 1.75 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

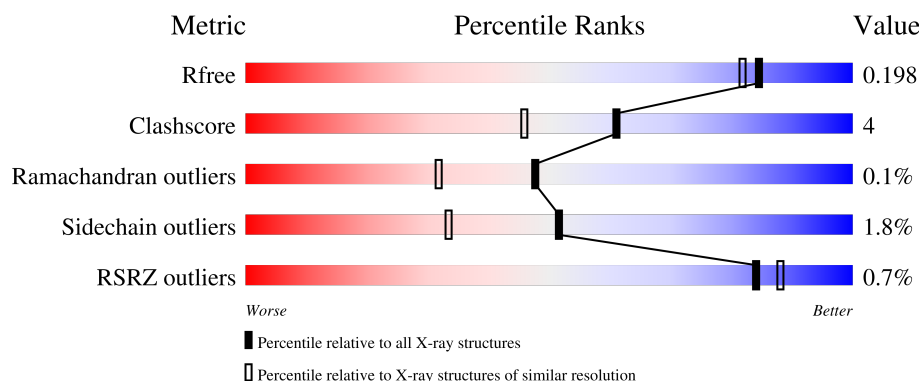
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	402	89% 8% .
1	B	402	% 90% 7% .
1	C	402	% 86% 12% ..
1	D	402	% 88% 9% .

2 Entry composition [i](#)

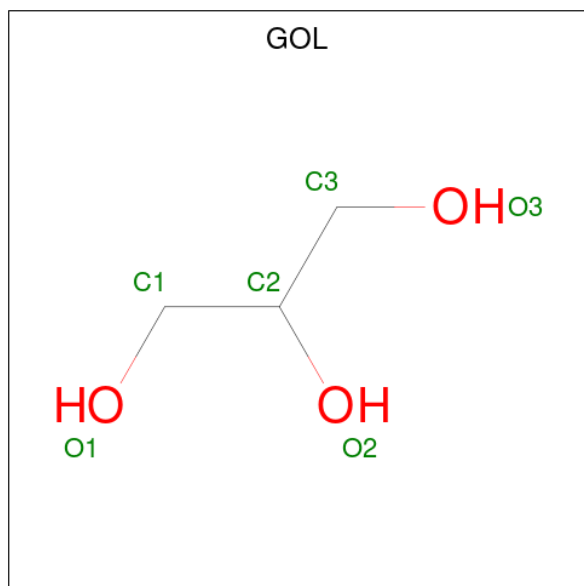
There are 6 unique types of molecules in this entry. The entry contains 15038 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ISOCITRATE DEHYDROGENASE NATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	49	4	0
			3234	2061	538	613	22			
1	B	401	Total	C	N	O	S	42	5	0
			3242	2066	539	614	23			
1	C	402	Total	C	N	O	S	66	7	0
			3271	2085	545	618	23			
1	D	402	Total	C	N	O	S	65	5	0
			3243	2067	539	615	22			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- 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	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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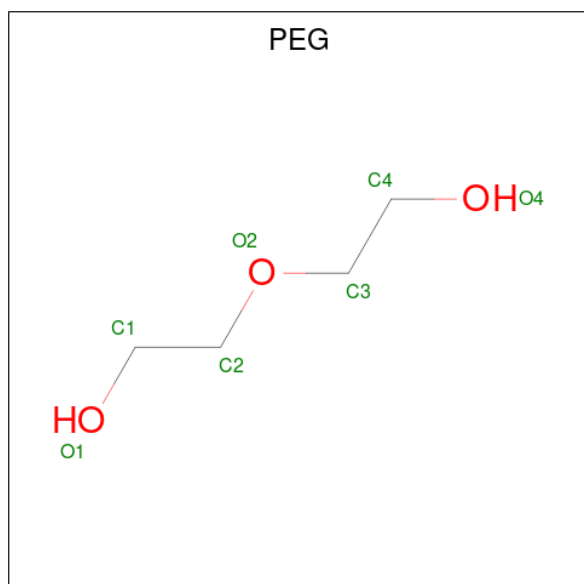
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 10 8 2	0	1
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 14 8 6	0	1

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	1
			14	8	6		

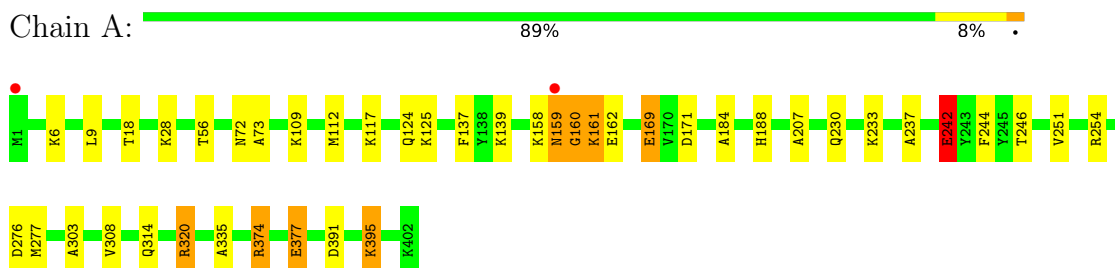
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	473	Total	O	0	0
			473	473		
6	B	513	Total	O	0	0
			513	513		
6	C	445	Total	O	0	0
			445	445		
6	D	452	Total	O	0	0
			452	452		

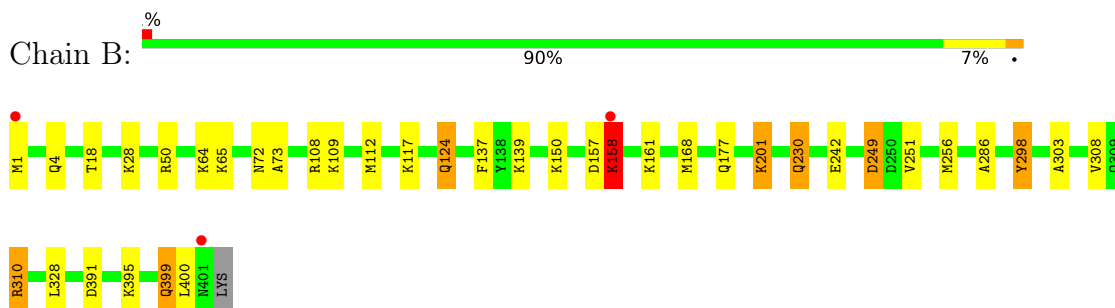
3 Residue-property plots

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.

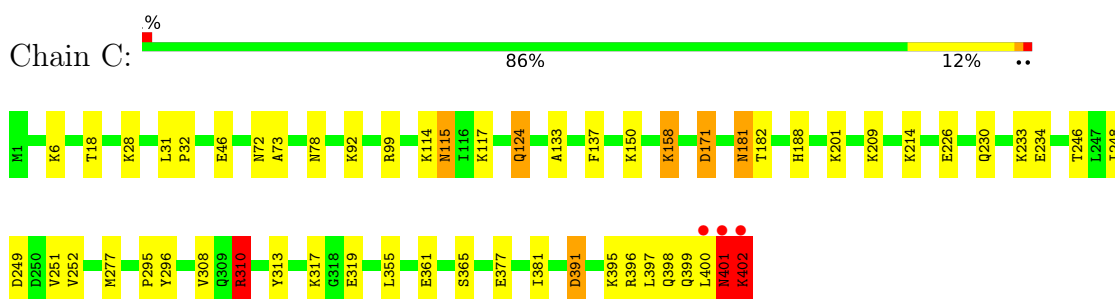
• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE



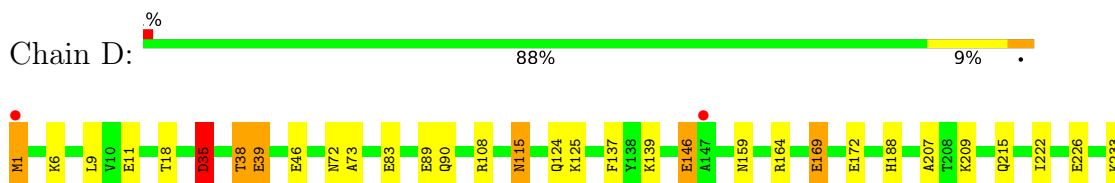
• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE

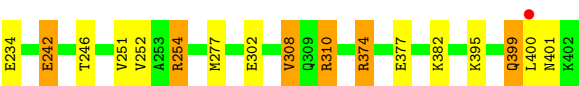


• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE



• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.32Å 73.28Å 126.41Å 98.90° 98.98° 113.88°	Depositor
Resolution (Å)	20.00 – 1.75 20.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-1.75) 86.3 (20.00-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.146 , 0.189 0.158 , 0.198	Depositor DCC
R_{free} test set	3243 reflections (1.72%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 75.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15038	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, PEG, GOL

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	1.68	21/3299 (0.6%)	1.64	27/4455 (0.6%)
1	B	1.89	15/3307 (0.5%)	1.22	18/4465 (0.4%)
1	C	1.49	25/3336 (0.7%)	1.55	38/4504 (0.8%)
1	D	1.81	22/3308 (0.7%)	1.32	33/4468 (0.7%)
All	All	1.72	83/13250 (0.6%)	1.44	116/17892 (0.6%)

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	A	0	7
1	B	0	3
1	C	0	3
1	D	0	6
All	All	0	19

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	LYS	CA-C	58.06	2.32	1.52
1	A	161	LYS	CA-C	42.45	2.05	1.52
1	D	400	LEU	C-N	37.37	1.84	1.33
1	B	158	LYS	C-O	-37.27	0.79	1.24
1	D	310	ARG	CD-NE	-34.39	0.98	1.46
1	B	310	ARG	CD-NE	-34.11	0.98	1.46
1	D	399	GLN	CG-CD	-31.89	0.72	1.52
1	D	35	ASP	CG-OD1	31.02	1.84	1.25
1	A	395	LYS	CE-NZ	25.56	2.26	1.49
1	C	391	ASP	CG-OD1	24.14	1.71	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	28	LYS	CE-NZ	-23.17	0.79	1.49
1	B	158	LYS	N-CA	21.87	1.71	1.46
1	B	310	ARG	NE-CZ	21.75	1.56	1.33
1	D	377	GLU	CD-OE2	-20.71	0.85	1.25
1	A	161	LYS	CB-CG	-18.94	0.95	1.52
1	A	242	GLU	CG-CD	18.80	1.99	1.52
1	D	169	GLU	CD-OE2	-18.57	0.90	1.25
1	A	160	GLY	CA-C	17.48	1.76	1.51
1	A	169	GLU	CD-OE2	-17.02	0.93	1.25
1	A	161	LYS	C-O	16.74	1.44	1.24
1	C	402	LYS	N-CA	15.93	1.76	1.46
1	D	83	GLU	CD-OE2	15.78	1.55	1.25
1	D	374	ARG	CD-NE	15.71	1.68	1.46
1	B	399	GLN	CD-NE2	-15.20	1.01	1.33
1	D	395	LYS	CG-CD	14.27	1.95	1.52
1	A	160	GLY	N-CA	14.20	1.66	1.45
1	D	6	LYS	CG-CD	-14.17	1.09	1.52
1	C	402	LYS	C-O	14.09	1.51	1.23
1	C	158	LYS	CD-CE	-13.98	1.10	1.52
1	C	46	GLU	CD-OE1	13.98	1.51	1.25
1	C	28	LYS	CD-CE	13.62	1.93	1.52
1	A	320	ARG	CZ-NH2	-13.45	1.16	1.33
1	A	233	LYS	CE-NZ	-13.15	1.09	1.49
1	A	117	LYS	CD-CE	-12.73	1.14	1.52
1	C	230	GLN	CD-NE2	12.12	1.58	1.33
1	B	310	ARG	CZ-NH1	-11.94	1.16	1.32
1	B	201	LYS	CG-CD	-11.73	1.17	1.52
1	B	395	LYS	CD-CE	-11.47	1.18	1.52
1	B	124	GLN	CD-OE1	-11.14	1.02	1.23
1	C	391	ASP	CG-OD2	-10.96	1.04	1.25
1	D	146	GLU	CD-OE1	10.72	1.45	1.25
1	D	209	LYS	CE-NZ	-10.68	1.17	1.49
1	C	395	LYS	CE-NZ	10.46	1.80	1.49
1	C	401	ASN	C-O	-10.45	1.10	1.24
1	C	124	GLN	CD-OE1	-10.41	1.03	1.23
1	C	92	LYS	CD-CE	-10.40	1.21	1.52
1	C	117	LYS	CD-CE	-10.23	1.21	1.52
1	C	402	LYS	CA-CB	10.05	1.73	1.53
1	A	314	GLN	CD-NE2	9.97	1.54	1.33
1	D	124	GLN	CD-NE2	9.92	1.54	1.33
1	A	395	LYS	CD-CE	-9.84	1.23	1.52
1	C	234	GLU	CB-CG	9.62	1.81	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	402	LYS	CB-CG	9.41	1.80	1.52
1	A	158	LYS	CB-CG	-9.18	1.25	1.52
1	B	400	LEU	CG-CD2	9.02	1.82	1.52
1	C	171	ASP	CG-OD2	-8.65	1.08	1.25
1	A	374	ARG	CZ-NH1	-8.49	1.20	1.32
1	D	233	LYS	CD-CE	8.37	1.77	1.52
1	C	158	LYS	CG-CD	8.32	1.77	1.52
1	D	254	ARG	CZ-NH2	-8.06	1.23	1.33
1	B	150	LYS	CE-NZ	7.55	1.72	1.49
1	D	125	LYS	CE-NZ	-7.55	1.26	1.49
1	C	150	LYS	CE-NZ	7.34	1.71	1.49
1	D	46	GLU	CD-OE2	7.08	1.38	1.25
1	B	124	GLN	CD-NE2	7.06	1.48	1.33
1	D	242	GLU	CD-OE1	6.85	1.38	1.25
1	D	89	GLU	CD-OE2	-6.73	1.12	1.25
1	D	401	ASN	N-CA	6.64	1.56	1.46
1	C	114	LYS	CG-CD	6.57	1.72	1.52
1	C	201	LYS	CG-CD	-6.40	1.33	1.52
1	D	382	LYS	CE-NZ	6.36	1.68	1.49
1	D	164	ARG	CZ-NH2	6.20	1.41	1.33
1	B	117	LYS	CE-NZ	-6.17	1.30	1.49
1	A	320	ARG	CZ-NH1	-6.11	1.24	1.32
1	B	256	MET	SD-CE	-5.94	1.64	1.79
1	C	319	GLU	CD-OE2	5.87	1.36	1.25
1	A	6	LYS	CD-CE	5.70	1.69	1.52
1	C	233	LYS	CD-CE	5.55	1.69	1.52
1	A	184	ALA	CA-CB	-5.53	1.44	1.53
1	C	317	LYS	CE-NZ	5.43	1.65	1.49
1	A	56	THR	CA-CB	5.41	1.61	1.53
1	A	124	GLN	CD-OE1	5.41	1.33	1.23
1	A	303	ALA	CA-CB	-5.07	1.46	1.52

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	GLY	CA-C-O	-34.95	59.76	120.57
1	A	320	ARG	NE-CZ-NH1	-34.28	87.22	121.50
1	C	398	GLN	CB-CG-CD	31.60	166.31	112.60
1	A	320	ARG	CD-NE-CZ	26.58	161.62	124.40
1	C	310	ARG	CD-NE-CZ	-26.52	87.28	124.40
1	A	159	ASN	CA-CB-CG	25.48	138.08	112.60
1	D	374	ARG	NE-CZ-NH2	-25.04	96.66	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LYS	N-CA-C	-24.54	68.72	109.46
1	B	158	LYS	CA-C-O	-24.39	92.49	121.02
1	C	310	ARG	NE-CZ-NH2	-24.10	97.51	119.20
1	A	242	GLU	CG-CD-OE1	-23.79	63.69	118.40
1	A	320	ARG	NH1-CZ-NH2	22.09	148.01	119.30
1	D	374	ARG	NE-CZ-NH1	21.65	143.15	121.50
1	C	310	ARG	NE-CZ-NH1	20.70	142.21	121.50
1	C	230	GLN	OE1-CD-NE2	-19.85	102.75	122.60
1	C	402	LYS	CA-C-O	-17.91	90.35	120.80
1	C	402	LYS	N-CA-C	-17.21	62.82	111.00
1	A	117	LYS	CG-CD-CE	16.74	149.79	111.30
1	B	310	ARG	CG-CD-NE	16.26	147.76	112.00
1	C	230	GLN	CG-CD-NE2	15.95	140.32	116.40
1	C	158	LYS	CB-CG-CD	-15.49	75.68	111.30
1	C	398	GLN	CG-CD-NE2	15.39	139.49	116.40
1	D	400	LEU	O-C-N	-15.39	94.64	122.34
1	D	164	ARG	NE-CZ-NH2	15.14	132.83	119.20
1	B	399	GLN	OE1-CD-NE2	-14.98	107.62	122.60
1	D	164	ARG	NH1-CZ-NH2	-13.92	101.21	119.30
1	A	242	GLU	CA-CB-CG	13.91	141.92	114.10
1	A	242	GLU	CG-CD-OE2	-12.45	89.77	118.40
1	D	310	ARG	CG-CD-NE	12.30	139.06	112.00
1	A	159	ASN	CB-CG-ND2	12.29	134.84	116.40
1	C	402	LYS	N-CA-CB	-11.70	90.61	110.50
1	A	158	LYS	CA-CB-CG	11.49	137.08	114.10
1	A	242	GLU	CB-CG-CD	11.31	131.83	112.60
1	C	171	ASP	OD1-CG-OD2	-11.00	96.50	122.90
1	B	158	LYS	O-C-N	10.66	135.10	122.20
1	B	161	LYS	CG-CD-CE	10.42	135.26	111.30
1	C	398	GLN	OE1-CD-NE2	-10.40	112.20	122.60
1	D	399	GLN	CB-CG-CD	10.37	130.24	112.60
1	B	161	LYS	CB-CG-CD	10.21	134.79	111.30
1	C	391	ASP	CB-CG-OD2	10.18	141.82	118.40
1	D	234	GLU	CG-CD-OE1	-10.16	95.03	118.40
1	D	377	GLU	CG-CD-OE2	10.15	141.74	118.40
1	D	374	ARG	CD-NE-CZ	10.04	138.45	124.40
1	D	377	GLU	OE1-CD-OE2	-9.94	99.04	122.90
1	A	159	ASN	CB-CG-OD1	-9.93	100.94	120.80
1	B	230	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	B	157	ASP	CA-C-N	9.57	136.41	121.19
1	B	157	ASP	C-N-CA	9.57	136.41	121.19
1	A	320	ARG	CG-CD-NE	9.52	132.94	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	399	GLN	OE1-CD-NE2	-9.50	113.10	122.60
1	C	158	LYS	CG-CD-CE	9.50	133.14	111.30
1	C	171	ASP	CB-CG-OD2	9.38	139.99	118.40
1	A	160	GLY	N-CA-C	9.30	135.22	113.18
1	C	402	LYS	CA-CB-CG	9.26	132.61	114.10
1	C	399	GLN	CA-CB-CG	9.25	132.60	114.10
1	D	124	GLN	OE1-CD-NE2	-9.17	113.43	122.60
1	C	401	ASN	CA-C-O	9.16	133.61	120.51
1	D	35	ASP	CB-CG-OD1	-9.03	97.63	118.40
1	D	1	MET	CB-CG-SD	8.93	139.50	112.70
1	D	233	LYS	CG-CD-CE	-8.91	90.80	111.30
1	A	159	ASN	CA-C-N	-8.47	104.82	121.41
1	A	159	ASN	C-N-CA	-8.47	104.82	121.41
1	A	374	ARG	NE-CZ-NH1	-8.24	113.26	121.50
1	C	402	LYS	CB-CG-CD	-8.15	92.55	111.30
1	C	391	ASP	OD1-CG-OD2	-8.15	103.35	122.90
1	D	254	ARG	NH1-CZ-NH2	-8.14	108.72	119.30
1	D	39	GLU	CG-CD-OE2	-8.14	99.69	118.40
1	C	401	ASN	O-C-N	8.01	133.25	122.59
1	D	234	GLU	OE1-CD-OE2	7.86	141.76	122.90
1	D	254	ARG	NE-CZ-NH2	7.76	126.19	119.20
1	C	124	GLN	OE1-CD-NE2	7.75	130.35	122.60
1	A	117	LYS	CD-CE-NZ	7.68	136.47	111.90
1	C	117	LYS	CG-CD-CE	7.55	128.68	111.30
1	A	237	ALA	N-CA-CB	7.49	120.87	110.01
1	C	124	GLN	CG-CD-NE2	-7.49	105.17	116.40
1	C	398	GLN	CG-CD-OE1	-7.36	106.08	120.80
1	B	310	ARG	NE-CZ-NH2	-7.21	112.72	119.20
1	B	249	ASP	CB-CG-OD2	7.09	134.71	118.40
1	D	209	LYS	CD-CE-NZ	6.89	133.95	111.90
1	B	201	LYS	CB-CG-CD	6.88	127.12	111.30
1	D	310	ARG	CD-NE-CZ	6.84	133.97	124.40
1	D	125	LYS	CD-CE-NZ	6.76	133.53	111.90
1	C	399	GLN	CG-CD-NE2	6.66	126.39	116.40
1	C	399	GLN	CB-CG-CD	6.65	123.91	112.60
1	D	233	LYS	CD-CE-NZ	-6.61	90.75	111.90
1	B	177	GLN	CA-C-N	6.51	126.08	121.65
1	B	177	GLN	C-N-CA	6.51	126.08	121.65
1	B	124	GLN	OE1-CD-NE2	-6.47	116.13	122.60
1	A	124	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	D	1	MET	CA-C-O	-6.37	109.97	120.80
1	D	374	ARG	CG-CD-NE	-6.30	98.14	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LYS	CA-CB-CG	6.27	126.64	114.10
1	C	92	LYS	CD-CE-NZ	6.27	131.97	111.90
1	D	146	GLU	CG-CD-OE1	-6.17	104.20	118.40
1	A	374	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	C	158	LYS	CD-CE-NZ	6.10	131.42	111.90
1	A	320	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	D	35	ASP	CA-CB-CG	5.97	118.57	112.60
1	D	1	MET	CB-CA-C	5.82	121.15	110.10
1	C	317	LYS	CD-CE-NZ	5.74	130.28	111.90
1	C	46	GLU	CG-CD-OE1	-5.71	105.27	118.40
1	A	377	GLU	OE1-CD-OE2	-5.65	109.33	122.90
1	B	399	GLN	CG-CD-NE2	-5.56	108.06	116.40
1	D	124	GLN	CG-CD-NE2	5.48	124.62	116.40
1	B	249	ASP	OD1-CG-OD2	-5.38	109.99	122.90
1	C	46	GLU	OE1-CD-OE2	5.33	135.70	122.90
1	B	230	GLN	CG-CD-NE2	5.32	124.38	116.40
1	C	92	LYS	CG-CD-CE	5.28	123.45	111.30
1	D	400	LEU	CA-C-N	5.24	129.81	122.36
1	D	400	LEU	C-N-CA	5.24	129.81	122.36
1	D	46	GLU	CG-CD-OE2	5.23	130.44	118.40
1	C	6	LYS	CB-CG-CD	-5.22	99.30	111.30
1	D	400	LEU	N-CA-C	-5.18	107.26	113.21
1	A	169	GLU	OE1-CD-OE2	-5.09	110.69	122.90
1	C	230	GLN	N-CA-C	5.05	116.87	111.36
1	C	401	ASN	CB-CG-ND2	-5.04	108.84	116.40

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLY	Mainchain,Peptide
1	A	169	GLU	Sidechain
1	A	171	ASP	Sidechain
1	A	242	GLU	Sidechain
1	A	374	ARG	Sidechain
1	A	377	GLU	Sidechain
1	B	158	LYS	Mainchain
1	B	310	ARG	Sidechain
1	B	399	GLN	Sidechain
1	C	124	GLN	Sidechain
1	C	171	ASP	Sidechain
1	C	313	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	146	GLU	Sidechain
1	D	169	GLU	Sidechain
1	D	242	GLU	Sidechain
1	D	254	ARG	Sidechain
1	D	35	ASP	Sidechain
1	D	39	GLU	Sidechain

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	3234	0	3209	26	0
1	B	3242	0	3217	22	0
1	C	3271	0	3250	35	0
1	D	3243	0	3216	33	0
2	A	18	0	24	0	0
2	B	6	0	8	1	0
2	C	18	0	24	0	0
2	D	18	0	24	2	0
3	A	5	0	0	1	0
3	B	30	0	0	2	0
3	C	10	0	0	1	0
3	D	10	0	0	1	0
4	A	1	0	0	0	0
5	A	14	0	20	0	0
5	B	14	0	20	1	0
5	C	21	0	30	1	0
6	A	473	0	0	12	2
6	B	513	0	0	12	2
6	C	445	0	0	8	0
6	D	452	0	0	6	0
All	All	15038	0	13042	108	2

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 (108) 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:A:254:ARG:HD2	6:A:2326:HOH:O	1.50	1.10
1:C:277[B]:MET:HG3	1:D:252[B]:VAL:HG22	1.35	1.06
5:B:1409:PEG:O4	6:B:2512:HOH:O	1.83	0.93
1:C:277[B]:MET:HG3	1:D:252[B]:VAL:CG2	2.07	0.84
3:D:1407:SO4:O1	6:D:2452:HOH:O	1.95	0.84
1:D:11:GLU:OE1	1:D:38:THR:HG21	1.75	0.84
1:C:226:GLU:OE2	6:C:2282:HOH:O	1.95	0.83
1:C:115:ASN:HD22	1:C:115:ASN:H	1.25	0.82
1:B:242:GLU:OE1	6:B:2342:HOH:O	1.98	0.80
1:D:108:ARG:HG3	6:D:2153:HOH:O	1.82	0.80
1:C:209:LYS:NZ	1:C:249:ASP:OD2	2.17	0.77
1:A:242:GLU:OE2	6:A:2312:HOH:O	2.03	0.77
1:A:188:HIS:ND1	6:A:2264:HOH:O	2.12	0.76
1:D:115:ASN:HD22	1:D:115:ASN:H	1.34	0.75
1:C:158:LYS:CG	1:C:158:LYS:CE	2.65	0.74
3:A:1406:SO4:O1	6:A:2470:HOH:O	2.08	0.72
1:B:109:LYS:HE2	6:B:2185:HOH:O	1.90	0.71
1:A:18:THR:HB	1:A:72:ASN:HD21	1.56	0.70
1:D:18:THR:HB	1:D:72:ASN:HD21	1.56	0.69
1:A:109:LYS:HE2	6:A:2176:HOH:O	1.91	0.69
1:C:181:ASN:HD22	1:C:182:THR:H	1.38	0.69
1:B:230:GLN:HG2	6:D:2250:HOH:O	1.93	0.69
1:C:18:THR:HB	1:C:72:ASN:HD21	1.58	0.67
3:B:1406:SO4:O3	6:B:2504:HOH:O	2.10	0.66
1:C:246:THR:CG2	1:C:251[A]:VAL:HG13	2.25	0.66
1:B:108:ARG:HG3	6:B:2177:HOH:O	1.96	0.66
1:B:18:THR:HB	1:B:72:ASN:HD21	1.61	0.65
1:D:308:VAL:HA	2:D:1403:GOL:H2	1.78	0.65
1:C:277[B]:MET:SD	1:D:277[B]:MET:SD	2.94	0.65
1:D:72:ASN:HD22	1:D:73:ALA:H	1.45	0.65
1:B:112:MET:HE3	6:B:2064:HOH:O	1.99	0.63
1:D:374:ARG:CD	1:D:374:ARG:CZ	2.77	0.63
1:B:64:LYS:HD3	1:D:159:ASN:HD21	1.63	0.63
1:B:298:TYR:OH	1:D:159:ASN:ND2	2.32	0.62
1:C:248:ILE:HA	1:C:251[A]:VAL:HG22	1.81	0.62
1:C:252[B]:VAL:HG22	1:D:277[B]:MET:HG3	1.82	0.62
1:C:188:HIS:ND1	6:C:2250:HOH:O	2.05	0.62
1:A:72:ASN:HD22	1:A:73:ALA:H	1.48	0.62
1:C:310:ARG:HD2	6:C:2346:HOH:O	1.99	0.62
1:D:35:ASP:OD1	1:D:35:ASP:CB	2.49	0.60
3:B:1407[B]:SO4:O4	6:B:2506:HOH:O	2.08	0.59
1:C:246:THR:HG23	1:C:251[A]:VAL:HG13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLU:CD	6:A:2313:HOH:O	2.44	0.59
1:D:139:LYS:NZ	6:D:2207:HOH:O	1.88	0.58
1:A:139:LYS:HG2	1:B:168:MET:CE	2.34	0.57
1:A:139:LYS:HG2	1:B:168:MET:HE2	1.84	0.57
1:C:72:ASN:HD22	1:C:73:ALA:H	1.53	0.57
1:C:391:ASP:CG	6:C:2429:HOH:O	2.46	0.57
1:B:28:LYS:NZ	1:B:391:ASP:OD1	2.37	0.56
1:B:65:LYS:HE2	6:B:2112:HOH:O	2.06	0.55
1:B:124:GLN:HG2	6:B:2210:HOH:O	2.06	0.55
1:C:214:LYS:NZ	1:D:90:GLN:OE1	2.39	0.55
1:C:277[B]:MET:CG	1:D:252[B]:VAL:HG22	2.24	0.55
1:A:9:LEU:HD11	1:A:335:ALA:HB1	1.89	0.54
1:D:246:THR:HG23	1:D:251[A]:VAL:HG13	1.89	0.54
1:A:112:MET:HE3	6:A:2057:HOH:O	2.09	0.52
1:C:401:ASN:C	1:C:402:LYS:CA	2.82	0.52
1:B:72:ASN:HD22	1:B:73:ALA:H	1.58	0.51
1:B:139:LYS:NZ	6:B:2241:HOH:O	2.20	0.51
1:A:207:ALA:HB2	1:A:251[A]:VAL:HG21	1.93	0.51
1:D:215:GLN:HG3	6:D:2269:HOH:O	2.11	0.51
1:B:108:ARG:CG	6:B:2177:HOH:O	2.56	0.49
1:D:72:ASN:HD22	1:D:73:ALA:N	2.11	0.49
1:C:361:GLU:HG3	6:C:2397:HOH:O	2.13	0.48
1:D:222:ILE:O	1:D:226:GLU:HG3	2.13	0.48
1:D:246:THR:CG2	1:D:251[B]:VAL:HG23	2.44	0.48
1:C:246:THR:CG2	1:C:251[A]:VAL:CG1	2.92	0.48
1:A:246:THR:HG21	6:A:2326:HOH:O	2.14	0.47
1:A:230:GLN:NE2	6:A:2301:HOH:O	2.47	0.47
1:D:38:THR:HG22	6:D:2049:HOH:O	2.14	0.47
1:D:302:GLU:OE2	2:D:1405:GOL:O3	2.24	0.47
1:D:399:GLN:O	1:D:399:GLN:HG3	2.15	0.47
1:A:244:PHE:HE2	6:A:2326:HOH:O	1.98	0.47
5:C:1409[A]:PEG:H42	1:D:172:GLU:OE1	2.16	0.46
1:B:230:GLN:O	1:D:188:HIS:CE1	2.69	0.46
1:D:246:THR:CG2	1:D:251[A]:VAL:CG1	2.94	0.46
1:C:295:PRO:HG2	1:C:296:TYR:CE2	2.51	0.46
1:D:18:THR:HB	1:D:72:ASN:ND2	2.27	0.45
1:C:252[B]:VAL:HG22	1:D:277[B]:MET:CG	2.44	0.45
1:D:246:THR:CG2	1:D:251[A]:VAL:HG13	2.47	0.45
1:A:246:THR:HG23	1:A:251[A]:VAL:HG23	2.00	0.44
1:A:395:LYS:NZ	1:A:395:LYS:CD	2.81	0.44
1:D:9:LEU:O	1:D:38:THR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:ALA:HB2	1:D:251[A]:VAL:HG11	1.99	0.44
1:A:254:ARG:CD	6:A:2326:HOH:O	2.32	0.44
1:B:65:LYS:NZ	6:B:2108:HOH:O	2.50	0.44
1:B:286:ALA:HB2	2:B:1402:GOL:H11	1.99	0.44
1:A:28:LYS:NZ	1:A:391:ASP:OD1	2.50	0.43
1:A:161:LYS:CA	1:A:162:GLU:N	2.81	0.43
1:C:78:ASN:HB2	3:C:1406:SO4:O2	2.18	0.43
1:A:72:ASN:HD22	1:A:73:ALA:N	2.15	0.42
1:A:246:THR:CG2	1:A:251[A]:VAL:CG2	2.98	0.42
1:A:246:THR:CG2	1:A:251[A]:VAL:HG22	2.49	0.42
1:C:402:LYS:C	6:C:2435:HOH:O	2.63	0.41
1:C:396:ARG:HD3	6:C:2398:HOH:O	2.21	0.41
1:A:125:LYS:NZ	6:A:2204:HOH:O	2.53	0.41
1:C:99[B]:ARG:HD2	1:C:133:ALA:HB1	2.02	0.41
1:C:72:ASN:HD22	1:C:73:ALA:N	2.16	0.41
1:A:277[A]:MET:HE2	1:A:277[A]:MET:HB3	1.89	0.41
1:C:377:GLU:HG2	6:C:2417:HOH:O	2.21	0.41
1:C:31:LEU:N	1:C:32:PRO:CD	2.84	0.40
1:C:355:LEU:HD13	1:C:397:LEU:HD11	2.03	0.40
1:B:1:MET:HE2	1:B:4:GLN:NE2	2.36	0.40
1:B:303:ALA:CB	1:B:328:LEU:HD23	2.51	0.40
1:C:248:ILE:O	1:C:251[A]:VAL:HG22	2.21	0.40
1:C:365:SER:O	1:C:381:ILE:HD12	2.21	0.40
1:A:276:ASP:OD2	1:B:249:ASP:HB2	2.20	0.40
1:C:158:LYS:CE	1:C:158:LYS:CB	2.98	0.40

All (2) 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)
6:A:2372:HOH:O	6:B:2511:HOH:O[1_445]	1.95	0.25
6:A:2086:HOH:O	6:B:2480:HOH:O[1_545]	2.11	0.09

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	404/402 (100%)	390 (96%)	14 (4%)	0	100	100
1	B	405/402 (101%)	393 (97%)	12 (3%)	0	100	100
1	C	408/402 (102%)	396 (97%)	11 (3%)	1 (0%)	43	27
1	D	405/402 (101%)	392 (97%)	13 (3%)	0	100	100
All	All	1622/1608 (101%)	1571 (97%)	50 (3%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	401	ASN

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	345/341 (101%)	341 (99%)	4 (1%)	63	49
1	B	346/341 (102%)	339 (98%)	7 (2%)	48	29
1	C	349/341 (102%)	342 (98%)	7 (2%)	48	29
1	D	346/341 (102%)	339 (98%)	7 (2%)	48	29
All	All	1386/1364 (102%)	1361 (98%)	25 (2%)	51	33

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	PHE
1	A	159	ASN
1	A	308	VAL
1	A	320	ARG
1	B	50	ARG
1	B	137	PHE
1	B	158	LYS

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Mol	Chain	Res	Type
1	B	201	LYS
1	B	251	VAL
1	B	298	TYR
1	B	308	VAL
1	C	115	ASN
1	C	137	PHE
1	C	181	ASN
1	C	308	VAL
1	C	310	ARG
1	C	400	LEU
1	C	402	LYS
1	D	1	MET
1	D	35	ASP
1	D	38	THR
1	D	115	ASN
1	D	137	PHE
1	D	308	VAL
1	D	310	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	215	GLN
1	A	309	GLN
1	A	399	GLN
1	B	4	GLN
1	B	72	ASN
1	B	309	GLN
1	B	399	GLN
1	C	72	ASN
1	C	90	GLN
1	C	115	ASN
1	C	159	ASN
1	C	181	ASN
1	D	72	ASN
1	D	115	ASN
1	D	159	ASN
1	D	230	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 ⓘ

Of 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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	GOL	A	1403	-	5,5,5	0.60	0	5,5,5	1.73	2 (40%)
2	GOL	A	1405	-	5,5,5	0.26	0	5,5,5	0.44	0
3	SO4	B	1407[B]	-	4,4,4	0.36	0	6,6,6	0.57	0
5	PEG	B	1409	-	6,6,6	0.52	0	5,5,5	0.63	0
2	GOL	B	1402	-	5,5,5	0.61	0	5,5,5	0.45	0
2	GOL	C	1404	-	5,5,5	0.56	0	5,5,5	0.59	0
5	PEG	B	1408	-	6,6,6	0.39	0	5,5,5	0.42	0
3	SO4	B	1406	-	4,4,4	0.24	0	6,6,6	0.67	0
2	GOL	C	1403	-	5,5,5	0.33	0	5,5,5	0.54	0
3	SO4	B	1407[A]	-	4,4,4	0.38	0	6,6,6	0.48	0
2	GOL	D	1404	-	5,5,5	0.50	0	5,5,5	0.58	0
3	SO4	C	1407	-	4,4,4	0.29	0	6,6,6	0.60	0
2	GOL	C	1405	-	5,5,5	0.51	0	5,5,5	0.85	0
2	GOL	D	1403	-	5,5,5	0.52	0	5,5,5	1.57	2 (40%)
3	SO4	B	1404	-	4,4,4	0.43	0	6,6,6	0.36	0
2	GOL	A	1404	-	5,5,5	0.73	0	5,5,5	1.46	1 (20%)
5	PEG	C	1409[B]	-	6,6,6	0.53	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	1406	-	4,4,4	0.23	0	6,6,6	0.17	0
3	SO4	D	1407	-	4,4,4	0.28	0	6,6,6	0.40	0
2	GOL	D	1405	-	5,5,5	0.36	0	5,5,5	0.73	0
5	PEG	C	1409[A]	-	6,6,6	0.35	0	5,5,5	0.21	0
3	SO4	B	1403	-	4,4,4	0.31	0	6,6,6	0.37	0
3	SO4	D	1406	-	4,4,4	0.33	0	6,6,6	0.39	0
5	PEG	A	1408[B]	-	6,6,6	0.46	0	5,5,5	0.41	0
3	SO4	B	1405	-	4,4,4	0.35	0	6,6,6	0.43	0
5	PEG	C	1408	-	6,6,6	0.41	0	5,5,5	0.29	0
3	SO4	A	1406	-	4,4,4	0.44	0	6,6,6	1.28	1 (16%)
5	PEG	A	1408[A]	-	6,6,6	0.40	0	5,5,5	0.18	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	GOL	A	1403	-	-	2/4/4/4	-
5	PEG	A	1408[B]	-	-	4/4/4/4	-
2	GOL	A	1405	-	-	4/4/4/4	-
2	GOL	D	1404	-	-	0/4/4/4	-
5	PEG	B	1409	-	-	3/4/4/4	-
2	GOL	C	1405	-	-	3/4/4/4	-
2	GOL	B	1402	-	-	3/4/4/4	-
2	GOL	D	1403	-	-	0/4/4/4	-
5	PEG	C	1408	-	-	1/4/4/4	-
2	GOL	C	1404	-	-	0/4/4/4	-
5	PEG	B	1408	-	-	3/4/4/4	-
5	PEG	C	1409[A]	-	-	3/4/4/4	-
2	GOL	A	1404	-	-	4/4/4/4	-
2	GOL	C	1403	-	-	2/4/4/4	-
5	PEG	C	1409[B]	-	-	2/4/4/4	-
5	PEG	A	1408[A]	-	-	2/4/4/4	-
2	GOL	D	1405	-	-	1/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1403	GOL	O1-C1-C2	-2.77	97.92	110.38
2	A	1403	GOL	O3-C3-C2	-2.51	99.09	110.38
2	A	1404	GOL	O1-C1-C2	2.45	121.42	110.38
3	A	1406	SO4	O3-S-O1	2.19	120.99	109.56
2	D	1403	GOL	O3-C3-C2	-2.10	100.91	110.38
2	D	1403	GOL	C3-C2-C1	2.04	119.30	111.80

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1403	GOL	O1-C1-C2-C3
2	A	1404	GOL	O1-C1-C2-C3
2	A	1404	GOL	C1-C2-C3-O3
2	A	1405	GOL	O1-C1-C2-C3
2	B	1402	GOL	O1-C1-C2-C3
2	C	1403	GOL	C1-C2-C3-O3
5	C	1408	PEG	O2-C3-C4-O4
5	A	1408[B]	PEG	O2-C3-C4-O4
5	B	1409	PEG	O1-C1-C2-O2
5	C	1409[B]	PEG	O1-C1-C2-O2
2	A	1405	GOL	C1-C2-C3-O3
2	C	1405	GOL	O1-C1-C2-C3
2	C	1405	GOL	C1-C2-C3-O3
2	A	1404	GOL	O1-C1-C2-O2
2	A	1405	GOL	O1-C1-C2-O2
2	B	1402	GOL	O1-C1-C2-O2
5	A	1408[B]	PEG	O1-C1-C2-O2
2	A	1404	GOL	O2-C2-C3-O3
2	C	1403	GOL	O2-C2-C3-O3
5	B	1408	PEG	O1-C1-C2-O2
5	B	1408	PEG	O2-C3-C4-O4
5	C	1409[A]	PEG	O2-C3-C4-O4
2	D	1405	GOL	O1-C1-C2-O2
2	A	1405	GOL	O2-C2-C3-O3
5	B	1408	PEG	C1-C2-O2-C3
5	A	1408[B]	PEG	C4-C3-O2-C2
5	A	1408[B]	PEG	C1-C2-O2-C3
5	C	1409[B]	PEG	C1-C2-O2-C3
5	C	1409[A]	PEG	O1-C1-C2-O2
2	A	1403	GOL	O1-C1-C2-O2
5	A	1408[A]	PEG	C4-C3-O2-C2
2	C	1405	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	C	1409[A]	PEG	C1-C2-O2-C3
5	B	1409	PEG	C1-C2-O2-C3
5	A	1408[A]	PEG	O2-C3-C4-O4
2	B	1402	GOL	O2-C2-C3-O3
5	B	1409	PEG	C4-C3-O2-C2

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1407[B]	SO4	1	0
5	B	1409	PEG	1	0
2	B	1402	GOL	1	0
3	B	1406	SO4	1	0
2	D	1403	GOL	1	0
3	C	1406	SO4	1	0
3	D	1407	SO4	1	0
2	D	1405	GOL	1	0
5	C	1409[A]	PEG	1	0
3	A	1406	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	400:LEU	C	401:ASN	N	1.84

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	402/402 (100%)	-0.52	2 (0%) 87 90	3, 15, 23, 31	40 (9%)
1	B	401/402 (99%)	-0.53	3 (0%) 84 88	3, 15, 24, 36	39 (9%)
1	C	402/402 (100%)	-0.45	3 (0%) 84 88	4, 16, 23, 31	51 (12%)
1	D	400/402 (99%)	-0.39	3 (0%) 82 86	7, 17, 26, 32	41 (10%)
All	All	1605/1608 (99%)	-0.47	11 (0%) 84 88	3, 16, 25, 36	171 (10%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	402	LYS	8.5
1	C	401	ASN	3.9
1	C	400	LEU	3.4
1	B	158	LYS	3.2
1	B	401	ASN	2.5
1	D	400	LEU	2.5
1	D	1	MET	2.4
1	A	159	ASN	2.4
1	A	1	MET	2.2
1	D	147	ALA	2.1
1	B	1	MET	2.1

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

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
5	PEG	B	1409	7/7	0.70	0.19	45,47,49,51	0
2	GOL	C	1405	6/6	0.72	0.16	42,45,48,50	0
2	GOL	A	1405	6/6	0.72	0.16	49,51,53,55	0
2	GOL	D	1405	6/6	0.76	0.16	40,43,44,46	2
3	SO4	B	1405	5/5	0.78	0.17	31,33,36,38	5
2	GOL	D	1403	6/6	0.78	0.17	30,35,38,41	0
2	GOL	C	1403	6/6	0.82	0.12	35,37,39,40	0
5	PEG	C	1409[A]	7/7	0.82	0.15	15,24,28,29	7
5	PEG	C	1409[B]	7/7	0.82	0.15	36,37,39,39	7
2	GOL	D	1404	6/6	0.83	0.12	32,35,37,39	0
2	GOL	A	1403	6/6	0.83	0.12	28,32,34,35	0
2	GOL	B	1402	6/6	0.87	0.10	27,31,33,37	0
2	GOL	C	1404	6/6	0.89	0.10	22,32,34,37	0
3	SO4	B	1407[A]	5/5	0.89	0.10	17,18,24,25	5
3	SO4	B	1407[B]	5/5	0.89	0.10	23,24,26,29	5
5	PEG	B	1408	7/7	0.90	0.11	39,40,42,44	0
3	SO4	B	1404	5/5	0.90	0.10	52,53,54,55	1
5	PEG	C	1408	7/7	0.92	0.09	38,38,39,41	0
5	PEG	A	1408[A]	7/7	0.92	0.08	20,21,22,23	7
5	PEG	A	1408[B]	7/7	0.92	0.08	26,27,30,31	7
3	SO4	C	1407	5/5	0.93	0.09	27,28,35,37	5
3	SO4	D	1407	5/5	0.94	0.08	35,35,39,41	5
3	SO4	A	1406	5/5	0.94	0.10	34,34,40,40	1
3	SO4	C	1406	5/5	0.94	0.08	27,29,32,32	5
2	GOL	A	1404	6/6	0.94	0.09	20,24,28,32	0
3	SO4	B	1406	5/5	0.95	0.08	26,28,31,34	5
3	SO4	D	1406	5/5	0.95	0.10	36,37,38,40	4
4	MG	A	1407	1/1	0.96	0.12	40,40,40,40	0
3	SO4	B	1403	5/5	0.97	0.08	35,38,39,40	0

6.5 Other polymers

There are no such residues in this entry.