Full wwPDB X-ray Structure Validation Report (i)

Dec 5, 2023 – 02:36 am GMT

PDB ID	:	2UXQ
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 (i) 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 (i)) were used in the production of this report:

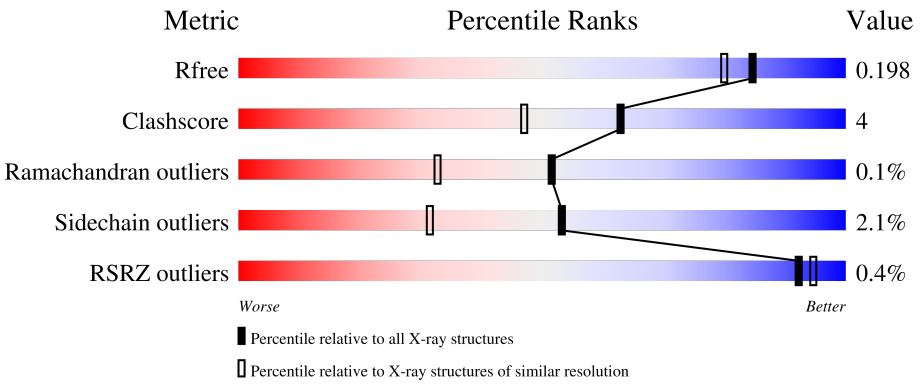
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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 <=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	90% 7% •
1	B	402	91% 7% •
1	C	402	% 85% 12% • •
1	D	402	86% 11% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	D	1405	-	-	X	-

2 Entry composition (i)

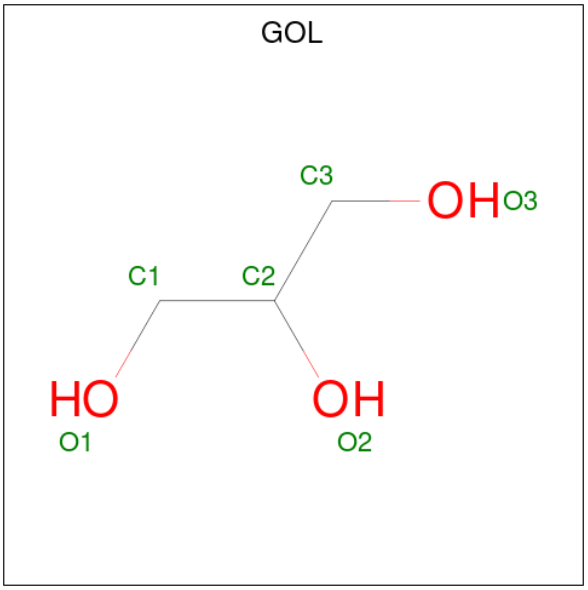
There are 6 unique types of molecules in this entry. The entry contains 15038 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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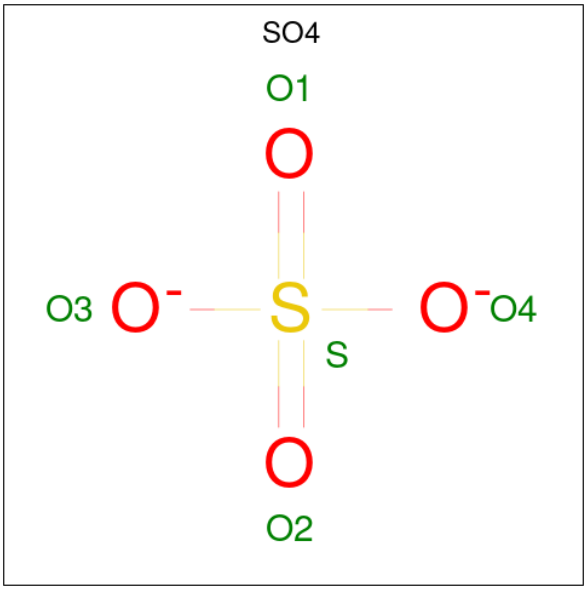
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	D	1	6	3	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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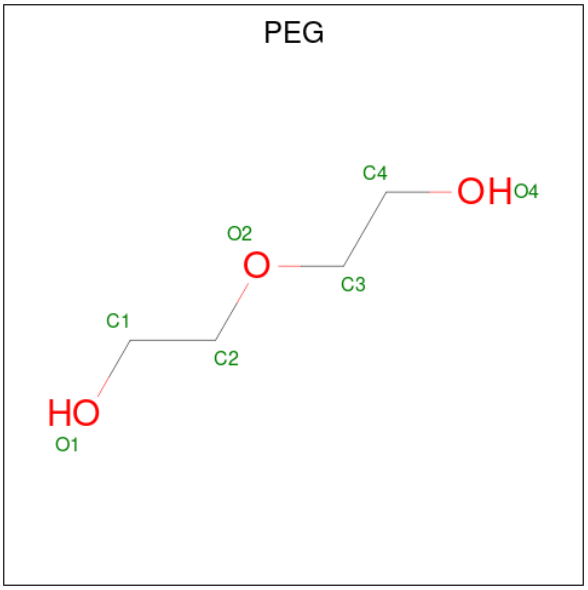
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 10 8 2	0	1
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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
			Total	C	O		
5	B	1	7	4	3	0	0
			Total	C	O		
5	B	1	7	4	3	0	0
			Total	C	O		
5	C	1	7	4	3	0	0
			Total	C	O		
5	C	1	14	8	6	0	1

- Molecule 6 is water.

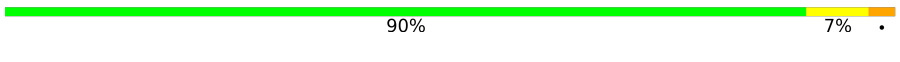
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	473	473	473	0	0
			Total	O		
6	B	513	513	513	0	0
			Total	O		
6	C	445	445	445	0	0
			Total	O		
6	D	452	452	452	0	0

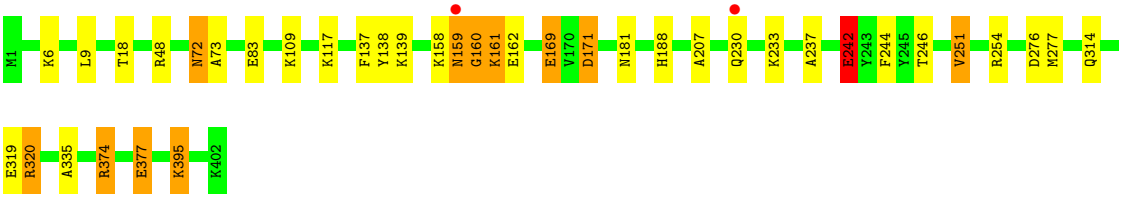
3 Residue-property plots (i)

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

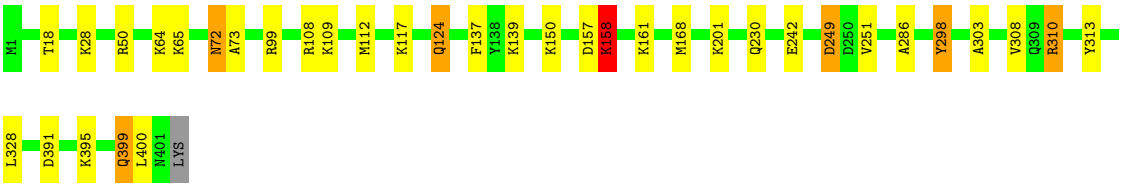
Chain A:





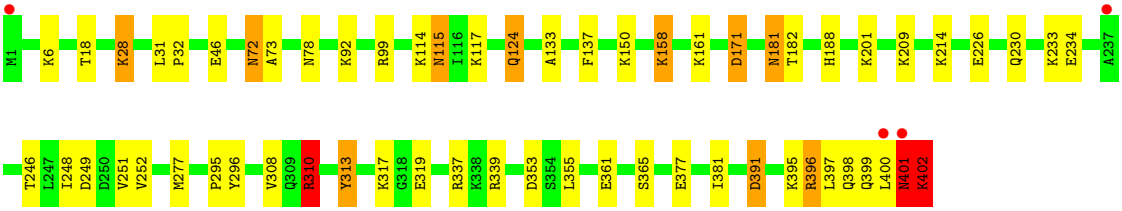
• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE

Chain B:



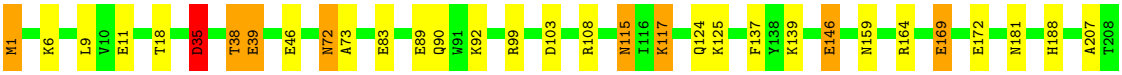
• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE

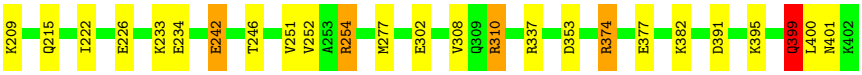
Chain C:



• Molecule 1: ISOCITRATE DEHYDROGENASE NATIVE

Chain D:




K209
Q215
I222
E226
K233
E234
E242
T246
V251
V252
A253
R254
M277
E302
V308
Q309
R310
R337
D353
R374
E377
K382
D391
K395
Q399
L400
N401
K402

4 Data and refinement statistics (i)

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 53.21 – 1.75	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-1.75) 86.3 (53.21-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (2.00%)	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)	0.37 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PEG, SO4, GOL, MG

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	1.59	21/3299 (0.6%)	1.74	33/4455 (0.7%)
1	B	1.40	14/3307 (0.4%)	1.06	14/4465 (0.3%)
1	C	1.46	28/3336 (0.8%)	1.66	39/4504 (0.9%)
1	D	1.80	25/3308 (0.8%)	1.63	36/4468 (0.8%)
All	All	1.57	88/13250 (0.7%)	1.55	122/17892 (0.7%)

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 (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	377	GLU	CD-OE2	-36.05	0.85	1.25
1	D	399	GLN	CG-CD	-34.22	0.72	1.51
1	D	169	GLU	CD-OE2	-32.34	0.90	1.25
1	A	242	GLU	CG-CD	31.39	1.99	1.51
1	A	395	LYS	CE-NZ	30.79	2.26	1.49
1	B	158	LYS	CA-C	30.59	2.32	1.52
1	A	169	GLU	CD-OE2	-29.66	0.93	1.25
1	D	310	ARG	CD-NE	-28.44	0.98	1.46
1	B	310	ARG	CD-NE	-28.21	0.98	1.46
1	C	28	LYS	CE-NZ	-27.69	0.79	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	GLU	CD-OE2	26.98	1.55	1.25
1	D	35	ASP	CG-OD1	25.62	1.84	1.25
1	C	46	GLU	CD-OE1	23.87	1.51	1.25
1	B	158	LYS	C-O	-23.36	0.79	1.23
1	D	400	LEU	C-N	21.89	1.84	1.34
1	A	161	LYS	CB-CG	-21.08	0.95	1.52
1	A	161	LYS	CA-C	20.18	2.05	1.52
1	C	391	ASP	CG-OD1	19.95	1.71	1.25
1	B	310	ARG	NE-CZ	18.41	1.56	1.33
1	D	146	GLU	CD-OE1	18.24	1.45	1.25
1	C	28	LYS	CD-CE	16.82	1.93	1.51
1	C	158	LYS	CD-CE	-16.30	1.10	1.51
1	A	233	LYS	CE-NZ	-15.67	1.09	1.49
1	A	160	GLY	CA-C	15.43	1.76	1.51
1	C	234	GLU	CB-CG	15.34	1.81	1.52
1	C	402	LYS	N-CA	15.09	1.76	1.46
1	C	402	LYS	C-O	14.94	1.51	1.23
1	A	117	LYS	CD-CE	-14.79	1.14	1.51
1	B	395	LYS	CD-CE	-13.29	1.18	1.51
1	A	160	GLY	N-CA	13.28	1.66	1.46
1	A	320	ARG	CZ-NH2	-13.14	1.16	1.33
1	B	310	ARG	CZ-NH1	-13.09	1.16	1.33
1	D	374	ARG	CD-NE	12.82	1.68	1.46
1	B	158	LYS	N-CA	12.71	1.71	1.46
1	D	209	LYS	CE-NZ	-12.70	1.17	1.49
1	C	395	LYS	CE-NZ	12.67	1.80	1.49
1	B	399	GLN	CD-NE2	-12.60	1.01	1.32
1	D	395	LYS	CG-CD	12.59	1.95	1.52
1	D	6	LYS	CG-CD	-12.50	1.09	1.52
1	C	92	LYS	CD-CE	-12.01	1.21	1.51
1	D	46	GLU	CD-OE2	11.96	1.38	1.25
1	D	89	GLU	CD-OE2	-11.90	1.12	1.25
1	C	117	LYS	CD-CE	-11.79	1.21	1.51
1	D	242	GLU	CD-OE1	11.56	1.38	1.25
1	A	395	LYS	CD-CE	-11.33	1.23	1.51
1	A	161	LYS	C-O	11.08	1.44	1.23
1	D	233	LYS	CD-CE	10.53	1.77	1.51
1	C	402	LYS	CB-CG	10.42	1.80	1.52
1	B	201	LYS	CG-CD	-10.35	1.17	1.52
1	C	230	GLN	CD-NE2	10.34	1.58	1.32
1	A	158	LYS	CB-CG	-10.24	1.25	1.52
1	C	319	GLU	CD-OE2	9.86	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	GLN	CD-OE1	-9.80	1.02	1.24
1	A	374	ARG	CZ-NH1	-9.38	1.20	1.33
1	B	150	LYS	CE-NZ	9.18	1.72	1.49
1	C	124	GLN	CD-OE1	-9.17	1.03	1.24
1	C	391	ASP	CG-OD2	-9.05	1.04	1.25
1	D	125	LYS	CE-NZ	-8.94	1.26	1.49
1	C	150	LYS	CE-NZ	8.93	1.71	1.49
1	C	402	LYS	CA-CB	8.91	1.73	1.53
1	A	314	GLN	CD-NE2	8.53	1.54	1.32
1	D	124	GLN	CD-NE2	8.50	1.54	1.32
1	B	400	LEU	CG-CD2	8.23	1.82	1.51
1	C	313	TYR	CG-CD2	7.81	1.49	1.39
1	D	254	ARG	CZ-NH2	-7.75	1.23	1.33
1	D	382	LYS	CE-NZ	7.75	1.68	1.49
1	C	158	LYS	CG-CD	7.34	1.77	1.52
1	A	6	LYS	CD-CE	7.33	1.69	1.51
1	B	117	LYS	CE-NZ	-7.29	1.30	1.49
1	C	171	ASP	CG-OD2	-7.14	1.08	1.25
1	C	233	LYS	CD-CE	7.14	1.69	1.51
1	D	39	GLU	CG-CD	6.88	1.62	1.51
1	A	320	ARG	CZ-NH1	-6.81	1.24	1.33
1	C	317	LYS	CE-NZ	6.63	1.65	1.49
1	C	401	ASN	C-O	-6.59	1.10	1.23
1	A	251[A]	VAL	CB-CG2	-6.53	1.39	1.52
1	A	251[B]	VAL	CB-CG2	-6.53	1.39	1.52
1	D	164	ARG	CZ-NH2	6.51	1.41	1.33
1	D	39	GLU	CB-CG	6.38	1.64	1.52
1	B	124	GLN	CD-NE2	6.09	1.48	1.32
1	A	319	GLU	CG-CD	5.81	1.60	1.51
1	C	114	LYS	CG-CD	5.79	1.72	1.52
1	C	201	LYS	CG-CD	-5.65	1.33	1.52
1	C	161	LYS	CB-CG	-5.58	1.37	1.52
1	A	138	TYR	CD2-CE2	5.19	1.47	1.39
1	D	401	ASN	N-CA	5.08	1.56	1.46
1	D	92	LYS	CE-NZ	5.05	1.61	1.49
1	C	6	LYS	CB-CG	-5.02	1.39	1.52

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	ARG	NE-CZ-NH1	-66.17	87.22	120.30
1	D	374	ARG	NE-CZ-NH2	-47.27	96.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	374	ARG	NE-CZ-NH1	45.70	143.15	120.30
1	C	310	ARG	NE-CZ-NH2	-45.58	97.51	120.30
1	C	310	ARG	NE-CZ-NH1	43.81	142.21	120.30
1	A	160	GLY	CA-C-O	-33.80	59.76	120.60
1	A	242	GLU	CG-CD-OE1	-27.30	63.69	118.30
1	A	320	ARG	CD-NE-CZ	27.16	161.62	123.60
1	C	391	ASP	CB-CG-OD2	26.13	141.82	118.30
1	A	320	ARG	NH1-CZ-NH2	26.01	148.01	119.40
1	C	310	ARG	CD-NE-CZ	-25.95	87.28	123.60
1	D	164	ARG	NE-CZ-NH2	25.05	132.83	120.30
1	C	171	ASP	CB-CG-OD2	24.09	139.99	118.30
1	D	35	ASP	CB-CG-OD1	-22.97	97.63	118.30
1	C	398	GLN	CB-CG-CD	21.04	166.31	111.60
1	D	377	GLU	OE1-CD-OE2	-20.22	99.04	123.30
1	B	158	LYS	CA-C-N	-19.49	74.32	117.20
1	B	249	ASP	CB-CG-OD2	18.24	134.71	118.30
1	C	402	LYS	N-CA-C	-17.84	62.82	111.00
1	D	400	LEU	O-C-N	-17.54	94.64	122.70
1	B	310	ARG	CG-CD-NE	17.12	147.76	111.80
1	D	164	ARG	NH1-CZ-NH2	-16.54	101.21	119.40
1	A	161	LYS	N-CA-C	-15.66	68.72	111.00
1	D	234	GLU	OE1-CD-OE2	15.39	141.76	123.30
1	B	310	ARG	NE-CZ-NH2	-15.17	112.72	120.30
1	A	242	GLU	CG-CD-OE2	-14.26	89.77	118.30
1	C	402	LYS	CA-C-O	-14.17	90.35	120.10
1	C	171	ASP	OD1-CG-OD2	-14.11	96.50	123.30
1	A	374	ARG	NE-CZ-NH1	-14.07	113.26	120.30
1	C	158	LYS	CB-CG-CD	-13.81	75.68	111.60
1	B	158	LYS	CA-C-O	-13.15	92.49	120.10
1	D	310	ARG	CG-CD-NE	12.98	139.06	111.80
1	A	242	GLU	CA-CB-CG	12.96	141.92	113.40
1	A	117	LYS	CG-CD-CE	12.63	149.79	111.90
1	C	401	ASN	CA-C-N	-12.34	90.05	117.20
1	D	254	ARG	NE-CZ-NH2	11.78	126.19	120.30
1	D	377	GLU	CG-CD-OE2	11.72	141.74	118.30
1	A	377	GLU	OE1-CD-OE2	-11.64	109.33	123.30
1	D	234	GLU	CG-CD-OE1	-11.63	95.03	118.30
1	A	159	ASN	CA-CB-CG	11.22	138.08	113.40
1	C	402	LYS	N-CA-CB	-11.11	90.61	110.60
1	A	117	LYS	CD-CE-NZ	10.77	136.47	111.70
1	A	158	LYS	CA-CB-CG	10.76	137.08	113.40
1	D	374	ARG	CD-NE-CZ	10.61	138.45	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169	GLU	OE1-CD-OE2	-10.51	110.69	123.30
1	C	391	ASP	OD1-CG-OD2	-10.50	103.35	123.30
1	C	46	GLU	OE1-CD-OE2	10.34	135.70	123.30
1	A	159	ASN	CB-CG-OD1	-10.33	100.94	121.60
1	A	320	ARG	CG-CD-NE	10.07	132.94	111.80
1	C	230	GLN	CG-CD-NE2	9.84	140.32	116.70
1	D	46	GLU	OE1-CD-OE2	-9.83	111.51	123.30
1	D	254	ARG	NH1-CZ-NH2	-9.71	108.72	119.40
1	D	209	LYS	CD-CE-NZ	9.67	133.95	111.70
1	C	398	GLN	CG-CD-NE2	9.49	139.49	116.70
1	D	125	LYS	CD-CE-NZ	9.49	133.53	111.70
1	D	39	GLU	CG-CD-OE2	-9.31	99.69	118.30
1	D	233	LYS	CD-CE-NZ	-9.11	90.75	111.70
1	D	1	MET	CB-CG-SD	9.03	139.50	112.40
1	B	161	LYS	CB-CG-CD	8.92	134.79	111.60
1	A	374	ARG	NE-CZ-NH2	8.91	124.75	120.30
1	A	160	GLY	N-CA-C	8.85	135.22	113.10
1	C	92	LYS	CD-CE-NZ	8.81	131.97	111.70
1	A	320	ARG	NE-CZ-NH2	8.75	124.67	120.30
1	C	402	LYS	CA-CB-CG	8.73	132.61	113.40
1	C	399	GLN	CA-CB-CG	8.73	132.60	113.40
1	C	158	LYS	CD-CE-NZ	8.57	131.42	111.70
1	D	146	GLU	OE1-CD-OE2	-8.54	113.05	123.30
1	C	319	GLU	OE1-CD-OE2	-8.37	113.26	123.30
1	C	230	GLN	OE1-CD-NE2	-8.33	102.75	121.90
1	A	159	ASN	C-N-CA	-8.32	104.82	122.30
1	C	317	LYS	CD-CE-NZ	8.08	130.28	111.70
1	D	242	GLU	OE1-CD-OE2	-7.97	113.73	123.30
1	B	161	LYS	CG-CD-CE	7.79	135.26	111.90
1	C	398	GLN	CG-CD-OE1	-7.76	106.08	121.60
1	B	158	LYS	O-C-N	7.75	135.10	122.70
1	A	237	ALA	N-CA-CB	7.69	120.87	110.10
1	A	159	ASN	CB-CG-ND2	7.56	134.84	116.70
1	D	310	ARG	CD-NE-CZ	7.41	133.97	123.60
1	C	402	LYS	CB-CG-CD	-7.33	92.55	111.60
1	D	399	GLN	CB-CG-CD	7.17	130.24	111.60
1	C	158	LYS	CG-CD-CE	7.08	133.14	111.90
1	D	146	GLU	CG-CD-OE1	-7.05	104.20	118.30
1	D	164	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	233	LYS	CG-CD-CE	-7.03	90.80	111.90
1	B	249	ASP	OD1-CG-OD2	-7.00	109.99	123.30
1	A	277[A]	MET	CG-SD-CE	-7.00	89.00	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277[B]	MET	CG-SD-CE	-7.00	89.00	100.20
1	A	233	LYS	CD-CE-NZ	6.72	127.16	111.70
1	C	401	ASN	O-C-N	6.59	133.25	122.70
1	C	117	LYS	CD-CE-NZ	6.54	126.73	111.70
1	A	242	GLU	CB-CG-CD	6.53	131.83	114.20
1	A	171	ASP	OD1-CG-OD2	-6.53	110.90	123.30
1	C	46	GLU	CG-CD-OE1	-6.51	105.27	118.30
1	D	374	ARG	CG-CD-NE	-6.51	98.14	111.80
1	C	339	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	48	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	C	401	ASN	CA-C-O	6.43	133.61	120.10
1	B	313	TYR	CZ-CE2-CD2	-6.23	114.20	119.80
1	B	399	GLN	OE1-CD-NE2	-6.21	107.62	121.90
1	A	48	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	D	46	GLU	CG-CD-OE2	6.07	130.44	118.30
1	A	83	GLU	OE1-CD-OE2	-6.02	116.08	123.30
1	A	161	LYS	CA-CB-CG	6.02	126.64	113.40
1	B	201	LYS	CB-CG-CD	5.97	127.12	111.60
1	D	117	LYS	CD-CE-NZ	5.94	125.36	111.70
1	A	171	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	157	ASP	C-N-CA	5.88	136.41	121.70
1	C	171	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	C	117	LYS	CG-CD-CE	5.59	128.68	111.90
1	C	391	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	D	103	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	1	MET	CB-CA-C	5.37	121.15	110.40
1	D	337	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	D	391[A]	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	391[B]	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	353	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	337	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	C	124	GLN	CG-CD-OE1	-5.13	111.33	121.60
1	C	150	LYS	CD-CE-NZ	-5.12	99.92	111.70
1	B	310	ARG	NH1-CZ-NH2	5.04	124.94	119.40
1	D	353	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	396	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLY	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
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
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 (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	3234	0	3209	23	0
1	B	3242	0	3217	23	0
1	C	3271	0	3250	35	0
1	D	3243	0	3216	37	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	5	0
3	A	5	0	0	1	0
3	B	30	0	0	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	473	0	0	10	2
6	B	513	0	0	12	2
6	C	445	0	0	7	0
6	D	452	0	0	7	0
All	All	15038	0	13042	109	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 (109) 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:D:99[A]:ARG:HH12	2:D:1405:GOL:H12	1.13	1.06
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:28:LYS:CD	1:C:28:LYS:NZ	2.34	0.89
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:D:99[A]:ARG:NH1	2:D:1405:GOL:H12	1.93	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:B:112:MET:HE3	6:B:2064:HOH:O	1.94	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99[A]:ARG:HH12	2:D:1405:GOL:C1	2.00	0.65
1:D:72:ASN:HD22	1:D:73:ALA:H	1.45	0.65
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
1:B:99[B]:ARG:NH1	3:B:1405:SO4:O3	2.30	0.59
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
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:C:72:ASN:HD22	1:C:73:ALA:H	1.53	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:A:242:GLU:CD	6:A:2313:HOH:O	2.44	0.54
1:A:139:LYS:HG2	1:B:168:MET:HE2	1.88	0.54
1:D:246:THR:HG23	1:D:251[A]:VAL:HG13	1.89	0.54
1:C:391:ASP:CG	6:C:2429:HOH:O	2.46	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:ASN:C	1:C:402:LYS:CA	2.82	0.47
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
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: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:D:117:LYS:NZ	6:D:2173:HOH:O	2.51	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:A:139:LYS:HG2	1:B:168:MET:HE1	2.01	0.42
1:C:396:ARG:HD3	6:C:2398:HOH:O	2.21	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: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: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%)	47	29
1	D	405/402 (101%)	392 (97%)	13 (3%)	0	100	100
All	All	1622/1608 (101%)	1571 (97%)	50 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	401	ASN

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	345/341 (101%)	340 (99%)	5 (1%)	67	52
1	B	346/341 (102%)	339 (98%)	7 (2%)	55	34
1	C	349/341 (102%)	341 (98%)	8 (2%)	50	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	346/341 (102%)	337 (97%)	9 (3%)	46	23
All	All	1386/1364 (102%)	1357 (98%)	29 (2%)	53	31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	137	PHE
1	A	159	ASN
1	A	181	ASN
1	A	320	ARG
1	B	50	ARG
1	B	72	ASN
1	B	137	PHE
1	B	158	LYS
1	B	251	VAL
1	B	298	TYR
1	B	308	VAL
1	C	72	ASN
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	72	ASN
1	D	115	ASN
1	D	137	PHE
1	D	181	ASN
1	D	310	ARG
1	D	399	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	309	GLN

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Mol	Chain	Res	Type
1	B	72	ASN
1	B	200	GLN
1	B	401	ASN
1	C	37	GLN
1	C	72	ASN
1	C	90	GLN
1	C	115	ASN
1	C	181	ASN
1	D	72	ASN
1	D	115	ASN
1	D	159	ASN
1	D	177	GLN
1	D	200	GLN
1	D	309	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	1404	-	5,5,5	0.53	0	5,5,5	0.58	0
5	PEG	C	1408	-	6,6,6	0.40	0	5,5,5	0.30	0
2	GOL	D	1403	-	5,5,5	0.50	0	5,5,5	1.48	0
3	SO4	A	1406	-	4,4,4	0.36	0	6,6,6	1.29	1 (16%)
2	GOL	D	1405	-	5,5,5	0.35	0	5,5,5	0.68	0
3	SO4	B	1403	-	4,4,4	0.24	0	6,6,6	0.38	0
5	PEG	B	1409	-	6,6,6	0.52	0	5,5,5	0.63	0
2	GOL	A	1405	-	5,5,5	0.26	0	5,5,5	0.42	0
5	PEG	C	1409[A]	-	6,6,6	0.34	0	5,5,5	0.20	0
5	PEG	A	1408[B]	-	6,6,6	0.45	0	5,5,5	0.42	0
5	PEG	B	1408	-	6,6,6	0.38	0	5,5,5	0.43	0
3	SO4	C	1406	-	4,4,4	0.32	0	6,6,6	0.15	0
2	GOL	B	1402	-	5,5,5	0.58	0	5,5,5	0.44	0
3	SO4	D	1406	-	4,4,4	0.23	0	6,6,6	0.36	0
2	GOL	C	1403	-	5,5,5	0.32	0	5,5,5	0.50	0
3	SO4	B	1407[A]	-	4,4,4	0.28	0	6,6,6	0.54	0
3	SO4	B	1406	-	4,4,4	0.23	0	6,6,6	0.75	0
2	GOL	A	1404	-	5,5,5	0.69	0	5,5,5	1.40	1 (20%)
3	SO4	C	1407	-	4,4,4	0.21	0	6,6,6	0.66	0
5	PEG	C	1409[B]	-	6,6,6	0.52	0	5,5,5	0.23	0
3	SO4	B	1405	-	4,4,4	0.25	0	6,6,6	0.41	0
3	SO4	D	1407	-	4,4,4	0.18	0	6,6,6	0.40	0
3	SO4	B	1404	-	4,4,4	0.32	0	6,6,6	0.40	0
2	GOL	A	1403	-	5,5,5	0.57	0	5,5,5	1.60	2 (40%)
5	PEG	A	1408[A]	-	6,6,6	0.40	0	5,5,5	0.18	0
2	GOL	D	1404	-	5,5,5	0.49	0	5,5,5	0.54	0
3	SO4	B	1407[B]	-	4,4,4	0.26	0	6,6,6	0.62	0
2	GOL	C	1405	-	5,5,5	0.48	0	5,5,5	0.82	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	C	1404	-	-	0/4/4/4	-
5	PEG	C	1408	-	-	1/4/4/4	-
2	GOL	D	1403	-	-	0/4/4/4	-
5	PEG	A	1408[B]	-	-	4/4/4/4	-
5	PEG	A	1408[A]	-	-	2/4/4/4	-
5	PEG	B	1408	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1402	-	-	3/4/4/4	-
2	GOL	A	1404	-	-	4/4/4/4	-
2	GOL	D	1405	-	-	1/4/4/4	-
5	PEG	C	1409[B]	-	-	2/4/4/4	-
5	PEG	B	1409	-	-	3/4/4/4	-
5	PEG	C	1409[A]	-	-	3/4/4/4	-
2	GOL	A	1405	-	-	4/4/4/4	-
2	GOL	D	1404	-	-	0/4/4/4	-
2	GOL	A	1403	-	-	2/4/4/4	-
2	GOL	C	1403	-	-	2/4/4/4	-
2	GOL	C	1405	-	-	3/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1403	GOL	O1-C1-C2	-2.56	97.92	110.20
2	A	1404	GOL	O1-C1-C2	2.34	121.42	110.20
2	A	1403	GOL	O3-C3-C2	-2.32	99.09	110.20
3	A	1406	SO4	O3-S-O1	2.24	120.99	109.31

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	C	1409[B]	PEG	O1-C1-C2-O2
5	B	1409	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

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

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1403	GOL	1	0
3	A	1406	SO4	1	0
2	D	1405	GOL	4	0
5	B	1409	PEG	1	0
5	C	1409[A]	PEG	1	0
3	C	1406	SO4	1	0
2	B	1402	GOL	1	0
3	B	1406	SO4	1	0
3	B	1405	SO4	1	0
3	D	1407	SO4	1	0
3	B	1407[B]	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%)	-0.31	2 (0%) 91 93	9, 16, 25, 38	36 (8%)
1	B	401/402 (99%)	-0.40	0 100 100	10, 15, 25, 40	34 (8%)
1	C	402/402 (100%)	-0.32	4 (0%) 82 87	10, 17, 26, 45	44 (10%)
1	D	400/402 (99%)	-0.28	0 100 100	11, 18, 28, 34	37 (9%)
All	All	1605/1608 (99%)	-0.33	6 (0%) 92 94	9, 16, 26, 45	151 (9%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ASN	3.3
1	C	400	LEU	3.3
1	C	401	ASN	3.1
1	C	1	MET	2.4
1	A	230	GLN	2.2
1	C	237	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 monosaccharides 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
2	GOL	C	1405	6/6	0.69	0.18	42,45,48,50	0
5	PEG	B	1409	7/7	0.69	0.23	45,47,49,51	0
2	GOL	D	1405	6/6	0.80	0.16	40,43,44,46	2
2	GOL	D	1403	6/6	0.83	0.18	30,35,38,41	0
2	GOL	A	1405	6/6	0.84	0.21	49,51,53,55	0
3	SO4	B	1405	5/5	0.85	0.23	31,33,36,38	5
5	PEG	C	1409[A]	7/7	0.86	0.45	15,24,28,29	7
5	PEG	C	1409[B]	7/7	0.86	0.45	36,37,39,39	7
2	GOL	C	1403	6/6	0.87	0.10	35,37,39,40	0
2	GOL	C	1404	6/6	0.88	0.13	22,32,34,37	0
2	GOL	A	1403	6/6	0.88	0.16	28,32,34,35	0
2	GOL	D	1404	6/6	0.89	0.11	32,35,37,39	0
5	PEG	B	1408	7/7	0.90	0.14	39,40,42,44	0
2	GOL	B	1402	6/6	0.90	0.09	27,31,33,37	0
5	PEG	C	1408	7/7	0.91	0.10	38,38,39,41	0
2	GOL	A	1404	6/6	0.93	0.10	20,24,28,32	0
5	PEG	A	1408[B]	7/7	0.94	0.17	26,27,30,31	7
5	PEG	A	1408[A]	7/7	0.94	0.17	20,21,22,23	7
3	SO4	A	1406	5/5	0.96	0.12	34,34,40,40	1
3	SO4	B	1407[A]	5/5	0.96	0.11	17,18,24,25	5
3	SO4	B	1407[B]	5/5	0.96	0.11	23,24,26,29	5
3	SO4	C	1406	5/5	0.96	0.11	27,29,32,32	5
3	SO4	C	1407	5/5	0.96	0.13	27,28,35,37	5
3	SO4	B	1404	5/5	0.96	0.10	52,53,54,55	1
3	SO4	D	1407	5/5	0.97	0.09	35,35,39,41	5
3	SO4	D	1406	5/5	0.97	0.08	36,37,38,40	4
4	MG	A	1407	1/1	0.98	0.08	40,40,40,40	0
3	SO4	B	1406	5/5	0.98	0.10	26,28,31,34	5
3	SO4	B	1403	5/5	0.99	0.09	35,38,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.