



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:54 AM UTC

PDB ID : 8OON / pdb_00008oon
Title : Glutamine synthetase from Methanothermococcus thermolithotrophicus at a resolution of 2.43 Å
Authors : Mueller, M.-C.; Lemaire, O.N.; Wagner, T.
Deposited on : 2023-04-05
Resolution : 2.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

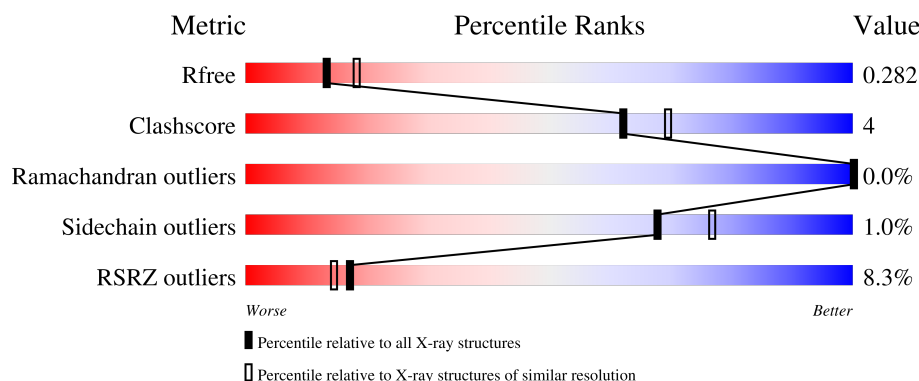
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	448	10% 88% 11% .
1	B	448	10% 87% 11% ..
1	C	448	9% 92% 7% .
1	D	448	8% 89% 9% .
1	E	448	7% 87% 12% .

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Mol	Chain	Length	Quality of chain
1	F	448	5% 92% 7%

2 Entry composition [i](#)

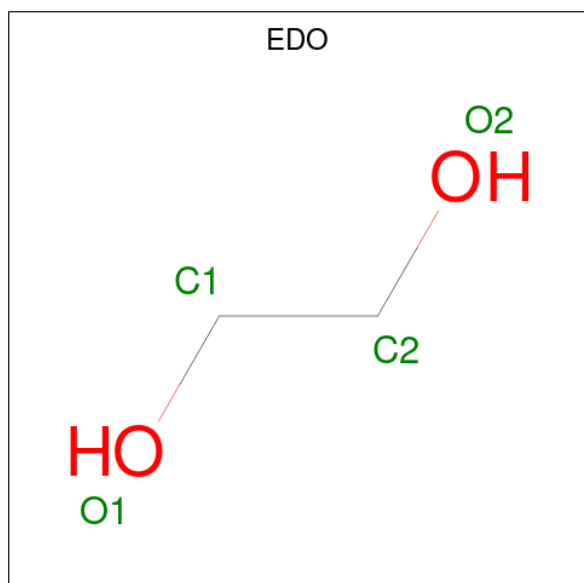
There are 5 unique types of molecules in this entry. The entry contains 21529 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase from *Methanothermococcus thermolithotrophicus*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	2	0
			3517	2256	583	662	16			
1	B	444	Total	C	N	O	S	0	1	0
			3513	2251	584	662	16			
1	C	443	Total	C	N	O	S	0	0	0
			3505	2247	582	660	16			
1	D	443	Total	C	N	O	S	0	1	0
			3512	2254	582	659	17			
1	E	444	Total	C	N	O	S	0	2	0
			3524	2262	584	661	17			
1	F	445	Total	C	N	O	S	0	0	0
			3511	2248	584	663	16			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		
4	E	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	43	Total	O	0	0
			43	43		
5	C	43	Total	O	0	0
			43	43		
5	D	45	Total	O	0	0
			45	45		
5	E	52	Total	O	0	0
			52	52		

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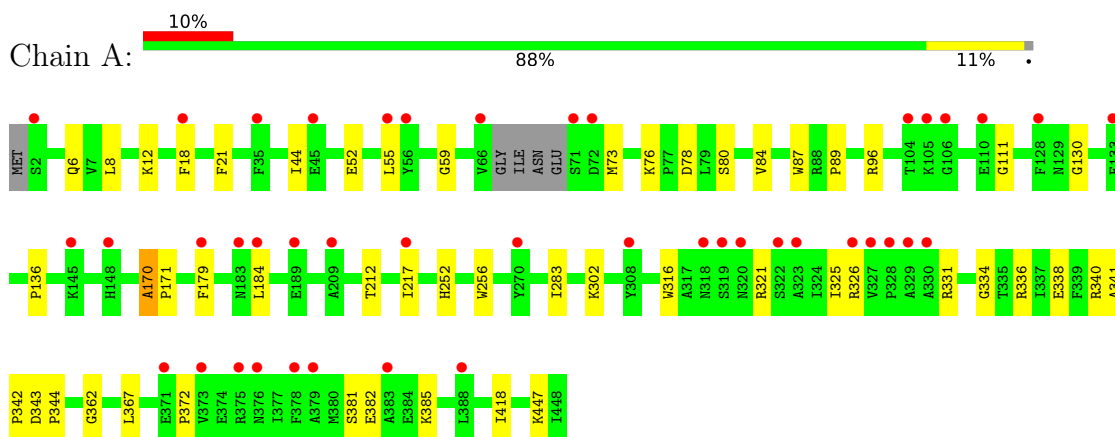
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	57	Total	O	0	0
			57	57		

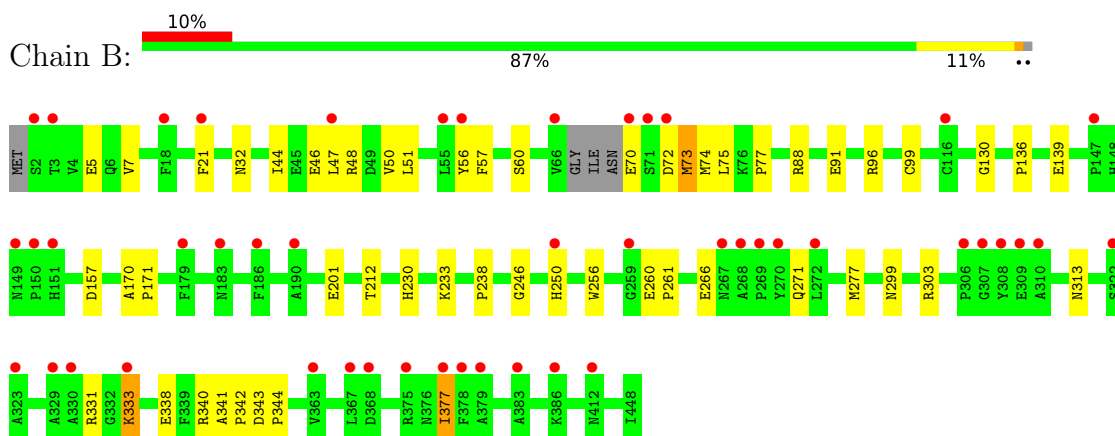
3 Residue-property plots [i](#)

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.

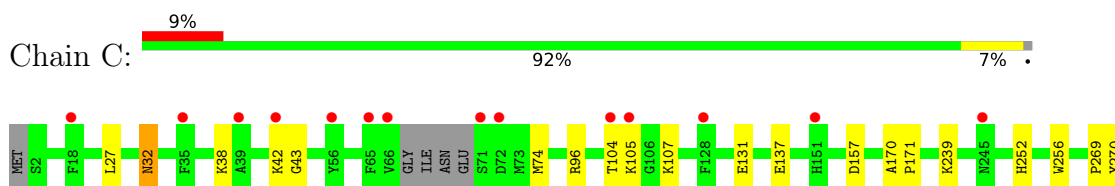
- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*



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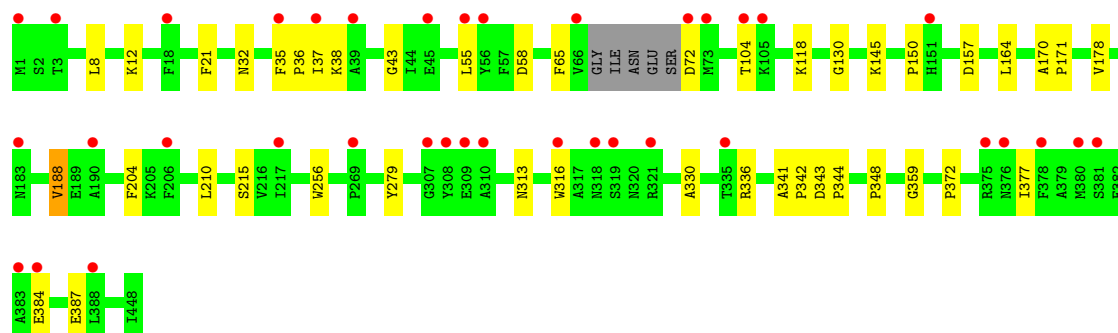
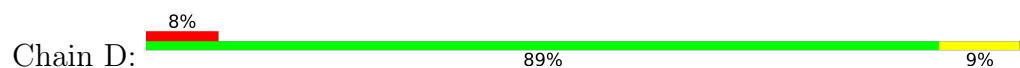


- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*

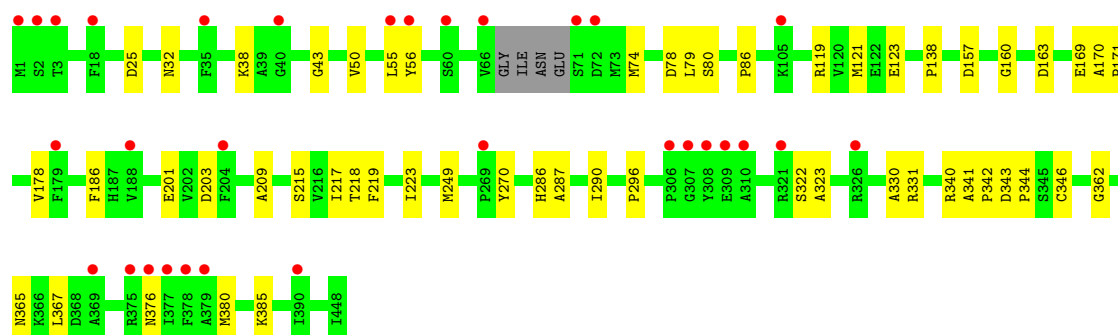
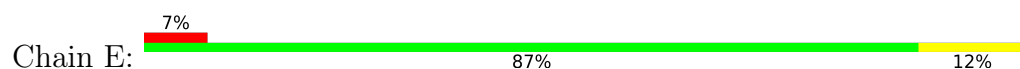




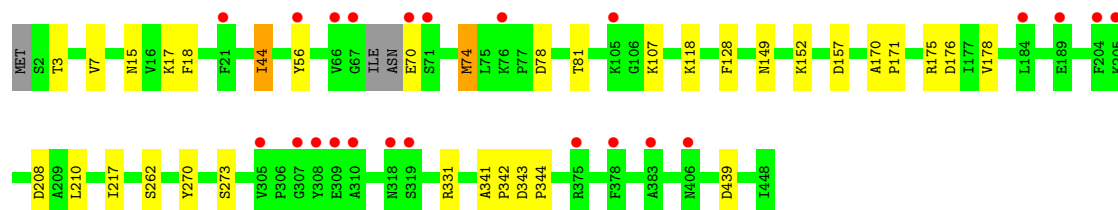
- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*



- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*



- Molecule 1: Glutamine synthetase from *Methanothermococcus thermolithotrophicus*



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.65Å 230.24Å 205.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.89 – 2.43 58.89 – 2.43	Depositor EDS
% Data completeness (in resolution range)	86.6 (58.89-2.43) 86.6 (58.89-2.43)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.229 , 0.268 0.246 , 0.282	Depositor DCC
R_{free} test set	4910 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.074 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.095 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21529	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4577e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EDO, GOL, NA

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	0.30	0/3613	0.44	0/4891
1	B	0.31	0/3605	0.44	0/4880
1	C	0.23	0/3595	0.37	0/4868
1	D	0.30	1/3605 (0.0%)	0.43	3/4881 (0.1%)
1	E	0.22	0/3620	0.37	0/4900
1	F	0.22	0/3600	0.37	1/4874 (0.0%)
All	All	0.26	1/21638 (0.0%)	0.40	4/29294 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	348	PRO	N-CD	10.24	1.62	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	PRO	CA-C-N	-5.67	113.21	121.71
1	D	36	PRO	C-N-CA	-5.67	113.21	121.71
1	D	37	ILE	N-CA-C	-5.57	101.64	109.21
1	F	176	ASP	N-CA-C	-5.38	104.97	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3517	0	3450	32	0
1	B	3513	0	3443	41	0
1	C	3505	0	3431	19	0
1	D	3512	0	3449	28	0
1	E	3524	0	3467	35	0
1	F	3511	0	3433	22	0
2	A	36	0	54	0	0
2	B	24	0	36	2	0
2	C	36	0	54	2	0
2	D	20	0	30	0	0
2	E	16	0	24	0	0
2	F	8	0	12	0	0
3	B	6	0	8	1	0
3	F	6	0	8	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	53	0	0	1	0
5	B	43	0	0	1	0
5	C	43	0	0	0	0
5	D	45	0	0	0	0
5	E	52	0	0	0	0
5	F	57	0	0	0	0
All	All	21529	0	20899	173	0

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 (173) 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:F:175:ARG:HG2	1:F:175:ARG:O	1.96	0.65
1:A:170:ALA:N	1:A:171:PRO:CD	2.65	0.59
1:F:70:GLU:O	1:F:70:GLU:HG3	2.02	0.59
1:A:338:GLU:HG2	1:A:338:GLU:O	2.04	0.58
1:B:57:PHE:CD1	1:B:75:LEU:HG	2.42	0.55
1:A:252:HIS:HB3	1:A:336:ARG:HD2	1.89	0.54
1:A:179:PHE:C	1:A:179:PHE:CD1	2.86	0.53
1:D:313:ASN:CG	1:D:377:ILE:HG21	2.34	0.53
1:A:283:ILE:CG2	1:A:325:ILE:HD11	2.38	0.52
1:D:58:ASP:C	1:D:58:ASP:OD1	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ARG:HA	1:C:326:ARG:HH22	1.76	0.51
1:F:118:LYS:HE2	1:F:210:LEU:HD21	1.92	0.51
1:D:38:LYS:HB2	1:D:43:GLY:HA2	1.91	0.51
1:C:38:LYS:HB2	1:C:43:GLY:HA2	1.93	0.50
1:E:56:TYR:HD1	1:E:74:MET:HG2	1.77	0.50
1:C:27:LEU:HD22	2:C:503:EDO:H21	1.93	0.50
1:D:21:PHE:CD2	1:D:55:LEU:HD21	2.46	0.50
1:B:250:HIS:CD2	1:B:338:GLU:OE2	2.65	0.50
1:C:256:TRP:HH2	1:C:333:LYS:HG2	1.77	0.50
1:F:3:THR:O	1:F:7:VAL:HG23	2.11	0.50
1:A:447:LYS:NZ	5:A:703:HOH:O	2.44	0.49
1:C:32:ASN:C	1:C:32:ASN:HD22	2.20	0.49
1:B:77:PRO:HA	1:B:99:CYS:HA	1.95	0.49
1:F:56:TYR:CD1	1:F:74:MET:HG3	2.47	0.49
1:B:256:TRP:HH2	1:B:333:LYS:HD3	1.77	0.49
1:D:118:LYS:HE2	1:D:210:LEU:HD21	1.94	0.49
1:F:262:SER:O	1:F:273:SER:OG	2.29	0.48
1:D:38:LYS:HB2	1:D:43:GLY:CA	2.43	0.48
1:C:42:LYS:HE3	1:C:42:LYS:HA	1.95	0.48
1:D:21:PHE:HD2	1:D:55:LEU:HD21	1.78	0.48
1:E:38:LYS:HB3	1:E:43:GLY:HA2	1.96	0.48
1:D:330:ALA:HB3	1:D:336:ARG:HH12	1.77	0.48
1:B:70:GLU:OE2	1:B:72:ASP:HB2	2.13	0.48
1:A:381:SER:OG	1:A:382:GLU:N	2.47	0.48
1:D:343:ASP:HB2	1:D:344:PRO:HD2	1.95	0.47
1:E:380:MET:HE2	1:E:385:LYS:HG2	1.95	0.47
1:C:27:LEU:HD21	1:C:426:LYS:HE2	1.96	0.47
1:C:341:ALA:N	1:C:342:PRO:CD	2.77	0.47
1:C:105:LYS:HD2	1:C:107:LYS:HE3	1.96	0.47
1:E:376:ASN:O	1:E:380:MET:HG3	2.14	0.47
1:B:170:ALA:N	1:B:171:PRO:CD	2.77	0.47
1:B:250:HIS:NE2	1:B:340:ARG:NH1	2.62	0.47
1:B:341:ALA:N	1:B:342:PRO:CD	2.78	0.47
1:E:50:VAL:HG13	1:E:55:LEU:HB3	1.97	0.47
1:E:157:ASP:HB3	1:E:169:GLU:HB2	1.97	0.47
1:E:178:VAL:HB	1:F:18:PHE:HZ	1.80	0.47
1:E:186:PHE:HD1	1:E:215:SER:HG	1.62	0.47
1:E:323:ALA:O	1:E:340:ARG:NH1	2.48	0.47
1:E:341:ALA:N	1:E:342:PRO:CD	2.78	0.47
1:F:341:ALA:N	1:F:342:PRO:CD	2.78	0.47
1:A:316:TRP:CZ2	1:A:372:PRO:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:NH1	1:B:60:SER:OG	2.48	0.47
1:B:271:GLN:HB2	1:B:331:ARG:HE	1.79	0.47
1:A:170:ALA:N	1:A:171:PRO:HD2	2.30	0.46
1:F:170:ALA:N	1:F:171:PRO:CD	2.78	0.46
1:B:7:VAL:HG11	1:B:51:LEU:CD2	2.46	0.46
1:E:138:PRO:HB3	1:E:249:MET:HE3	1.98	0.46
1:F:107:LYS:HD2	1:F:107:LYS:C	2.40	0.46
1:D:341:ALA:N	1:D:342:PRO:CD	2.79	0.46
1:D:384:GLU:OE2	1:D:387:GLU:OE1	2.33	0.46
1:E:380:MET:CE	1:E:385:LYS:HG2	2.46	0.46
1:D:204:PHE:HE2	1:D:215:SER:HG	1.60	0.46
1:A:341:ALA:N	1:A:342:PRO:CD	2.79	0.46
1:E:56:TYR:HE1	1:E:74:MET:SD	2.38	0.46
1:E:79:LEU:HD22	1:E:79:LEU:H	1.81	0.46
1:F:270:TYR:O	1:F:331:ARG:NH1	2.48	0.46
1:C:239:LYS:N	1:C:299:ASN:OD1	2.44	0.45
1:D:145:LYS:NZ	1:D:150:PRO:O	2.45	0.45
1:A:326:ARG:HB2	1:A:340:ARG:HD2	1.97	0.45
1:D:55:LEU:N	1:D:55:LEU:HD23	2.32	0.45
1:F:343:ASP:HB2	1:F:344:PRO:HD2	1.98	0.45
1:A:8:LEU:O	1:A:12:LYS:HG3	2.16	0.45
1:B:21:PHE:HB3	1:B:75:LEU:HD13	1.99	0.45
1:C:439:ASP:N	1:C:439:ASP:OD1	2.49	0.45
1:F:439:ASP:N	1:F:439:ASP:OD1	2.48	0.45
1:B:139:GLU:HG2	1:B:201:GLU:HB2	1.98	0.45
1:B:313:ASN:HB3	1:B:377:ILE:HG21	1.99	0.45
1:E:201:GLU:OE2	1:E:203:ASP:OD1	2.35	0.45
1:F:149:ASN:ND2	1:F:152:LYS:HD2	2.32	0.45
1:D:170:ALA:N	1:D:171:PRO:CD	2.80	0.45
1:E:296:PRO:HG3	1:E:346:CYS:HA	1.98	0.45
1:D:8:LEU:O	1:D:12:LYS:HG3	2.17	0.44
1:D:157:ASP:OD1	1:D:157:ASP:C	2.61	0.44
1:A:18:PHE:HZ	1:F:178:VAL:HB	1.83	0.44
1:B:343:ASP:HB2	1:B:344:PRO:HD2	1.99	0.44
1:C:321:ARG:HA	1:C:326:ARG:NH2	2.31	0.44
1:E:38:LYS:HB3	1:E:43:GLY:CA	2.47	0.44
1:E:86:PRO:HG2	1:E:218:THR:HG23	1.99	0.44
1:A:52:GLU:O	1:A:76:LYS:NZ	2.48	0.44
1:B:5:GLU:OE2	1:B:48:ARG:NH1	2.34	0.44
1:B:21:PHE:O	1:B:32:ASN:HA	2.17	0.44
1:B:46:GLU:O	1:B:50:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASN:CB	1:B:377:ILE:HG21	2.47	0.44
1:C:170:ALA:N	1:C:171:PRO:CD	2.81	0.44
1:A:78:ASP:OD1	1:A:80:SER:OG	2.31	0.44
1:A:111:GLY:HA2	1:A:418:ILE:HG13	1.99	0.44
1:A:343:ASP:HB2	1:A:344:PRO:HD2	2.00	0.44
1:B:47:LEU:CD1	1:B:51:LEU:HD11	2.47	0.44
1:C:27:LEU:HD22	2:C:503:EDO:C2	2.48	0.44
1:C:343:ASP:HB2	1:C:344:PRO:HD2	2.00	0.44
1:B:277:MET:HE2	1:B:277:MET:N	2.33	0.44
1:B:56:TYR:HD1	1:B:74:MET:HG2	1.83	0.43
1:E:160:GLY:N	1:E:163:ASP:OD2	2.51	0.43
1:E:170:ALA:N	1:E:171:PRO:CD	2.80	0.43
1:B:303:ARG:HG3	3:B:502:GOL:H11	2.00	0.43
1:E:119:ARG:O	1:E:123:GLU:HG3	2.18	0.43
1:E:287:ALA:HA	1:E:290:ILE:HD12	1.99	0.43
1:B:157:ASP:OD1	1:B:157:ASP:C	2.61	0.43
1:B:266:GLU:OE1	1:B:266:GLU:N	2.49	0.43
1:F:128:PHE:CD1	1:F:128:PHE:N	2.86	0.43
1:A:316:TRP:O	1:A:372:PRO:HA	2.19	0.43
1:E:365:ASN:HB2	1:E:367:LEU:HD21	1.99	0.43
1:B:246:GLY:O	2:B:501:EDO:O2	2.36	0.43
1:D:316:TRP:CZ2	1:D:372:PRO:HG3	2.54	0.43
1:A:84:VAL:HG21	1:A:89:PRO:O	2.18	0.43
1:A:381:SER:O	1:A:385:LYS:HG3	2.18	0.43
1:D:72:ASP:O	1:D:104:THR:OG1	2.34	0.43
1:E:219:PHE:O	1:E:223:ILE:HG22	2.19	0.43
1:F:78:ASP:O	1:F:81:THR:OG1	2.33	0.43
1:E:56:TYR:CD1	1:E:74:MET:HG2	2.54	0.43
1:A:362:GLY:HA2	1:A:367:LEU:HG	2.01	0.42
1:B:233:LYS:HB3	2:B:504:EDO:H21	2.01	0.42
1:E:121:MET:HE3	1:E:209:ALA:HB3	2.01	0.42
1:E:343:ASP:HB2	1:E:344:PRO:HD2	2.00	0.42
1:F:208:ASP:OD1	1:F:208:ASP:C	2.61	0.42
1:D:65:PHE:CD1	1:D:65:PHE:N	2.86	0.42
1:E:286:HIS:O	1:E:290:ILE:HG13	2.18	0.42
1:A:84:VAL:CG1	1:A:184:LEU:HD11	2.50	0.42
1:B:130:GLY:HA2	1:B:256:TRP:O	2.20	0.42
1:C:157:ASP:C	1:C:157:ASP:OD1	2.62	0.42
1:E:78:ASP:OD1	1:E:80:SER:OG	2.29	0.42
1:D:65:PHE:N	1:D:65:PHE:HD1	2.18	0.42
1:B:88:ARG:NH1	1:B:91:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:GLU:O	1:B:271:GLN:NE2	2.53	0.42
1:E:362:GLY:HA2	1:E:367:LEU:HG	2.00	0.42
1:A:334:GLY:O	1:A:336:ARG:NH1	2.52	0.42
1:B:47:LEU:O	1:B:50:VAL:N	2.44	0.42
1:E:330:ALA:O	1:E:331:ARG:NE	2.53	0.42
1:F:44:ILE:HD13	1:F:44:ILE:HA	1.89	0.42
1:A:130:GLY:HA2	1:A:256:TRP:O	2.19	0.42
1:A:283:ILE:HG21	1:A:325:ILE:HD11	2.01	0.41
1:B:277:MET:HE2	1:B:277:MET:HA	2.01	0.41
1:D:178:VAL:HG13	1:D:188:VAL:CG2	2.51	0.41
1:D:279:TYR:CE1	1:D:359:GLY:HA3	2.55	0.41
1:B:44:ILE:HD13	1:B:44:ILE:N	2.35	0.41
1:B:47:LEU:HG	1:B:51:LEU:HD11	2.02	0.41
1:B:230:HIS:HE1	5:B:631:HOH:O	2.01	0.41
1:A:59:GLY:HA3	1:A:73:MET:HE3	2.03	0.41
1:B:260:GLU:OE1	1:B:261:PRO:HD2	2.20	0.41
1:F:15:ASN:O	1:F:17:LYS:NZ	2.50	0.41
1:C:137:GLU:OE2	1:C:252:HIS:NE2	2.54	0.41
1:D:21:PHE:CD2	1:D:55:LEU:CD2	3.03	0.41
1:B:57:PHE:CE1	1:B:73:MET:HB3	2.56	0.41
1:B:136:PRO:HD3	1:B:212:THR:HG21	2.02	0.41
1:D:343:ASP:OD1	1:D:343:ASP:C	2.63	0.41
1:F:208:ASP:OD1	1:F:210:LEU:N	2.53	0.41
1:D:164:LEU:HD11	1:E:32:ASN:HB3	2.02	0.41
1:A:59:GLY:HA3	1:A:73:MET:CE	2.50	0.41
1:A:136:PRO:HD3	1:A:212:THR:HG21	2.03	0.41
1:B:47:LEU:O	1:B:48:ARG:C	2.63	0.41
1:C:270:TYR:O	1:C:331:ARG:NH1	2.54	0.41
1:F:157:ASP:OD1	1:F:157:ASP:C	2.62	0.41
1:A:44:ILE:N	1:A:44:ILE:HD13	2.36	0.41
1:A:302:LYS:N	1:A:302:LYS:HD2	2.35	0.41
1:B:56:TYR:CD1	1:B:74:MET:HG2	2.55	0.41
1:B:238:PRO:HD2	1:B:299:ASN:OD1	2.21	0.41
1:D:35:PHE:CD1	1:D:35:PHE:N	2.90	0.40
1:A:21:PHE:HD2	1:A:55:LEU:HD22	1.87	0.40
1:C:269:PRO:C	1:C:271:GLN:H	2.29	0.40
1:E:25:ASP:C	1:E:25:ASP:OD1	2.65	0.40
1:D:130:GLY:HA2	1:D:256:TRP:O	2.21	0.40
1:E:55:LEU:O	1:E:55:LEU:HD23	2.21	0.40
1:E:270:TYR:O	1:E:331:ARG:NH1	2.54	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	441/448 (98%)	428 (97%)	12 (3%)	1 (0%)	43	53
1	B	441/448 (98%)	427 (97%)	14 (3%)	0	100	100
1	C	439/448 (98%)	421 (96%)	18 (4%)	0	100	100
1	D	440/448 (98%)	424 (96%)	16 (4%)	0	100	100
1	E	442/448 (99%)	427 (97%)	15 (3%)	0	100	100
1	F	441/448 (98%)	425 (96%)	16 (4%)	0	100	100
All	All	2644/2688 (98%)	2552 (96%)	91 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ALA

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	381/383 (100%)	376 (99%)	5 (1%)	61	72
1	B	380/383 (99%)	376 (99%)	4 (1%)	65	75
1	C	379/383 (99%)	373 (98%)	6 (2%)	55	68
1	D	380/383 (99%)	378 (100%)	2 (0%)	81	87
1	E	382/383 (100%)	379 (99%)	3 (1%)	73	81
1	F	379/383 (99%)	376 (99%)	3 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2281/2298 (99%)	2258 (99%)	23 (1%)	68 77

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	87	TRP
1	A	96	ARG
1	A	217	ILE
1	A	331	ARG
1	B	73	MET
1	B	96	ARG
1	B	333	LYS
1	B	377	ILE
1	C	32	ASN
1	C	74	MET
1	C	96	ARG
1	C	104	THR
1	C	131	GLU
1	C	277	MET
1	D	32	ASN
1	D	188	VAL
1	E	217[A]	ILE
1	E	217[B]	ILE
1	E	322	SER
1	F	44	ILE
1	F	74	MET
1	F	217	ILE

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	192	HIS
1	A	365	ASN
1	A	406	ASN
1	B	129	ASN
1	B	148	HIS
1	B	271	GLN
1	D	32	ASN
1	D	129	ASN
1	D	258	ASN

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Mol	Chain	Res	Type
1	D	278	ASN
1	D	295	ASN
1	E	148	HIS
1	E	271	GLN
1	E	278	ASN
1	F	151	HIS
1	F	252	HIS
1	F	406	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 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	EDO	C	501	-	3,3,3	0.47	0	2,2,2	0.42	0
2	EDO	C	504	-	3,3,3	0.48	0	2,2,2	0.40	0
2	EDO	C	506	-	3,3,3	0.47	0	2,2,2	0.40	0
2	EDO	E	502	-	3,3,3	0.46	0	2,2,2	0.50	0
2	EDO	D	502	-	3,3,3	0.46	0	2,2,2	0.49	0
2	EDO	D	505	-	3,3,3	0.50	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	508	-	3,3,3	0.06	0	2,2,2	0.11	0
2	EDO	A	604	-	3,3,3	0.47	0	2,2,2	0.57	0
2	EDO	B	504	-	3,3,3	0.52	0	2,2,2	0.42	0
2	EDO	A	605	-	3,3,3	0.49	0	2,2,2	0.39	0
2	EDO	C	502	-	3,3,3	0.44	0	2,2,2	0.47	0
2	EDO	C	505	-	3,3,3	0.46	0	2,2,2	0.47	0
2	EDO	A	608	-	3,3,3	0.48	0	2,2,2	0.55	0
2	EDO	C	509	-	3,3,3	0.05	0	2,2,2	0.11	0
2	EDO	A	606	-	3,3,3	0.06	0	2,2,2	0.11	0
2	EDO	A	603	-	3,3,3	0.49	0	2,2,2	0.35	0
2	EDO	D	501	-	3,3,3	0.49	0	2,2,2	0.36	0
2	EDO	E	504	-	3,3,3	0.46	0	2,2,2	0.44	0
2	EDO	B	506	-	3,3,3	0.06	0	2,2,2	0.12	0
3	GOL	B	502	-	5,5,5	0.90	0	5,5,5	1.18	1 (20%)
2	EDO	B	501	-	3,3,3	0.48	0	2,2,2	0.50	0
2	EDO	F	501	-	3,3,3	0.46	0	2,2,2	0.48	0
2	EDO	E	501	-	3,3,3	0.47	0	2,2,2	0.43	0
2	EDO	D	504	-	3,3,3	0.47	0	2,2,2	0.46	0
2	EDO	A	609	-	3,3,3	0.06	0	2,2,2	0.11	0
2	EDO	C	507	-	3,3,3	0.51	0	2,2,2	0.33	0
2	EDO	E	503	-	3,3,3	0.50	0	2,2,2	0.27	0
2	EDO	B	507	-	3,3,3	0.48	0	2,2,2	0.53	0
2	EDO	A	607	-	3,3,3	0.49	0	2,2,2	0.29	0
2	EDO	F	503	-	3,3,3	0.46	0	2,2,2	0.42	0
2	EDO	B	505	-	3,3,3	0.47	0	2,2,2	0.43	0
2	EDO	D	503	-	3,3,3	0.50	0	2,2,2	0.27	0
2	EDO	A	601	-	3,3,3	0.47	0	2,2,2	0.33	0
2	EDO	A	602	-	3,3,3	0.45	0	2,2,2	0.48	0
2	EDO	C	503	-	3,3,3	0.46	0	2,2,2	0.35	0
2	EDO	B	503	-	3,3,3	0.49	0	2,2,2	0.37	0
3	GOL	F	502	-	5,5,5	0.73	0	5,5,5	0.97	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	EDO	C	501	-	-	1/1/1/1	-
2	EDO	C	504	-	-	1/1/1/1	-
2	EDO	C	506	-	-	0/1/1/1	-
2	EDO	E	502	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	502	-	-	1/1/1/1	-
2	EDO	D	505	-	-	1/1/1/1	-
2	EDO	C	508	-	-	0/1/1/1	-
2	EDO	A	604	-	-	1/1/1/1	-
2	EDO	B	504	-	-	1/1/1/1	-
2	EDO	A	605	-	-	1/1/1/1	-
2	EDO	C	502	-	-	1/1/1/1	-
2	EDO	C	505	-	-	1/1/1/1	-
2	EDO	A	608	-	-	0/1/1/1	-
2	EDO	C	509	-	-	1/1/1/1	-
2	EDO	A	606	-	-	0/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	E	504	-	-	1/1/1/1	-
2	EDO	B	506	-	-	0/1/1/1	-
3	GOL	B	502	-	-	0/4/4/4	-
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	F	501	-	-	1/1/1/1	-
2	EDO	E	501	-	-	1/1/1/1	-
2	EDO	D	504	-	-	0/1/1/1	-
2	EDO	A	609	-	-	1/1/1/1	-
2	EDO	C	507	-	-	1/1/1/1	-
2	EDO	E	503	-	-	1/1/1/1	-
2	EDO	B	507	-	-	0/1/1/1	-
2	EDO	A	607	-	-	1/1/1/1	-
2	EDO	F	503	-	-	0/1/1/1	-
2	EDO	B	505	-	-	1/1/1/1	-
2	EDO	D	503	-	-	1/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	C	503	-	-	1/1/1/1	-
2	EDO	B	503	-	-	1/1/1/1	-
3	GOL	F	502	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	GOL	C3-C2-C1	-2.17	103.84	111.80

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	502	GOL	O1-C1-C2-O2
3	F	502	GOL	O1-C1-C2-C3
3	F	502	GOL	C1-C2-C3-O3
2	B	503	EDO	O1-C1-C2-O2
2	E	504	EDO	O1-C1-C2-O2
2	A	602	EDO	O1-C1-C2-O2
2	C	502	EDO	O1-C1-C2-O2
2	C	505	EDO	O1-C1-C2-O2
2	D	502	EDO	O1-C1-C2-O2
2	E	502	EDO	O1-C1-C2-O2
2	F	501	EDO	O1-C1-C2-O2
2	B	504	EDO	O1-C1-C2-O2
2	D	503	EDO	O1-C1-C2-O2
2	D	505	EDO	O1-C1-C2-O2
2	C	503	EDO	O1-C1-C2-O2
2	C	504	EDO	O1-C1-C2-O2
2	E	503	EDO	O1-C1-C2-O2
3	F	502	GOL	O2-C2-C3-O3
2	A	607	EDO	O1-C1-C2-O2
2	C	509	EDO	O1-C1-C2-O2
2	D	501	EDO	O1-C1-C2-O2
2	C	507	EDO	O1-C1-C2-O2
2	E	501	EDO	O1-C1-C2-O2
2	A	609	EDO	O1-C1-C2-O2
2	C	501	EDO	O1-C1-C2-O2
2	B	505	EDO	O1-C1-C2-O2
2	A	604	EDO	O1-C1-C2-O2
2	A	605	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	504	EDO	1	0
3	B	502	GOL	1	0
2	B	501	EDO	1	0
2	C	503	EDO	2	0

5.7 Other polymers [i](#)

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	443/448 (98%)	0.72	43 (9%) 13 10	26, 49, 86, 132	2 (0%)
1	B	444/448 (99%)	0.80	47 (10%) 11 8	28, 51, 91, 129	1 (0%)
1	C	443/448 (98%)	0.58	39 (8%) 15 13	19, 46, 87, 122	0
1	D	443/448 (98%)	0.72	37 (8%) 17 14	30, 52, 86, 129	1 (0%)
1	E	444/448 (99%)	0.62	31 (6%) 22 19	25, 49, 85, 141	2 (0%)
1	F	445/448 (99%)	0.56	23 (5%) 33 29	30, 47, 81, 163	0
All	All	2662/2688 (99%)	0.67	220 (8%) 17 14	19, 49, 87, 163	6 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	66	VAL	6.2
1	E	71	SER	5.9
1	B	308	TYR	5.6
1	F	67	GLY	5.6
1	B	66	VAL	5.2
1	D	308	TYR	4.8
1	F	309	GLU	4.8
1	C	308	TYR	4.8
1	C	66	VAL	4.7
1	D	1	MET	4.4
1	E	308	TYR	4.3
1	F	308	TYR	4.3
1	A	308	TYR	4.2
1	C	378	PHE	4.2
1	B	2	SER	4.1
1	B	269	PRO	4.1
1	D	66	VAL	4.1
1	A	378	PHE	4.0
1	E	18	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	72	ASP	3.9
1	A	318	ASN	3.9
1	B	21	PHE	3.8
1	B	70	GLU	3.8
1	E	375	ARG	3.6
1	C	379	ALA	3.6
1	A	18	PHE	3.6
1	B	183	ASN	3.6
1	E	369	ALA	3.6
1	C	71	SER	3.5
1	D	319	SER	3.5
1	A	105	LYS	3.5
1	D	321	ARG	3.5
1	D	217[A]	ILE	3.5
1	A	183	ASN	3.4
1	C	388	LEU	3.4
1	F	375	ARG	3.4
1	B	55	LEU	3.4
1	F	383	ALA	3.4
1	C	105	LYS	3.4
1	F	71	SER	3.4
1	D	376	ASN	3.3
1	D	316	TRP	3.3
1	A	319	SER	3.3
1	F	70	GLU	3.3
1	E	321	ARG	3.2
1	E	3	THR	3.2
1	D	310	ALA	3.2
1	A	326	ARG	3.2
1	B	368	ASP	3.2
1	A	375	ARG	3.2
1	B	72	ASP	3.1
1	B	310	ALA	3.1
1	A	71	SER	3.1
1	D	269	PRO	3.1
1	B	3	THR	3.1
1	F	105	LYS	3.1
1	D	18	PHE	3.1
1	A	66	VAL	3.1
1	A	329	ALA	3.1
1	A	179	PHE	3.1
1	C	377	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	179	PHE	3.0
1	E	55	LEU	3.0
1	B	378	PHE	3.0
1	E	379	ALA	2.9
1	B	383	ALA	2.9
1	B	322	SER	2.9
1	F	205	LYS	2.9
1	C	65	PHE	2.9
1	A	376	ASN	2.9
1	E	188	VAL	2.9
1	F	66	VAL	2.9
1	D	104	THR	2.8
1	B	272	LEU	2.8
1	E	179	PHE	2.8
1	A	145[A]	LYS	2.8
1	A	133	PHE	2.8
1	C	390	ILE	2.7
1	C	56	TYR	2.7
1	C	323	ALA	2.7
1	B	309	GLU	2.7
1	C	331	ARG	2.7
1	C	272	LEU	2.7
1	F	184	LEU	2.7
1	E	310	ALA	2.7
1	E	378	PHE	2.7
1	D	388	LEU	2.7
1	B	330	ALA	2.7
1	C	18	PHE	2.7
1	E	1	MET	2.7
1	B	71	SER	2.7
1	E	326	ARG	2.7
1	B	270	TYR	2.7
1	A	56	TYR	2.6
1	C	72	ASP	2.6
1	C	318	ASN	2.6
1	B	307	GLY	2.6
1	D	378	PHE	2.6
1	D	55	LEU	2.6
1	B	412	ASN	2.6
1	E	376	ASN	2.6
1	A	270	TYR	2.6
1	D	380	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	388	LEU	2.6
1	D	39	ALA	2.6
1	E	2	SER	2.6
1	B	375	ARG	2.5
1	C	307	GLY	2.5
1	E	306	PRO	2.5
1	E	307	GLY	2.5
1	B	149	ASN	2.5
1	A	148	HIS	2.5
1	C	39	ALA	2.5
1	A	104	THR	2.5
1	E	204	PHE	2.5
1	C	329	ALA	2.5
1	E	269	PRO	2.5
1	A	110	GLU	2.5
1	D	35	PHE	2.5
1	A	373	VAL	2.5
1	B	151	HIS	2.5
1	C	330	ALA	2.5
1	B	386	LYS	2.5
1	B	363	VAL	2.5
1	C	321	ARG	2.5
1	A	2	SER	2.5
1	A	328	PRO	2.4
1	F	189	GLU	2.4
1	D	384	GLU	2.4
1	F	310	ALA	2.4
1	D	3	THR	2.4
1	A	322	SER	2.4
1	D	105	LYS	2.4
1	D	307	GLY	2.4
1	A	320	ASN	2.4
1	A	379	ALA	2.4
1	E	40	GLY	2.4
1	A	128	PHE	2.4
1	B	18	PHE	2.4
1	B	56	TYR	2.4
1	A	383	ALA	2.4
1	C	383	ALA	2.4
1	A	189	GLU	2.4
1	D	309	GLU	2.4
1	B	150	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	335	THR	2.3
1	F	319	SER	2.3
1	B	250	HIS	2.3
1	A	323	ALA	2.3
1	C	382	GLU	2.3
1	B	367	LEU	2.3
1	D	37	ILE	2.3
1	F	56	TYR	2.3
1	A	330	ALA	2.3
1	A	55	LEU	2.3
1	C	42	LYS	2.3
1	B	186	PHE	2.3
1	B	323	ALA	2.3
1	F	406	ASN	2.3
1	B	259	GLY	2.3
1	E	390	ILE	2.3
1	B	116	CYS	2.3
1	A	217	ILE	2.2
1	E	377	ILE	2.2
1	A	72	ASP	2.2
1	C	35	PHE	2.2
1	D	206	PHE	2.2
1	D	318	ASN	2.2
1	D	56	TYR	2.2
1	C	373	VAL	2.2
1	E	105	LYS	2.2
1	D	73	MET	2.2
1	C	322	SER	2.2
1	F	378	PHE	2.2
1	B	379	ALA	2.2
1	C	151	HIS	2.2
1	C	104	THR	2.2
1	C	309	GLU	2.2
1	E	72	ASP	2.2
1	B	147	PRO	2.2
1	B	306	PRO	2.2
1	A	35	PHE	2.2
1	C	128	PHE	2.2
1	A	327	VAL	2.1
1	B	329	ALA	2.1
1	C	310	ALA	2.1
1	A	184	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	307	GLY	2.1
1	B	377	ILE	2.1
1	A	371	GLU	2.1
1	D	375	ARG	2.1
1	B	190	ALA	2.1
1	D	190	ALA	2.1
1	B	47	LEU	2.1
1	A	45	GLU	2.1
1	C	375	ARG	2.1
1	F	76	LYS	2.1
1	A	209	ALA	2.1
1	D	383	ALA	2.1
1	D	183	ASN	2.1
1	E	60	SER	2.1
1	D	151	HIS	2.1
1	F	21	PHE	2.1
1	F	305	VAL	2.1
1	B	268	ALA	2.1
1	A	106	GLY	2.1
1	D	45	GLU	2.1
1	B	333	LYS	2.1
1	D	381	SER	2.1
1	E	35	PHE	2.0
1	F	204	PHE	2.0
1	C	336	ARG	2.0
1	C	376	ASN	2.0
1	C	326	ARG	2.0
1	C	317	ALA	2.0
1	E	309	GLU	2.0
1	B	267	ASN	2.0
1	C	245	ASN	2.0
1	F	318	ASN	2.0
1	E	56	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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	EDO	A	606	4/4	0.58	0.24	40,53,56,61	0
2	EDO	A	609	4/4	0.74	0.18	48,51,57,63	0
2	EDO	A	604	4/4	0.75	0.17	38,47,57,80	0
2	EDO	E	501	4/4	0.76	0.16	34,36,39,43	0
2	EDO	C	509	4/4	0.77	0.16	41,44,50,53	0
2	EDO	C	501	4/4	0.77	0.20	34,51,56,57	0
3	GOL	F	502	6/6	0.77	0.17	43,51,65,66	0
2	EDO	B	506	4/4	0.79	0.16	53,53,54,56	0
2	EDO	C	504	4/4	0.79	0.17	36,42,47,49	0
2	EDO	F	503	4/4	0.79	0.21	38,47,52,75	0
2	EDO	C	508	4/4	0.79	0.15	39,46,46,62	0
2	EDO	C	507	4/4	0.80	0.23	25,29,31,38	0
2	EDO	C	502	4/4	0.80	0.21	31,36,37,42	0
3	GOL	B	502	6/6	0.80	0.13	35,41,43,56	0
2	EDO	B	503	4/4	0.80	0.28	45,49,49,58	0
2	EDO	B	507	4/4	0.81	0.20	36,37,48,54	0
2	EDO	B	504	4/4	0.82	0.15	25,32,35,53	0
2	EDO	D	502	4/4	0.82	0.28	43,53,60,63	0
2	EDO	A	603	4/4	0.82	0.18	44,51,52,55	0
2	EDO	A	607	4/4	0.83	0.21	35,38,43,47	0
2	EDO	D	501	4/4	0.83	0.21	35,42,43,56	0
2	EDO	E	502	4/4	0.83	0.24	43,47,51,59	0
2	EDO	B	501	4/4	0.84	0.13	37,40,40,52	0
2	EDO	C	506	4/4	0.84	0.15	21,24,30,43	0
2	EDO	E	503	4/4	0.85	0.16	33,34,46,54	0
2	EDO	F	501	4/4	0.85	0.12	31,33,42,47	0
2	EDO	D	504	4/4	0.85	0.18	30,39,50,51	0
2	EDO	A	602	4/4	0.85	0.19	50,56,57,58	0
2	EDO	C	505	4/4	0.85	0.19	45,47,52,57	0
2	EDO	D	505	4/4	0.87	0.14	51,57,64,68	0
2	EDO	B	505	4/4	0.87	0.15	31,35,38,49	0
2	EDO	A	605	4/4	0.88	0.11	42,49,52,59	0
2	EDO	E	504	4/4	0.88	0.14	48,58,59,64	0
4	NA	D	506	1/1	0.91	0.06	30,30,30,30	0
4	NA	E	505	1/1	0.91	0.14	46,46,46,46	0
2	EDO	A	608	4/4	0.92	0.20	27,38,39,49	0
2	EDO	A	601	4/4	0.92	0.09	33,41,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	C	503	4/4	0.93	0.17	27,27,29,41	0
2	EDO	D	503	4/4	0.93	0.14	19,34,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.