



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:52 PM GMT

PDB ID : 3OOQ
Title : CRYSTAL STRUCTURE OF amidohydrolase from *Thermotoga maritima* MSB8
Authors : Malashkevich, V.N.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-08-31
Resolution : 2.06 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

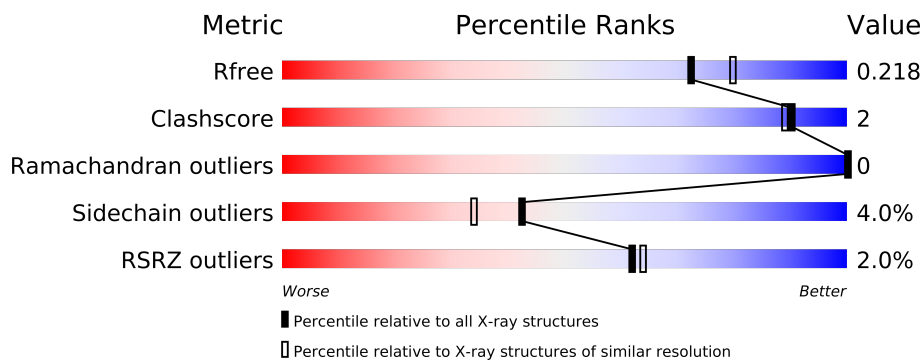
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.06 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}	66092	1224 (2.08-2.04)
Clashscore	79885	1390 (2.08-2.04)
Ramachandran outliers	78287	1381 (2.08-2.04)
Sidechain outliers	78261	1381 (2.08-2.04)
RSRZ outliers	66119	1225 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	396	
1	B	396	
1	C	396	
1	D	396	
1	E	396	
1	F	396	
1	G	396	
1	H	396	
1	I	396	
1	J	396	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	C	500	-	X
2	GOL	E	500	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31584 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	Se	0	1	0
			2985	1914	502	556	2	11			
1	B	383	Total	C	N	O	S	Se	0	0	0
			2970	1905	501	551	2	11			
1	C	384	Total	C	N	O	S	Se	0	3	0
			2996	1921	503	559	2	11			
1	D	384	Total	C	N	O	S	Se	0	0	0
			2979	1910	502	554	2	11			
1	E	383	Total	C	N	O	S	Se	0	0	0
			2970	1905	501	551	2	11			
1	F	385	Total	C	N	O	S	Se	0	0	0
			2986	1915	503	555	2	11			
1	G	383	Total	C	N	O	S	Se	0	1	0
			2974	1908	501	552	2	11			
1	H	383	Total	C	N	O	S	Se	0	1	0
			2976	1909	502	552	2	11			
1	I	383	Total	C	N	O	S	Se	0	1	0
			2976	1909	501	553	2	11			
1	J	383	Total	C	N	O	S	Se	0	0	0
			2970	1905	501	551	2	11			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q9X247
A	2	SER	-	expression tag	UNP Q9X247
A	3	LEU	-	expression tag	UNP Q9X247
A	389	GLU	-	expression tag	UNP Q9X247
A	390	GLY	-	expression tag	UNP Q9X247
A	391	HIS	-	expression tag	UNP Q9X247
A	392	HIS	-	expression tag	UNP Q9X247
A	393	HIS	-	expression tag	UNP Q9X247
A	394	HIS	-	expression tag	UNP Q9X247

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Chain	Residue	Modelled	Actual	Comment	Reference
A	395	HIS	-	expression tag	UNP Q9X247
A	396	HIS	-	expression tag	UNP Q9X247
B	1	MSE	-	expression tag	UNP Q9X247
B	2	SER	-	expression tag	UNP Q9X247
B	3	LEU	-	expression tag	UNP Q9X247
B	389	GLU	-	expression tag	UNP Q9X247
B	390	GLY	-	expression tag	UNP Q9X247
B	391	HIS	-	expression tag	UNP Q9X247
B	392	HIS	-	expression tag	UNP Q9X247
B	393	HIS	-	expression tag	UNP Q9X247
B	394	HIS	-	expression tag	UNP Q9X247
B	395	HIS	-	expression tag	UNP Q9X247
B	396	HIS	-	expression tag	UNP Q9X247
C	1	MSE	-	expression tag	UNP Q9X247
C	2	SER	-	expression tag	UNP Q9X247
C	3	LEU	-	expression tag	UNP Q9X247
C	389	GLU	-	expression tag	UNP Q9X247
C	390	GLY	-	expression tag	UNP Q9X247
C	391	HIS	-	expression tag	UNP Q9X247
C	392	HIS	-	expression tag	UNP Q9X247
C	393	HIS	-	expression tag	UNP Q9X247
C	394	HIS	-	expression tag	UNP Q9X247
C	395	HIS	-	expression tag	UNP Q9X247
C	396	HIS	-	expression tag	UNP Q9X247
D	1	MSE	-	expression tag	UNP Q9X247
D	2	SER	-	expression tag	UNP Q9X247
D	3	LEU	-	expression tag	UNP Q9X247
D	389	GLU	-	expression tag	UNP Q9X247
D	390	GLY	-	expression tag	UNP Q9X247
D	391	HIS	-	expression tag	UNP Q9X247
D	392	HIS	-	expression tag	UNP Q9X247
D	393	HIS	-	expression tag	UNP Q9X247
D	394	HIS	-	expression tag	UNP Q9X247
D	395	HIS	-	expression tag	UNP Q9X247
D	396	HIS	-	expression tag	UNP Q9X247
E	1	MSE	-	expression tag	UNP Q9X247
E	2	SER	-	expression tag	UNP Q9X247
E	3	LEU	-	expression tag	UNP Q9X247
E	389	GLU	-	expression tag	UNP Q9X247
E	390	GLY	-	expression tag	UNP Q9X247
E	391	HIS	-	expression tag	UNP Q9X247
E	392	HIS	-	expression tag	UNP Q9X247

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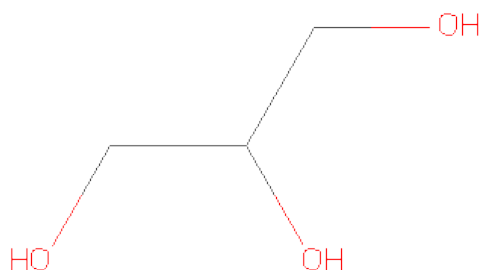
Chain	Residue	Modelled	Actual	Comment	Reference
E	393	HIS	-	expression tag	UNP Q9X247
E	394	HIS	-	expression tag	UNP Q9X247
E	395	HIS	-	expression tag	UNP Q9X247
E	396	HIS	-	expression tag	UNP Q9X247
F	1	MSE	-	expression tag	UNP Q9X247
F	2	SER	-	expression tag	UNP Q9X247
F	3	LEU	-	expression tag	UNP Q9X247
F	389	GLU	-	expression tag	UNP Q9X247
F	390	GLY	-	expression tag	UNP Q9X247
F	391	HIS	-	expression tag	UNP Q9X247
F	392	HIS	-	expression tag	UNP Q9X247
F	393	HIS	-	expression tag	UNP Q9X247
F	394	HIS	-	expression tag	UNP Q9X247
F	395	HIS	-	expression tag	UNP Q9X247
F	396	HIS	-	expression tag	UNP Q9X247
G	1	MSE	-	expression tag	UNP Q9X247
G	2	SER	-	expression tag	UNP Q9X247
G	3	LEU	-	expression tag	UNP Q9X247
G	389	GLU	-	expression tag	UNP Q9X247
G	390	GLY	-	expression tag	UNP Q9X247
G	391	HIS	-	expression tag	UNP Q9X247
G	392	HIS	-	expression tag	UNP Q9X247
G	393	HIS	-	expression tag	UNP Q9X247
G	394	HIS	-	expression tag	UNP Q9X247
G	395	HIS	-	expression tag	UNP Q9X247
G	396	HIS	-	expression tag	UNP Q9X247
H	1	MSE	-	expression tag	UNP Q9X247
H	2	SER	-	expression tag	UNP Q9X247
H	3	LEU	-	expression tag	UNP Q9X247
H	389	GLU	-	expression tag	UNP Q9X247
H	390	GLY	-	expression tag	UNP Q9X247
H	391	HIS	-	expression tag	UNP Q9X247
H	392	HIS	-	expression tag	UNP Q9X247
H	393	HIS	-	expression tag	UNP Q9X247
H	394	HIS	-	expression tag	UNP Q9X247
H	395	HIS	-	expression tag	UNP Q9X247
H	396	HIS	-	expression tag	UNP Q9X247
I	1	MSE	-	expression tag	UNP Q9X247
I	2	SER	-	expression tag	UNP Q9X247
I	3	LEU	-	expression tag	UNP Q9X247
I	389	GLU	-	expression tag	UNP Q9X247
I	390	GLY	-	expression tag	UNP Q9X247

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Chain	Residue	Modelled	Actual	Comment	Reference
I	391	HIS	-	expression tag	UNP Q9X247
I	392	HIS	-	expression tag	UNP Q9X247
I	393	HIS	-	expression tag	UNP Q9X247
I	394	HIS	-	expression tag	UNP Q9X247
I	395	HIS	-	expression tag	UNP Q9X247
I	396	HIS	-	expression tag	UNP Q9X247
J	1	MSE	-	expression tag	UNP Q9X247
J	2	SER	-	expression tag	UNP Q9X247
J	3	LEU	-	expression tag	UNP Q9X247
J	389	GLU	-	expression tag	UNP Q9X247
J	390	GLY	-	expression tag	UNP Q9X247
J	391	HIS	-	expression tag	UNP Q9X247
J	392	HIS	-	expression tag	UNP Q9X247
J	393	HIS	-	expression tag	UNP Q9X247
J	394	HIS	-	expression tag	UNP Q9X247
J	395	HIS	-	expression tag	UNP Q9X247
J	396	HIS	-	expression tag	UNP Q9X247

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	229	Total	O	0	0
			229	229		
3	B	179	Total	O	0	0
			179	179		
3	C	213	Total	O	0	0
			213	213		
3	D	188	Total	O	0	0
			188	188		
3	E	167	Total	O	0	0
			167	167		
3	F	199	Total	O	0	0
			199	199		
3	G	170	Total	O	0	0
			170	170		
3	H	149	Total	O	0	0
			149	149		
3	I	136	Total	O	0	0
			136	136		
3	J	142	Total	O	0	0
			142	142		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: amidohydrolase

Chain A: 



- Molecule 1: amidohydrolase

Chain B: 



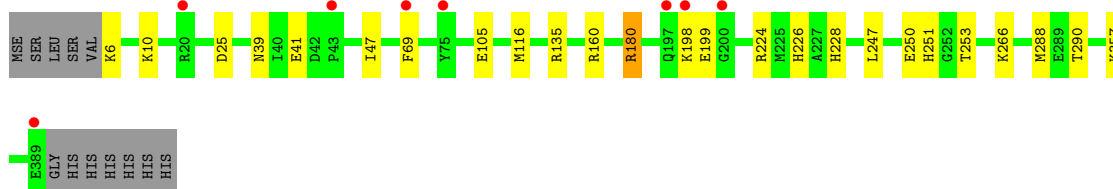
- Molecule 1: amidohydrolase

Chain C: 



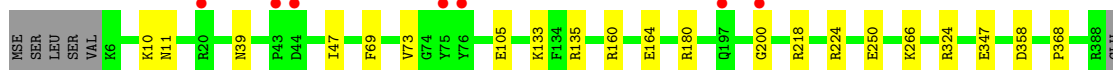
- Molecule 1: amidohydrolase

Chain D: 



- Molecule 1: amidohydrolase

Chain E: 



GLY
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 1: amidohydrolase

Chain F:

MSE SER LEU SER VAL K10 E38 E41 D42 P43 D44 I47 F69 S130 R135 E141 D146 K166 L195 A196 Q197 K198 E199 G200 K201 V212 H226 L247 H251 K266 M288 E313 K357 P368 E389 GLY HIS HIS HIS

HIS
HIS
HIS

- Molecule 1: amidohydrolase

Chain G:

MSE SER LEU SER VAL K6 R20 K23 P43 D44 I47 Y75 Q100 M116 R135 K166 K185 Q197 G198 E199 G200 H226 A227 H228 H251 G252 T253 K260 M323 R324 E347 K357 F369 R388 GLY HIS HIS HIS HIS HIS HIS

HIS

- Molecule 1: amidohydrolase

Chain H:

MSE SER LEU SER VAL K6 K10 R20 N30 E34 E38 N39 I40 E41 D42 P43 D44 L55 F69 V73 G74 Y75 E105 M116 R135 R160 K166 R180 K185 E194 E199 G200 E205 R224 M225 H226 L247 E250 H251

K265 K356 K357 P368 R388 GLY HIS HIS HIS HIS HIS HIS

- Molecule 1: amidohydrolase

Chain I:

MSE SER LEU SER VAL K6 R20 K23 N30 E38 N39 P43 D44 I47 F69 Y75 K92 M116 R135 E140 R160 K166 R180 L195 A196 Q197 K198 E199 G200 H226 H251 K257 K260 K266 D285 M288

E313 R324 P368 R388 GLY HIS HIS HIS HIS HIS HIS

- Molecule 1: amidohydrolase

Chain J:

MSE SER LEU SER VAL K6 K10 R20 K23 E38 N39 I40 E41 D42 P43 D44 L55 F69 V73 G74 Y75 L94 M116 R135 I143 R160 R180 K185 E194 Q197 K198 H226 H251 M288 R324 E347 K357

R388 GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.45Å 148.30Å 195.02Å 90.00° 105.31° 90.00°	Depositor
Resolution (Å)	19.92 – 2.06 19.92 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.92-2.06) 98.4 (19.92-2.06)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.167 , 0.213 0.173 , 0.218	Depositor DCC
R_{free} test set	12737 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 252990 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31584	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	0/3034	0.68	0/4078
1	B	0.53	0/3016	0.64	0/4054
1	C	0.58	0/3051	0.67	1/4101 (0.0%)
1	D	0.56	0/3025	0.63	0/4066
1	E	0.56	0/3016	0.65	0/4054
1	F	0.57	0/3032	0.64	0/4076
1	G	0.54	0/3023	0.65	0/4064
1	H	0.53	0/3025	0.65	0/4066
1	I	0.53	0/3025	0.62	0/4066
1	J	0.52	0/3016	0.61	0/4054
All	All	0.55	0/30263	0.65	1/40679 (0.0%)

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	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	200	GLY	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2985	0	0	7	0
1	B	2970	0	0	6	0
1	C	2996	0	0	6	0
1	D	2979	0	0	6	0
1	E	2970	0	0	7	0
1	F	2986	0	0	6	0
1	G	2974	0	0	5	0
1	H	2976	0	0	7	0
1	I	2976	0	0	11	0
1	J	2970	0	0	6	0
2	A	6	0	8	1	0
2	C	6	0	8	2	0
2	E	6	0	8	1	0
2	F	6	0	8	0	0
2	H	6	0	8	0	0
3	A	229	0	0	3	0
3	B	179	0	0	2	0
3	C	213	0	0	2	0
3	D	188	0	0	2	0
3	E	167	0	0	4	0
3	F	199	0	0	1	0
3	G	170	0	0	1	0
3	H	149	0	0	3	0
3	I	136	0	0	6	0
3	J	142	0	0	1	0
All	All	31584	0	40	63	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:180:ARG:NH1	3:H:1715:HOH:O	2.28	0.66
1:G:323:MSE:CE	1:G:369:PHE:CD2	2.79	0.64
1:J:160:ARG:NE	3:J:751:HOH:O	2.31	0.63
1:C:247:LEU:O	2:C:500:GOL:H32	1.99	0.62
1:A:288:MSE:N	2:A:500:GOL:HO1	1.99	0.60
1:I:313:GLU:OE1	3:I:931:HOH:O	2.15	0.59
1:E:160:ARG:NE	3:E:1132:HOH:O	2.35	0.59
1:E:180:ARG:NH1	3:E:613:HOH:O	2.35	0.59
1:G:226:HIS:CD2	1:G:251:HIS:CD2	2.91	0.58
1:A:160:ARG:NE	3:A:492:HOH:O	2.37	0.58
1:F:313:GLU:OE1	3:F:1123:HOH:O	2.18	0.54
1:D:226:HIS:CD2	1:D:251:HIS:CD2	2.97	0.53
1:B:226:HIS:CD2	1:B:251:HIS:CD2	2.97	0.53
1:A:116:MSE:CE	1:A:224:ARG:NH1	2.72	0.53
1:I:180:ARG:NH1	3:I:814:HOH:O	2.42	0.52
2:E:500:GOL:HO3	1:I:288:MSE:N	2.08	0.51
1:A:388:ARG:O	1:A:389:GLU:CB	2.60	0.50
1:B:195:LEU:O	1:B:199:GLU:CG	2.61	0.49
1:C:6:LYS:N	3:C:486:HOH:O	2.45	0.48
1:C:389:GLU:CD	1:C:389:GLU:N	2.66	0.48
1:E:133:LYS:NZ	1:E:358:ASP:OD2	2.47	0.48
1:I:166:LYS:NZ	3:I:1054:HOH:O	2.47	0.48
3:E:426:HOH:O	1:H:205:GLU:CG	2.61	0.48
1:I:195:LEU:O	1:I:199:GLU:CG	2.62	0.48
1:G:100:GLN:NE2	3:G:828:HOH:O	2.47	0.47
1:B:180:ARG:NH1	3:B:789:HOH:O	2.47	0.47
1:F:226:HIS:CD2	1:F:251:HIS:CD2	3.02	0.47
1:J:94:LEU:CD1	1:J:143:ILE:CD1	2.93	0.46
1:I:226:HIS:CD2	1:I:251:HIS:CD2	3.03	0.46
1:B:160:ARG:NE	3:B:506:HOH:O	2.48	0.46
1:D:10:LYS:NZ	1:D:25:ASP:OD2	2.48	0.46
1:C:247:LEU:O	2:C:500:GOL:H12	2.15	0.46
1:C:257:LYS:NZ	1:C:285:ASP:OD2	2.49	0.46
1:F:130:SER:OG	1:F:146:ASP:OD1	2.34	0.45
1:H:226:HIS:CD2	1:H:251:HIS:CD2	3.04	0.45
1:B:228:HIS:ND1	1:B:253:THR:OG1	2.50	0.44
1:H:224:ARG:NE	1:H:250:GLU:OE1	2.51	0.44
1:A:228:HIS:ND1	1:A:253:THR:OG1	2.50	0.44
1:I:257:LYS:NZ	1:I:285:ASP:OD2	2.50	0.44
1:H:160:ARG:NE	3:H:1446:HOH:O	2.51	0.44
1:D:160:ARG:NE	3:D:547:HOH:O	2.51	0.44
1:D:180:ARG:NH1	3:D:1694:HOH:O	2.50	0.44
1:G:228:HIS:ND1	1:G:253:THR:OG1	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:368:PRO:O	1:G:324:ARG:NH2	2.51	0.43
1:E:368:PRO:O	1:I:324:ARG:NH2	2.51	0.43
1:A:313:GLU:OE1	3:A:690:HOH:O	2.21	0.43
1:C:349:ARG:NH2	3:C:1011:HOH:O	2.51	0.43
1:E:224:ARG:NE	1:E:250:GLU:OE1	2.52	0.43
1:I:160:ARG:NE	3:I:919:HOH:O	2.52	0.42
3:I:1364:HOH:O	1:J:180:ARG:NH1	2.52	0.42
1:D:224:ARG:NE	1:D:250:GLU:OE1	2.52	0.42
1:H:368:PRO:O	1:J:324:ARG:NH2	2.51	0.42
1:F:135:ARG:CD	1:F:141:GLU:O	2.67	0.42
1:A:349:ARG:NH2	3:A:1603:HOH:O	2.52	0.42
1:H:265:LYS:NZ	3:H:645:HOH:O	2.52	0.42
1:E:324:ARG:NH2	1:I:368:PRO:O	2.53	0.42
1:B:10:LYS:NZ	1:B:25:ASP:OD2	2.53	0.41
1:E:218:ARG:NH2	3:E:1183:HOH:O	2.53	0.41
1:J:226:HIS:CD2	1:J:251:HIS:CD2	3.09	0.41
1:I:92:LYS:CE	3:I:1162:HOH:O	2.68	0.41
1:F:195:LEU:O	1:F:199:GLU:CG	2.69	0.41
1:D:228:HIS:ND1	1:D:253:THR:OG1	2.53	0.41
1:J:347:GLU:O	1:J:357:LYS:NZ	2.55	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	383/396 (97%)	373 (97%)	10 (3%)	0	100	100
1	B	381/396 (96%)	369 (97%)	12 (3%)	0	100	100
1	C	385/396 (97%)	372 (97%)	13 (3%)	0	100	100
1	D	382/396 (96%)	370 (97%)	12 (3%)	0	100	100
1	E	381/396 (96%)	367 (96%)	14 (4%)	0	100	100
1	F	383/396 (97%)	369 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	382/396 (96%)	372 (97%)	10 (3%)	0	100	100
1	H	382/396 (96%)	370 (97%)	12 (3%)	0	100	100
1	I	382/396 (96%)	369 (97%)	13 (3%)	0	100	100
1	J	381/396 (96%)	370 (97%)	11 (3%)	0	100	100
All	All	3822/3960 (96%)	3701 (97%)	121 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	323/321 (101%)	309 (96%)	14 (4%)	40	31
1	B	321/321 (100%)	311 (97%)	10 (3%)	52	45
1	C	325/321 (101%)	314 (97%)	11 (3%)	49	42
1	D	322/321 (100%)	306 (95%)	16 (5%)	34	23
1	E	321/321 (100%)	310 (97%)	11 (3%)	49	42
1	F	323/321 (101%)	310 (96%)	13 (4%)	42	34
1	G	322/321 (100%)	309 (96%)	13 (4%)	42	34
1	H	322/321 (100%)	305 (95%)	17 (5%)	32	21
1	I	322/321 (100%)	313 (97%)	9 (3%)	56	50
1	J	321/321 (100%)	307 (96%)	14 (4%)	39	29
All	All	3222/3210 (100%)	3094 (96%)	128 (4%)	42	34

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	41	GLU
1	A	47	ILE
1	A	69	PHE
1	A	73	VAL

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Mol	Chain	Res	Type
1	A	105	GLU
1	A	116	MSE
1	A	166	LYS
1	A	197	GLN
1	A	198	LYS
1	A	205	GLU
1	A	266	LYS
1	A	288	MSE
1	A	389	GLU
1	B	23	LYS
1	B	41	GLU
1	B	69	PHE
1	B	73	VAL
1	B	116	MSE
1	B	185	LYS
1	B	198	LYS
1	B	247	LEU
1	B	266	LYS
1	B	288	MSE
1	C	39	ASN
1	C	47	ILE
1	C	69	PHE
1	C	73	VAL
1	C	116	MSE
1	C	128	GLN
1	C	135	ARG
1	C	185	LYS
1	C	266	LYS
1	C	288	MSE
1	C	389	GLU
1	D	6	LYS
1	D	39	ASN
1	D	41	GLU
1	D	47	ILE
1	D	69	PHE
1	D	105	GLU
1	D	116	MSE
1	D	135	ARG
1	D	180	ARG
1	D	198	LYS
1	D	199	GLU
1	D	247	LEU

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Mol	Chain	Res	Type
1	D	266	LYS
1	D	288	MSE
1	D	290	THR
1	D	357	LYS
1	E	10	LYS
1	E	11	ASN
1	E	39	ASN
1	E	47	ILE
1	E	69	PHE
1	E	73	VAL
1	E	105	GLU
1	E	135	ARG
1	E	164	GLU
1	E	266	LYS
1	E	347	GLU
1	F	10	LYS
1	F	38	GLU
1	F	41	GLU
1	F	47	ILE
1	F	69	PHE
1	F	135	ARG
1	F	166	LYS
1	F	198	LYS
1	F	212	VAL
1	F	247	LEU
1	F	266	LYS
1	F	288	MSE
1	F	357	LYS
1	G	20	ARG
1	G	23	LYS
1	G	44	ASP
1	G	47	ILE
1	G	116	MSE
1	G	135	ARG
1	G	166	LYS
1	G	185	LYS
1	G	198	LYS
1	G	199	GLU
1	G	260	LYS
1	G	347	GLU
1	G	357	LYS
1	H	6	LYS

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Mol	Chain	Res	Type
1	H	10	LYS
1	H	34	GLU
1	H	39	ASN
1	H	41	GLU
1	H	55	LEU
1	H	69	PHE
1	H	73	VAL
1	H	105	GLU
1	H	116	MSE
1	H	135	ARG
1	H	166	LYS
1	H	185	LYS
1	H	194	GLU
1	H	199	GLU
1	H	247	LEU
1	H	357	LYS
1	I	23	LYS
1	I	39	ASN
1	I	47	ILE
1	I	116	MSE
1	I	135	ARG
1	I	140	GLU
1	I	198	LYS
1	I	266	LYS
1	I	288	MSE
1	J	10	LYS
1	J	20	ARG
1	J	23	LYS
1	J	38	GLU
1	J	39	ASN
1	J	55	LEU
1	J	69	PHE
1	J	73	VAL
1	J	116	MSE
1	J	135	ARG
1	J	185	LYS
1	J	194	GLU
1	J	198	LYS
1	J	288	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	500	-	5,5,5	0.39	0	5,5,5	0.36	0
2	GOL	C	500	-	5,5,5	0.37	0	5,5,5	0.60	0
2	GOL	E	500	-	5,5,5	0.31	0	5,5,5	0.72	0
2	GOL	F	500	-	5,5,5	0.31	0	5,5,5	0.52	0
2	GOL	H	500	-	5,5,5	0.29	0	5,5,5	0.48	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	500	-	-	0/4/4/4	0/0/0/0
2	GOL	C	500	-	-	0/4/4/4	0/0/0/0
2	GOL	E	500	-	-	0/4/4/4	0/0/0/0
2	GOL	F	500	-	-	0/4/4/4	0/0/0/0
2	GOL	H	500	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	384/396 (96%)	-0.42	4 (1%) 79 81	15, 21, 40, 54	0
1	B	383/396 (96%)	-0.25	10 (2%) 53 55	16, 25, 51, 73	0
1	C	384/396 (96%)	-0.42	4 (1%) 79 81	16, 23, 37, 53	0
1	D	384/396 (96%)	-0.30	8 (2%) 60 62	17, 24, 46, 68	0
1	E	383/396 (96%)	-0.37	7 (1%) 65 68	17, 26, 42, 65	0
1	F	385/396 (97%)	-0.33	9 (2%) 57 59	16, 24, 44, 67	0
1	G	383/396 (96%)	-0.27	6 (1%) 68 72	17, 26, 48, 69	0
1	H	383/396 (96%)	-0.26	10 (2%) 53 55	17, 27, 52, 71	0
1	I	383/396 (96%)	-0.15	12 (3%) 47 47	18, 29, 56, 81	0
1	J	383/396 (96%)	-0.18	8 (2%) 60 62	19, 30, 53, 78	0
All	All	3835/3960 (96%)	-0.29	78 (2%) 62 64	15, 26, 49, 81	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	200	GLY	6.4
1	D	200	GLY	5.8
1	H	44	ASP	5.4
1	J	75	TYR	5.4
1	G	75	TYR	5.3
1	I	75	TYR	5.1
1	I	43	PRO	4.6
1	B	198	LYS	4.5
1	B	43	PRO	4.3
1	J	20	ARG	4.3
1	G	200	GLY	4.3
1	A	75	TYR	4.3
1	C	75	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	75	TYR	4.2
1	H	75	TYR	4.0
1	D	75	TYR	3.9
1	B	38	GLU	3.9
1	E	200	GLY	3.6
1	C	389	GLU	3.5
1	B	197	GLN	3.4
1	F	44	ASP	3.4
1	D	197	GLN	3.4
1	J	43	PRO	3.4
1	I	44	ASP	3.3
1	I	20	ARG	3.3
1	B	200	GLY	3.2
1	H	43	PRO	3.1
1	A	389	GLU	3.0
1	C	43	PRO	3.0
1	E	44	ASP	2.9
1	D	389	GLU	2.9
1	F	5	VAL	2.9
1	F	389	GLU	2.9
1	F	43	PRO	2.8
1	J	44	ASP	2.8
1	E	43	PRO	2.7
1	G	198	LYS	2.7
1	I	47	ILE	2.7
1	H	200	GLY	2.6
1	G	197	GLN	2.6
1	H	30	ASN	2.6
1	I	69	PHE	2.6
1	E	20	ARG	2.6
1	H	39	ASN	2.5
1	B	75	TYR	2.5
1	B	201	LYS	2.4
1	F	198	LYS	2.4
1	H	38	GLU	2.4
1	A	76	TYR	2.4
1	I	198	LYS	2.4
1	B	199	GLU	2.4
1	I	30	ASN	2.4
1	I	197	GLN	2.3
1	I	260	LYS	2.3
1	E	197	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	43	PRO	2.3
1	F	199	GLU	2.3
1	H	356	GLY	2.3
1	F	201	LYS	2.3
1	J	198	LYS	2.2
1	G	20	ARG	2.2
1	H	20	ARG	2.2
1	B	76	TYR	2.2
1	F	197	GLN	2.2
1	D	198	LYS	2.2
1	D	43	PRO	2.2
1	I	38	GLU	2.1
1	D	69	PHE	2.1
1	J	41	GLU	2.1
1	D	20	ARG	2.1
1	C	44	ASP	2.1
1	J	197	GLN	2.1
1	F	200	GLY	2.1
1	B	44	ASP	2.1
1	E	76	TYR	2.1
1	H	41	GLU	2.0
1	J	38	GLU	2.0
1	A	43	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	E	500	6/6	0.18	2.45	38,41,42,42	0
2	GOL	C	500	6/6	0.23	2.41	50,52,56,56	0
2	GOL	H	500	6/6	0.15	1.92	54,54,56,56	0
2	GOL	F	500	6/6	0.14	1.58	27,28,29,29	0
2	GOL	A	500	6/6	0.12	0.88	36,37,37,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.