



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 08:07 AM EST

PDB ID : 2IGS  
Title : Crystal Structure of the Protein of Unknown Function from *Pseudomonas aeruginosa*  
Authors : Kim, Y.; Joachimiak, A.; Skarina, T.; Egorova, O.; Edwards, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2006-09-25  
Resolution : 2.17 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](mailto: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:

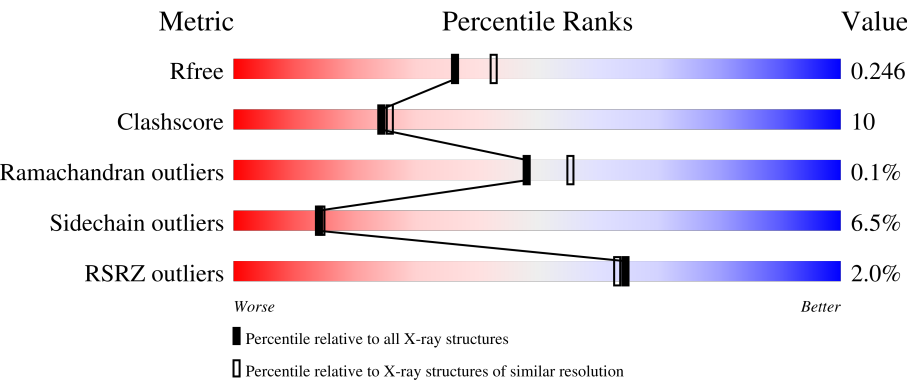
MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 2.17 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 <sub>free</sub>	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (2.20-2.16)

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  $\geq 3$ , 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	219	<div><div>3%</div><div>82%</div><div>14%</div><div>..</div></div>
1	B	219	<div><div>2%</div><div>80%</div><div>15%</div><div>..</div></div>
1	C	219	<div><div>%</div><div>79%</div><div>15%</div><div>..</div></div>
1	D	219	<div><div>79%</div><div>15%</div><div>..</div></div>
1	E	219	<div><div>3%</div><div>73%</div><div>21%</div><div>..</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	219	<p>2% 72% 20% 6%</p>
1	G	219	<p>1% 79% 16%</p>
1	H	219	<p>4% 80% 14%</p>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15080 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 Hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	Se	0	9	0
			1721	1095	295	326	2	3			
1	B	214	Total	C	N	O	S	Se	0	10	0
			1752	1110	305	332	2	3			
1	C	213	Total	C	N	O	S	Se	0	11	0
			1757	1113	307	332	2	3			
1	D	213	Total	C	N	O	S	Se	0	7	0
			1700	1081	293	321	2	3			
1	E	214	Total	C	N	O	S	Se	0	13	0
			1770	1119	314	332	2	3			
1	F	215	Total	C	N	O	S	Se	0	13	0
			1774	1123	311	335	2	3			
1	G	214	Total	C	N	O	S	Se	0	11	0
			1740	1102	301	332	2	3			
1	H	214	Total	C	N	O	S	Se	0	7	0
			1704	1083	290	326	2	3			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q9I1P7
A	0	HIS	-	cloning artifact	UNP Q9I1P7
A	1	MSE	MET	modified residue	UNP Q9I1P7
A	81	MSE	MET	modified residue	UNP Q9I1P7
A	100	MSE	MET	modified residue	UNP Q9I1P7
A	165	MSE	MET	modified residue	UNP Q9I1P7
A	216	GLY	-	cloning artifact	UNP Q9I1P7
A	217	SER	-	cloning artifact	UNP Q9I1P7
B	-1	GLY	-	cloning artifact	UNP Q9I1P7
B	0	HIS	-	cloning artifact	UNP Q9I1P7
B	1	MSE	MET	modified residue	UNP Q9I1P7
B	81	MSE	MET	modified residue	UNP Q9I1P7
B	100	MSE	MET	modified residue	UNP Q9I1P7

*Continued on next page...*

*Continued from previous page...*

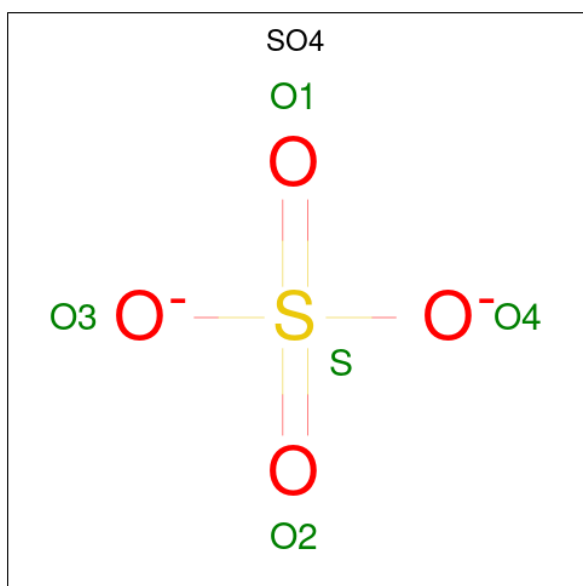
Chain	Residue	Modelled	Actual	Comment	Reference
B	165	MSE	MET	modified residue	UNP Q9I1P7
B	216	GLY	-	cloning artifact	UNP Q9I1P7
B	217	SER	-	cloning artifact	UNP Q9I1P7
C	-1	GLY	-	cloning artifact	UNP Q9I1P7
C	0	HIS	-	cloning artifact	UNP Q9I1P7
C	1	MSE	MET	modified residue	UNP Q9I1P7
C	81	MSE	MET	modified residue	UNP Q9I1P7
C	100	MSE	MET	modified residue	UNP Q9I1P7
C	165	MSE	MET	modified residue	UNP Q9I1P7
C	216	GLY	-	cloning artifact	UNP Q9I1P7
C	217	SER	-	cloning artifact	UNP Q9I1P7
D	-1	GLY	-	cloning artifact	UNP Q9I1P7
D	0	HIS	-	cloning artifact	UNP Q9I1P7
D	1	MSE	MET	modified residue	UNP Q9I1P7
D	81	MSE	MET	modified residue	UNP Q9I1P7
D	100	MSE	MET	modified residue	UNP Q9I1P7
D	165	MSE	MET	modified residue	UNP Q9I1P7
D	216	GLY	-	cloning artifact	UNP Q9I1P7
D	217	SER	-	cloning artifact	UNP Q9I1P7
E	-1	GLY	-	cloning artifact	UNP Q9I1P7
E	0	HIS	-	cloning artifact	UNP Q9I1P7
E	1	MSE	MET	modified residue	UNP Q9I1P7
E	81	MSE	MET	modified residue	UNP Q9I1P7
E	100	MSE	MET	modified residue	UNP Q9I1P7
E	165	MSE	MET	modified residue	UNP Q9I1P7
E	216	GLY	-	cloning artifact	UNP Q9I1P7
E	217	SER	-	cloning artifact	UNP Q9I1P7
F	-1	GLY	-	cloning artifact	UNP Q9I1P7
F	0	HIS	-	cloning artifact	UNP Q9I1P7
F	1	MSE	MET	modified residue	UNP Q9I1P7
F	81	MSE	MET	modified residue	UNP Q9I1P7
F	100	MSE	MET	modified residue	UNP Q9I1P7
F	165	MSE	MET	modified residue	UNP Q9I1P7
F	216	GLY	-	cloning artifact	UNP Q9I1P7
F	217	SER	-	cloning artifact	UNP Q9I1P7
G	-1	GLY	-	cloning artifact	UNP Q9I1P7
G	0	HIS	-	cloning artifact	UNP Q9I1P7
G	1	MSE	MET	modified residue	UNP Q9I1P7
G	81	MSE	MET	modified residue	UNP Q9I1P7
G	100	MSE	MET	modified residue	UNP Q9I1P7
G	165	MSE	MET	modified residue	UNP Q9I1P7
G	216	GLY	-	cloning artifact	UNP Q9I1P7

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	217	SER	-	cloning artifact	UNP Q9I1P7
H	-1	GLY	-	cloning artifact	UNP Q9I1P7
H	0	HIS	-	cloning artifact	UNP Q9I1P7
H	1	MSE	MET	modified residue	UNP Q9I1P7
H	81	MSE	MET	modified residue	UNP Q9I1P7
H	100	MSE	MET	modified residue	UNP Q9I1P7
H	165	MSE	MET	modified residue	UNP Q9I1P7
H	216	GLY	-	cloning artifact	UNP Q9I1P7
H	217	SER	-	cloning artifact	UNP Q9I1P7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



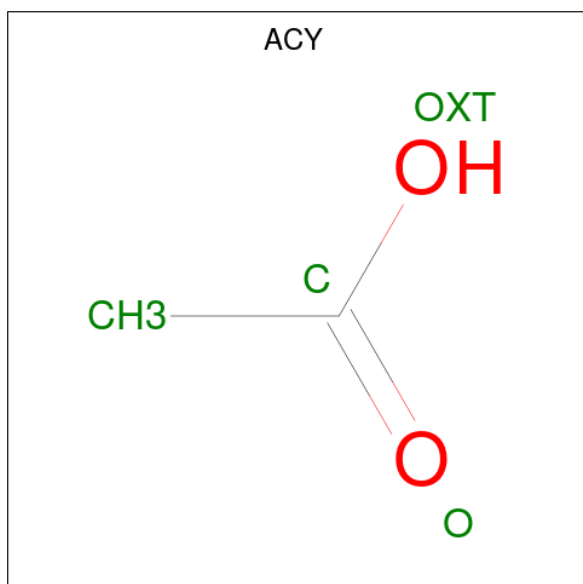
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



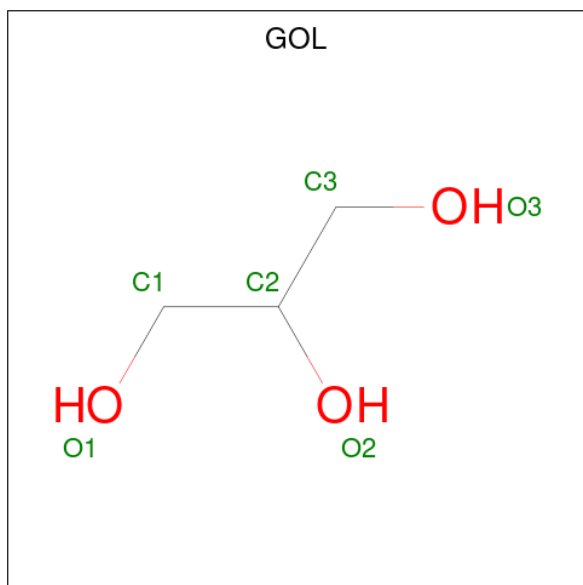
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	135	Total	O	0	0
			135	135		
5	B	141	Total	O	0	2
			141	141		
5	C	130	Total	O	0	2
			130	130		
5	D	130	Total	O	0	0
			130	130		
5	E	136	Total	O	0	4
			136	136		

Continued on next page...

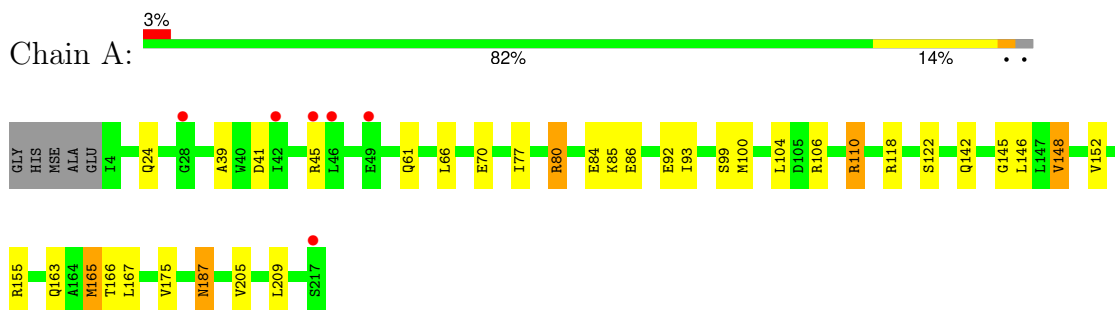
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	117	Total 117	O 117	0	0
5	G	135	Total 135	O 135	0	0
5	H	135	Total 135	O 135	0	0

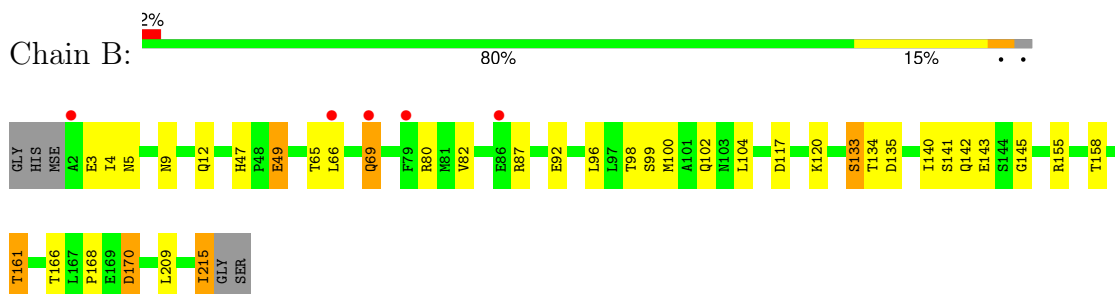
### 3 Residue-property plots [i](#)

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.

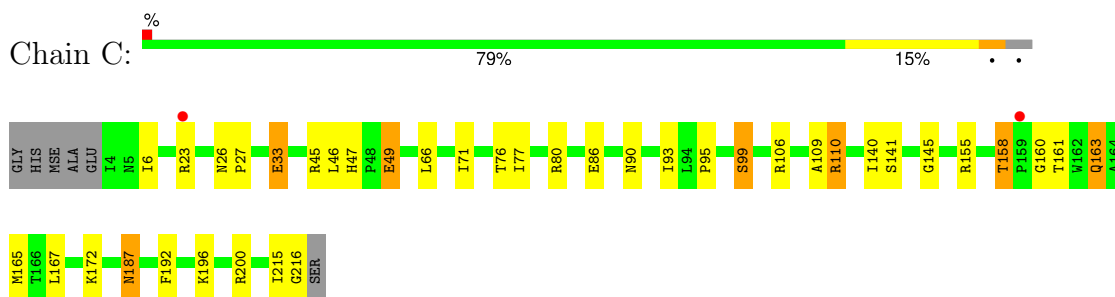
#### • Molecule 1: Hypothetical protein



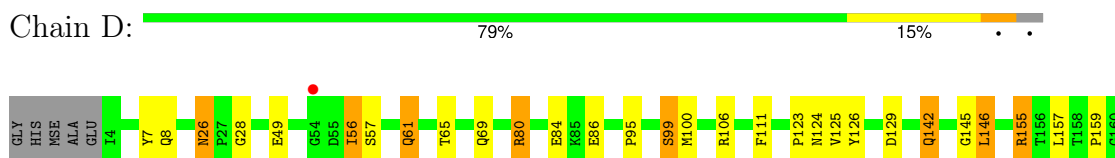
#### • Molecule 1: Hypothetical protein



#### • Molecule 1: Hypothetical protein



#### • Molecule 1: Hypothetical protein

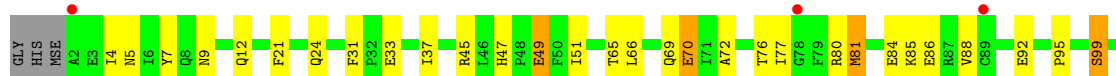




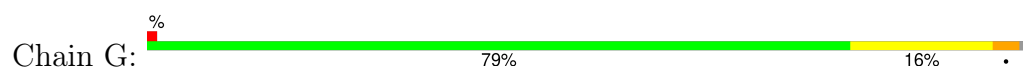
- Molecule 1: Hypothetical protein



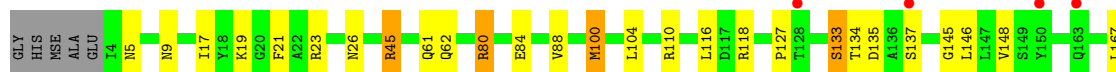
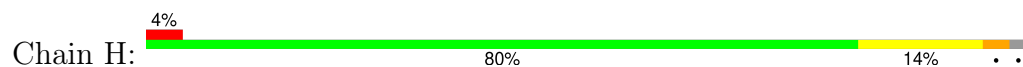
- Molecule 1: Hypothetical protein



- Molecule 1: Hypothetical protein



- Molecule 1: Hypothetical protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.42Å 100.46Å 140.84Å 90.00° 100.33° 90.00°	Depositor
Resolution (Å)	28.52 – 2.17 28.52 – 2.17	Depositor EDS
% Data completeness (in resolution range)	96.6 (28.52-2.17) 96.5 (28.52-2.17)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.187 , 0.250 0.185 , 0.246	Depositor DCC
$R_{free}$ test set	10729 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtrriage
Anisotropy	0.583	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.43 % 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 2.7407e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.59	0/1754	0.71	2/2377 (0.1%)
1	B	0.64	0/1785	0.70	0/2418
1	C	0.57	0/1789	0.66	0/2421
1	D	0.61	0/1733	0.71	2/2350 (0.1%)
1	E	0.62	0/1803	0.71	1/2441 (0.0%)
1	F	0.56	0/1807	0.70	0/2446
1	G	0.65	0/1773	0.72	2/2403 (0.1%)
1	H	0.62	0/1737	0.74	3/2356 (0.1%)
All	All	0.61	0/14181	0.71	10/19212 (0.1%)

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	H	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	216	GLY	N-CA-C	-7.15	95.22	113.10
1	A	80	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	H	80	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	80	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	80	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	H	80	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	E	80	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	D	155	ARG	NE-CZ-NH2	-5.22	117.69	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	170[A]	ASP	CB-CG-OD1	5.18	122.96	118.30
1	G	170[B]	ASP	CB-CG-OD1	5.18	122.96	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	215	ILE	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1721	0	1704	25	0
1	B	1752	0	1727	30	0
1	C	1757	0	1733	28	0
1	D	1700	0	1680	40	0
1	E	1770	0	1751	57	1
1	F	1774	0	1749	61	0
1	G	1740	0	1709	29	0
1	H	1704	0	1678	28	0
2	A	15	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	F	5	0	0	0	0
2	G	10	0	0	0	0
2	H	15	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	8	0	6	0	0
3	F	8	0	6	0	0
3	G	4	0	3	0	0
3	H	4	0	3	0	0
4	D	6	0	8	3	0
5	A	135	0	0	4	0
5	B	141	0	0	4	0
5	C	130	0	0	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	130	0	0	2	0
5	E	136	0	0	15	0
5	F	117	0	0	9	0
5	G	135	0	0	6	1
5	H	135	0	0	7	0
All	All	15080	0	13763	275	1

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 10.

All (275) 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:G:157:LEU:HG	5:G:2137:HOH:O	1.18	1.30
1:D:161:THR:HG22	1:D:165:MSE:CE	1.75	1.16
1:D:8[B]:GLN:HE22	1:D:56:ILE:HG21	1.10	1.08
1:E:156:THR:HG21	5:E:226:HOH:O	1.56	1.04
1:F:158:THR:HB	1:F:161:THR:CG2	1.99	0.93
1:D:161:THR:HG22	1:D:165:MSE:HE3	1.53	0.90
1:B:134:THR:HG22	1:B:135:ASP:O	1.73	0.88
1:D:200:ARG:HH22	4:D:2022:GOL:H32	1.40	0.87
1:A:100:MSE:HE1	1:A:205:VAL:HG12	1.57	0.87
1:D:8[B]:GLN:NE2	1:D:56:ILE:HG21	1.88	0.87
1:F:157:LEU:CD1	1:F:165:MSE:HE1	2.04	0.87
1:C:196:LYS:HE3	1:G:189:SER:HB3	1.55	0.86
1:F:156:THR:HG22	5:F:2021:HOH:O	1.78	0.84
1:F:157:LEU:HD11	1:F:165:MSE:HE1	1.59	0.84
1:F:158:THR:HB	1:F:161:THR:HG23	1.56	0.84
1:D:161:THR:HG22	1:D:165:MSE:HE2	1.60	0.82
1:E:83:ASN:HB2	5:E:304:HOH:O	1.78	0.82
1:F:77:ILE:HD11	5:F:2027:HOH:O	1.77	0.82
1:E:79:PHE:O	1:E:82:VAL:HG22	1.79	0.81
1:A:187:ASN:HD22	1:A:187:ASN:H	1.27	0.80
1:F:157:LEU:HD11	1:F:165:MSE:CE	2.10	0.80
1:C:163[C]:GLN:NE2	1:D:126:TYR:OH	2.16	0.79
1:E:81:MSE:HE2	1:E:85:LYS:HA	1.66	0.78
1:C:158:THR:HG21	5:D:2131:HOH:O	1.83	0.78
1:A:106:ARG:NH1	1:D:216:GLY:O	2.17	0.78
1:E:45[B]:ARG:HD2	1:E:116:LEU:HD11	1.66	0.77
1:D:161:THR:CG2	1:D:165:MSE:CE	2.61	0.77
1:F:187:ASN:HD22	1:F:187:ASN:H	1.32	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110[A]:ARG:HH22	1:F:216:GLY:HA2	1.52	0.75
1:G:156:THR:HG21	5:G:2136:HOH:O	1.86	0.74
1:B:140:ILE:H	1:D:142:GLN:HE21	1.35	0.74
1:B:134:THR:HG21	1:F:134:THR:HG21	1.70	0.74
1:G:24:GLN:HB3	1:G:81:MSE:HE2	1.69	0.74
1:A:100:MSE:CE	1:A:205:VAL:HG12	2.16	0.74
1:D:200:ARG:HH22	4:D:2022:GOL:C3	2.01	0.73
1:F:106[A]:ARG:O	1:F:110[A]:ARG:HG3	1.89	0.73
1:H:170[A]:ASP:OD2	5:H:2145:HOH:O	2.07	0.73
1:G:19:LYS:HD3	5:G:2088:HOH:O	1.89	0.72
1:B:65:THR:O	1:B:69[B]:GLN:HG3	1.89	0.72
1:D:161:THR:CG2	1:D:165:MSE:HE2	2.20	0.72
1:F:81:MSE:HE2	1:F:81:MSE:HA	1.71	0.71
1:H:45:ARG:HG2	1:H:116:LEU:HD11	1.73	0.70
1:H:216:GLY:HA3	1:H:217:SER:C	2.12	0.70
1:A:61:GLN:HG3	5:A:2092:HOH:O	1.91	0.70
1:F:189:SER:HB3	5:F:2067:HOH:O	1.91	0.70
1:B:47:HIS:ND1	1:B:49[A]:GLU:OE1	2.21	0.70
1:C:158:THR:HG22	1:C:161:THR:H	1.57	0.69
1:A:100:MSE:HE2	1:A:209:LEU:HD12	1.74	0.69
1:D:200:ARG:NH2	4:D:2022:GOL:H32	2.07	0.68
1:D:8[B]:GLN:HE22	1:D:56:ILE:CG2	1.96	0.68
1:C:187[A]:ASN:H	1:C:187[A]:ASN:HD22	1.42	0.68
1:E:45[B]:ARG:NH2	5:E:313:HOH:O	2.22	0.68
1:E:92:GLU:OE2	5:E:341:HOH:O	2.12	0.68
1:F:86[B]:GLU:HG3	5:F:2086:HOH:O	1.92	0.68
1:D:159:PRO:O	1:D:163[B]:GLN:HG2	1.94	0.68
1:G:157:LEU:HD13	1:G:211:TYR:HE1	1.57	0.67
1:F:4:ILE:HD13	1:F:12:GLN:HG2	1.77	0.67
1:E:142:GLN:HA	1:E:183:LEU:HD11	1.77	0.67
1:C:76:THR:O	1:C:80[B]:ARG:HG2	1.94	0.67
1:D:26:ASN:HD22	1:D:28:GLY:H	1.42	0.67
1:F:110[A]:ARG:NH2	1:F:216:GLY:HA2	2.10	0.66
1:B:4:ILE:HD13	1:B:12:GLN:HG2	1.76	0.66
1:D:61:GLN:NE2	1:E:27:PRO:HD3	2.11	0.66
1:D:145:GLY:HA3	1:D:155:ARG:HB2	1.77	0.66
1:E:88:VAL:HG11	5:E:343:HOH:O	1.97	0.64
1:B:134:THR:CG2	1:B:135:ASP:O	2.45	0.64
1:F:134:THR:HG22	1:F:135:ASP:O	1.97	0.64
1:B:87[B]:ARG:NH2	1:B:170[B]:ASP:OD1	2.30	0.64
1:E:81:MSE:HE2	1:E:81:MSE:HA	1.79	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:THR:HG22	1:F:160:GLY:H	1.64	0.63
1:F:202:THR:HG21	5:F:2026:HOH:O	1.98	0.63
1:D:8[B]:GLN:NE2	1:D:56:ILE:CG2	2.59	0.63
1:H:193:ASN:HA	5:H:2135:HOH:O	1.99	0.62
1:C:192:PHE:CE1	1:G:193[B]:ASN:ND2	2.68	0.62
1:H:100:MSE:HG2	1:H:209:LEU:HD12	1.81	0.62
1:E:158:THR:HG22	1:E:160:GLY:H	1.65	0.61
1:B:170[A]:ASP:OD1	5:B:2087:HOH:O	2.16	0.61
1:B:215:ILE:C	5:B:2152:HOH:O	2.38	0.61
1:G:24:GLN:HB3	1:G:81:MSE:CE	2.31	0.60
1:F:31:PHE:HD1	1:F:33[B]:GLU:HG3	1.67	0.60
1:G:156:THR:HG22	5:G:2023:HOH:O	2.01	0.60
1:E:80:ARG:HD2	1:E:84:GLU:OE2	2.01	0.59
1:E:102[B]:GLN:OE1	1:E:106[B]:ARG:HD3	2.02	0.59
1:B:80:ARG:NH2	1:B:92:GLU:OE2	2.33	0.59
1:F:80:ARG:NH2	1:F:92:GLU:OE2	2.34	0.59
1:F:146:LEU:HD13	1:F:188:PHE:CZ	2.38	0.59
1:H:61:GLN:HG2	5:H:2027:HOH:O	2.02	0.59
1:E:145:GLY:HA3	1:E:155:ARG:HB2	1.84	0.59
1:G:95:PRO:O	1:G:99:SER:HB3	2.03	0.59
1:E:163:GLN:HE21	1:H:26:ASN:HD22	1.51	0.58
1:C:77:ILE:HG21	1:C:93:ILE:HD11	1.86	0.58
1:B:134:THR:HG21	1:F:134:THR:CG2	2.34	0.58
1:D:123:PRO:HG2	5:D:2148:HOH:O	2.04	0.58
1:F:157:LEU:HD13	1:F:165:MSE:HE1	1.83	0.58
1:H:110:ARG:HH22	1:H:216:GLY:H	1.51	0.58
1:F:81:MSE:HE3	1:F:88:VAL:HB	1.86	0.57
1:C:95:PRO:O	1:C:99:SER:HB3	2.04	0.57
1:C:106:ARG:O	1:C:110:ARG:HG2	2.04	0.57
1:F:81:MSE:HA	1:F:81:MSE:CE	2.34	0.57
1:C:165:MSE:HE2	1:C:167:LEU:HD22	1.86	0.57
5:B:2057:HOH:O	1:F:156:THR:HG21	2.05	0.57
1:A:100:MSE:HE1	1:A:205:VAL:CG1	2.32	0.56
1:A:187:ASN:H	1:A:187:ASN:ND2	2.02	0.56
1:C:109:ALA:HB2	5:C:2077:HOH:O	2.03	0.56
1:E:156:THR:HG22	5:E:222:HOH:O	2.05	0.56
1:G:81:MSE:HE1	1:G:85:LYS:HE3	1.88	0.56
1:E:200:ARG:NH2	5:E:334:HOH:O	2.38	0.56
1:A:99:SER:HB2	1:A:166:THR:HG22	1.86	0.56
1:A:24:GLN:O	1:A:85:LYS:NZ	2.39	0.56
1:C:145:GLY:HA3	1:C:155:ARG:HB2	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:MSE:CE	1:E:85:LYS:HA	2.35	0.56
1:H:133:SER:HB3	1:H:145:GLY:H	1.71	0.55
1:E:102[B]:GLN:OE1	1:E:106[B]:ARG:CD	2.54	0.55
1:F:157:LEU:HD11	1:F:165:MSE:HE3	1.89	0.55
1:H:134:THR:HG22	1:H:135:ASP:O	2.06	0.55
1:E:40:TRP:CZ2	1:E:202:THR:HG23	2.41	0.55
1:C:6:ILE:HD12	1:C:71:ILE:HD11	1.88	0.55
1:E:81:MSE:HE3	1:E:88:VAL:HB	1.86	0.55
1:H:19:LYS:HE3	1:H:23[B]:ARG:HH22	1.72	0.55
1:C:45:ARG:NH1	5:C:2034:HOH:O	2.38	0.55
1:D:181:LEU:HD21	1:D:188:PHE:HA	1.88	0.55
1:B:5:ASN:H	1:B:9:ASN:HD22	1.53	0.54
1:E:3:GLU:HG3	1:E:4:ILE:H	1.73	0.54
1:F:161:THR:HG21	5:F:2031:HOH:O	2.06	0.54
1:H:167:LEU:HB3	1:H:172:LYS:HG3	1.89	0.54
1:F:81:MSE:CE	1:F:85:LYS:HA	2.37	0.54
1:H:216:GLY:CA	1:H:217:SER:C	2.76	0.54
1:F:202:THR:CG2	5:F:2026:HOH:O	2.56	0.53
1:E:174:LEU:HD12	1:E:194:THR:HG22	1.90	0.53
1:D:57:SER:HA	1:E:23[A]:ARG:HH21	1.74	0.53
1:E:158:THR:CG2	5:E:235[A]:HOH:O	2.56	0.53
1:C:192:PHE:HE1	1:G:193[B]:ASN:ND2	2.06	0.53
1:D:7:TYR:CZ	1:E:23[B]:ARG:HD2	2.44	0.53
1:G:181:LEU:HD12	1:G:182[A]:ARG:HH21	1.73	0.53
1:H:5:ASN:H	1:H:9:ASN:HD22	1.54	0.53
1:D:26:ASN:ND2	1:D:28:GLY:H	2.07	0.53
1:F:134:THR:CG2	1:F:135:ASP:O	2.55	0.53
1:A:80:ARG:HD2	1:A:84:GLU:OE1	2.09	0.52
1:E:117:ASP:OD1	1:E:120:LYS:HE2	2.08	0.52
1:B:158:THR:OG1	1:B:161:THR:HG23	2.09	0.52
1:E:81:MSE:HE3	1:E:88:VAL:CG1	2.40	0.52
1:F:65:THR:O	1:F:69[A]:GLN:HG3	2.09	0.52
1:C:160:GLY:HA2	1:C:163[C]:GLN:HE21	1.74	0.52
1:E:3:GLU:HG3	1:E:4:ILE:N	2.25	0.52
1:G:157:LEU:HD13	1:G:211:TYR:CE1	2.42	0.51
1:G:142:GLN:HG2	5:G:2040:HOH:O	2.09	0.51
1:D:80:ARG:HD2	1:D:84:GLU:OE2	2.11	0.51
1:B:3:GLU:HB2	5:B:2128:HOH:O	2.11	0.51
1:D:61:GLN:HE22	1:E:27:PRO:HD3	1.74	0.51
1:G:146:LEU:HD21	1:G:192:PHE:CD2	2.46	0.51
1:C:141:SER:HA	1:G:140:ILE:O	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:PRO:O	1:D:99:SER:HB3	2.11	0.51
1:E:45[B]:ARG:HD2	1:E:116:LEU:CD1	2.38	0.51
1:B:80:ARG:HH22	1:B:92:GLU:CD	2.15	0.50
1:F:70:GLU:OE1	1:F:202:THR:HB	2.10	0.50
1:E:45[B]:ARG:CD	1:E:116:LEU:HD11	2.38	0.50
1:G:143:GLU:HG3	1:G:155:ARG:HH21	1.77	0.50
1:A:77:ILE:HD11	5:A:2036:HOH:O	2.12	0.50
1:D:100:MSE:HG3	1:D:209:LEU:HD12	1.94	0.50
1:B:99:SER:HB2	1:B:166:THR:HG22	1.94	0.49
1:F:70:GLU:OE2	1:F:70:GLU:HA	2.12	0.49
1:F:158:THR:HG22	1:F:160:GLY:N	2.27	0.49
1:E:88:VAL:HG21	5:E:343:HOH:O	2.12	0.49
1:F:110[A]:ARG:HH22	1:F:216:GLY:CA	2.21	0.49
1:A:118:ARG:HH12	1:D:111:PHE:C	2.15	0.49
1:F:31:PHE:CD1	1:F:33[B]:GLU:HG3	2.46	0.49
1:A:41:ASP:O	1:A:45[A]:ARG:HG2	2.12	0.49
1:H:19:LYS:HE3	1:H:23[B]:ARG:NH2	2.27	0.49
1:E:3:GLU:CG	1:E:4:ILE:H	2.25	0.49
1:E:89:CYS:O	1:E:94:LEU:HG	2.12	0.49
1:G:162:TRP:HB2	5:G:2137:HOH:O	2.13	0.49
1:F:142:GLN:O	1:F:182[B]:ARG:HD2	2.13	0.49
1:C:23[A]:ARG:CZ	1:F:158:THR:HG21	2.43	0.48
1:G:21:PHE:HA	1:G:24:GLN:HE21	1.78	0.48
1:H:135:ASP:HB3	5:H:2142:HOH:O	2.12	0.48
1:E:12:GLN:HG3	5:E:240:HOH:O	2.12	0.48
1:G:106[B]:ARG:HD2	1:G:213:ALA:HB1	1.95	0.48
1:C:47:HIS:HA	1:C:49:GLU:OE1	2.13	0.48
1:E:106[A]:ARG:O	1:E:110[A]:ARG:HG3	2.12	0.48
1:C:167:LEU:HD23	1:C:172[A]:LYS:HG2	1.95	0.48
1:H:118:ARG:HD3	5:H:2054:HOH:O	2.14	0.48
1:F:81:MSE:HE3	1:F:88:VAL:CG1	2.44	0.48
1:E:38:GLU:OE1	1:E:108:LYS:HE3	2.14	0.47
1:F:80:ARG:HH22	1:F:92:GLU:CD	2.18	0.47
1:F:45[B]:ARG:NH1	5:F:2073:HOH:O	2.47	0.47
1:G:168:PRO:HG2	1:G:171:ILE:HD12	1.95	0.47
1:C:200:ARG:NE	5:C:2146:HOH:O	2.30	0.47
1:F:12:GLN:HA	1:F:37:ILE:HG12	1.96	0.47
1:A:100:MSE:HE2	1:A:209:LEU:CD1	2.43	0.47
1:A:148:VAL:HG22	1:A:152:VAL:HB	1.97	0.47
1:B:100:MSE:HG2	1:B:209:LEU:HD12	1.96	0.47
1:H:110:ARG:NH1	1:H:215:ILE:O	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ASN:H	1:E:187:ASN:HD22	1.63	0.47
1:F:157:LEU:CD1	1:F:165:MSE:CE	2.79	0.47
1:B:49[B]:GLU:CD	1:B:49[B]:GLU:H	2.18	0.46
1:B:140:ILE:H	1:D:142:GLN:NE2	2.07	0.46
1:G:145:GLY:HA3	1:G:155:ARG:HB2	1.97	0.46
1:H:80:ARG:HD2	1:H:84:GLU:OE2	2.14	0.46
1:A:86:GLU:HA	5:A:2083:HOH:O	2.16	0.46
1:H:189:SER:HA	5:H:2140:HOH:O	2.16	0.46
1:B:145:GLY:HA3	1:B:155:ARG:HB2	1.99	0.45
1:F:21:PHE:O	1:F:24:GLN:HB2	2.16	0.45
1:D:157:LEU:HD11	1:D:165:MSE:HE1	1.98	0.45
1:F:47:HIS:HA	1:F:49:GLU:OE1	2.16	0.45
1:C:33:GLU:HG2	5:C:2119:HOH:O	2.16	0.45
1:C:140:ILE:O	1:G:141:SER:HA	2.16	0.45
1:E:5:ASN:H	1:E:9:ASN:HD22	1.62	0.45
1:H:110:ARG:HH22	1:H:216:GLY:N	2.15	0.45
1:D:8[B]:GLN:N	1:D:8[B]:GLN:HE21	2.15	0.45
1:E:92:GLU:CD	5:E:341:HOH:O	2.52	0.45
1:E:106[B]:ARG:NH2	5:E:233:HOH:O	2.49	0.45
1:A:77:ILE:HD13	1:A:93:ILE:HD11	1.99	0.45
1:D:65:THR:O	1:D:69:GLN:HG3	2.17	0.45
1:A:110:ARG:HD2	1:D:215:ILE:O	2.16	0.45
1:H:215:ILE:HB	1:H:216:GLY:CA	2.47	0.45
1:E:3:GLU:CG	1:E:4:ILE:N	2.80	0.44
1:E:70:GLU:OE1	1:E:202:THR:HB	2.18	0.44
1:E:81:MSE:HE3	1:E:88:VAL:CB	2.47	0.44
1:B:98:THR:O	1:B:102:GLN:HG3	2.16	0.44
1:A:39:ALA:HB1	1:A:100:MSE:CE	2.46	0.44
1:E:211:TYR:O	1:E:215:ILE:HG23	2.18	0.44
1:G:153:ASN:OD1	1:G:156:THR:HB	2.16	0.44
1:F:12:GLN:HG3	5:F:2053:HOH:O	2.17	0.44
1:F:143:GLU:O	1:F:155:ARG:NE	2.47	0.44
1:E:99:SER:HB3	5:E:297[B]:HOH:O	2.18	0.44
1:E:202:THR:HG21	5:E:334:HOH:O	2.18	0.44
1:D:100:MSE:CG	1:D:209:LEU:HD12	2.48	0.43
1:E:102[B]:GLN:HG3	1:E:103:ASN:N	2.32	0.43
1:B:117:ASP:HA	1:B:120:LYS:HD2	2.01	0.43
1:B:134:THR:CG2	1:F:134:THR:HG21	2.45	0.43
1:H:214:ALA:C	1:H:215:ILE:O	2.56	0.43
1:E:187:ASN:H	1:E:187:ASN:ND2	2.17	0.43
1:G:80:ARG:HD2	1:G:84:GLU:OE1	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:MSE:HE3	1:F:88:VAL:CB	2.48	0.43
1:G:58[A]:LYS:HA	1:G:58[A]:LYS:HE3	2.01	0.43
1:C:215:ILE:HA	1:C:216:GLY:HA3	1.66	0.43
1:B:87[B]:ARG:HD3	1:B:92:GLU:OE1	2.19	0.43
1:F:7:TYR:HB3	1:F:51:ILE:HD11	2.01	0.43
1:B:100:MSE:CG	1:B:209:LEU:HD12	2.49	0.42
1:C:163[B]:GLN:CG	1:D:125:VAL:HG21	2.50	0.42
1:A:45[B]:ARG:HG2	5:A:2125:HOH:O	2.19	0.42
1:B:87[B]:ARG:HH21	1:B:170[B]:ASP:CG	2.22	0.42
1:F:81:MSE:HE2	1:F:85:LYS:HA	2.02	0.42
1:A:118:ARG:NH1	1:D:111:PHE:HA	2.35	0.42
1:F:72:ALA:O	1:F:76:THR:HG23	2.20	0.42
1:E:106[A]:ARG:O	1:E:106[A]:ARG:HD2	2.20	0.42
1:D:57:SER:HA	1:E:23[A]:ARG:NH2	2.35	0.41
1:F:5:ASN:H	1:F:9:ASN:HD22	1.67	0.41
1:C:86[B]:GLU:CD	1:C:90:ASN:HD22	2.24	0.41
1:H:84:GLU:O	1:H:88:VAL:HG23	2.19	0.41
1:F:142:GLN:HA	1:F:183:LEU:HD11	2.02	0.41
1:C:26:ASN:HA	1:C:27:PRO:HD2	1.83	0.41
1:F:167:LEU:HD12	1:F:168:PRO:HD2	2.02	0.41
1:E:98:THR:O	1:E:102[A]:GLN:HG3	2.21	0.41
1:E:104:LEU:HD13	1:E:108:LYS:HD2	2.01	0.41
1:H:17:ILE:HG22	1:H:21:PHE:CE2	2.56	0.41
1:A:165:MSE:HE2	1:A:167:LEU:HD22	2.03	0.41
1:D:146:LEU:HD13	1:D:188:PHE:CE1	2.55	0.41
1:E:158:THR:HG22	5:E:235[A]:HOH:O	2.18	0.41
1:H:127:PRO:O	1:H:204:ALA:HB1	2.20	0.41
1:A:80:ARG:NH2	1:A:92:GLU:OE2	2.35	0.41
1:E:134:THR:HG23	1:E:138:GLY:HA2	2.03	0.41
1:G:146:LEU:CD2	1:G:192:PHE:CD2	3.03	0.41
1:H:62:GLN:HG3	5:H:2037:HOH:O	2.20	0.41
1:B:96:LEU:HA	1:B:168:PRO:HG3	2.03	0.41
1:G:183:LEU:HA	1:G:188:PHE:CG	2.56	0.41
1:B:133:SER:HB2	1:B:145:GLY:H	1.86	0.41
1:B:141:SER:OG	1:B:143[B]:GLU:HB2	2.21	0.41
1:F:80:ARG:HD2	1:F:84:GLU:OE1	2.21	0.41
1:A:145:GLY:HA3	1:A:155:ARG:HB2	2.03	0.40
1:D:124:ASN:HB3	1:D:129:ASP:HB2	2.04	0.40
1:F:146:LEU:HD13	1:F:188:PHE:CE1	2.56	0.40
1:F:159:PRO:O	1:F:163[A]:GLN:HG3	2.21	0.40
1:F:95:PRO:O	1:F:99:SER:HB3	2.20	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:LEU:HD13	1:H:210:ALA:CB	2.52	0.40

All (1) 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)
1:E:118[B]:ARG:NH1	5:G:2100:HOH:O[2_646]	1.97	0.23

## 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	221/219 (101%)	216 (98%)	5 (2%)	0	100	100
1	B	223/219 (102%)	218 (98%)	5 (2%)	0	100	100
1	C	224/219 (102%)	220 (98%)	4 (2%)	0	100	100
1	D	218/219 (100%)	216 (99%)	2 (1%)	0	100	100
1	E	225/219 (103%)	218 (97%)	7 (3%)	0	100	100
1	F	226/219 (103%)	223 (99%)	3 (1%)	0	100	100
1	G	223/219 (102%)	220 (99%)	3 (1%)	0	100	100
1	H	219/219 (100%)	212 (97%)	6 (3%)	1 (0%)	25	26
All	All	1779/1752 (102%)	1743 (98%)	35 (2%)	1 (0%)	48	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	215	ILE

### 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	185/175 (106%)	172 (93%)	13 (7%)	12	12
1	B	187/175 (107%)	174 (93%)	13 (7%)	12	12
1	C	188/175 (107%)	176 (94%)	12 (6%)	14	15
1	D	182/175 (104%)	170 (93%)	12 (7%)	14	14
1	E	189/175 (108%)	175 (93%)	14 (7%)	11	11
1	F	189/175 (108%)	172 (91%)	17 (9%)	8	7
1	G	187/175 (107%)	169 (90%)	18 (10%)	7	6
1	H	183/175 (105%)	174 (95%)	9 (5%)	21	24
All	All	1490/1400 (106%)	1382 (93%)	108 (7%)	14	11

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	70	GLU
1	A	104	LEU
1	A	110	ARG
1	A	122	SER
1	A	142	GLN
1	A	146	LEU
1	A	148	VAL
1	A	163[A]	GLN
1	A	163[B]	GLN
1	A	165	MSE
1	A	175	VAL
1	A	187	ASN
1	B	49[A]	GLU
1	B	49[B]	GLU
1	B	66	LEU
1	B	69[A]	GLN
1	B	69[B]	GLN
1	B	82	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	104	LEU
1	B	133	SER
1	B	142	GLN
1	B	161	THR
1	B	170[A]	ASP
1	B	170[B]	ASP
1	B	215	ILE
1	C	33	GLU
1	C	46	LEU
1	C	49	GLU
1	C	66	LEU
1	C	99	SER
1	C	110	ARG
1	C	158	THR
1	C	163[A]	GLN
1	C	163[B]	GLN
1	C	163[C]	GLN
1	C	187[A]	ASN
1	C	187[B]	ASN
1	D	26	ASN
1	D	49	GLU
1	D	56	ILE
1	D	61	GLN
1	D	86	GLU
1	D	99	SER
1	D	106	ARG
1	D	142	GLN
1	D	146	LEU
1	D	169[A]	GLU
1	D	169[B]	GLU
1	D	183	LEU
1	E	24	GLN
1	E	49	GLU
1	E	92	GLU
1	E	104	LEU
1	E	108	LYS
1	E	110[A]	ARG
1	E	110[B]	ARG
1	E	134	THR
1	E	148	VAL
1	E	156	THR
1	E	170[A]	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	170[B]	ASP
1	E	183	LEU
1	E	187	ASN
1	F	49	GLU
1	F	66	LEU
1	F	70	GLU
1	F	81	MSE
1	F	99	SER
1	F	104	LEU
1	F	106[A]	ARG
1	F	106[B]	ARG
1	F	134	THR
1	F	142	GLN
1	F	146	LEU
1	F	156	THR
1	F	161	THR
1	F	183	LEU
1	F	187	ASN
1	F	202	THR
1	F	215	ILE
1	G	49	GLU
1	G	58[A]	LYS
1	G	58[B]	LYS
1	G	66	LEU
1	G	99	SER
1	G	104	LEU
1	G	120	LYS
1	G	122	SER
1	G	148	VAL
1	G	156	THR
1	G	163[A]	GLN
1	G	163[B]	GLN
1	G	170[A]	ASP
1	G	170[B]	ASP
1	G	175	VAL
1	G	182[A]	ARG
1	G	182[B]	ARG
1	G	189	SER
1	H	45	ARG
1	H	100	MSE
1	H	104	LEU
1	H	133	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	137	SER
1	H	146	LEU
1	H	148	VAL
1	H	170[A]	ASP
1	H	170[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	103	ASN
1	A	142	GLN
1	A	187	ASN
1	B	9	ASN
1	B	103	ASN
1	B	142	GLN
1	C	24	GLN
1	C	90	ASN
1	C	103	ASN
1	D	9	ASN
1	D	16	ASN
1	D	26	ASN
1	D	61	GLN
1	D	73	ASN
1	D	102	GLN
1	D	103	ASN
1	D	142	GLN
1	E	9	ASN
1	E	90	ASN
1	E	163	GLN
1	E	187	ASN
1	F	9	ASN
1	F	73	ASN
1	F	187	ASN
1	G	9	ASN
1	G	24	GLN
1	G	103	ASN
1	H	9	ASN
1	H	103	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

22 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	SO4	G	2011	-	4,4,4	0.22	0	6,6,6	0.32	0
2	SO4	C	2001	-	4,4,4	0.25	0	6,6,6	0.25	0
2	SO4	D	2009	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	H	2005	-	4,4,4	0.25	0	6,6,6	0.33	0
2	SO4	A	2007	-	4,4,4	0.23	0	6,6,6	0.13	0
3	ACY	B	2017	-	3,3,3	1.00	0	3,3,3	1.07	0
3	ACY	G	2020	-	3,3,3	0.78	0	3,3,3	0.93	0
3	ACY	C	2019	-	3,3,3	0.80	0	3,3,3	0.84	0
2	SO4	H	2008	-	4,4,4	0.92	0	6,6,6	0.36	0
3	ACY	C	2015	-	3,3,3	0.92	0	3,3,3	0.90	0
2	SO4	A	2003	-	4,4,4	0.28	0	6,6,6	0.32	0
2	SO4	D	2002	-	4,4,4	0.19	0	6,6,6	0.56	0
2	SO4	C	2004	-	4,4,4	0.28	0	6,6,6	0.28	0
2	SO4	H	2010	-	4,4,4	0.26	0	6,6,6	0.18	0
2	SO4	F	2013	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	A	2006	-	4,4,4	0.24	0	6,6,6	0.26	0
4	GOL	D	2022	-	5,5,5	0.53	0	5,5,5	0.65	0
2	SO4	G	2012	-	4,4,4	0.29	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACY	H	2021	-	3,3,3	0.81	0	3,3,3	0.83	0
3	ACY	F	2014	-	3,3,3	0.99	0	3,3,3	1.06	0
3	ACY	F	2016	-	3,3,3	0.76	0	3,3,3	1.05	0
3	ACY	A	2018	-	3,3,3	0.79	0	3,3,3	1.10	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
4	GOL	D	2022	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2022	GOL	C1-C2-C3-O3
4	D	2022	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2022	GOL	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	211/219 (96%)	0.14	6 (2%)	55	54	8, 20, 26, 28	9 (4%)
1	B	211/219 (96%)	-0.20	5 (2%)	59	58	3, 16, 25, 30	10 (4%)
1	C	210/219 (95%)	-0.17	2 (0%)	79	78	5, 18, 25, 28	11 (5%)
1	D	210/219 (95%)	-0.09	1 (0%)	87	86	9, 18, 26, 27	7 (3%)
1	E	211/219 (96%)	0.08	6 (2%)	55	54	8, 20, 27, 29	13 (6%)
1	F	212/219 (96%)	0.04	4 (1%)	66	65	9, 23, 30, 33	13 (6%)
1	G	211/219 (96%)	-0.08	2 (0%)	81	80	9, 20, 26, 28	11 (5%)
1	H	211/219 (96%)	0.01	8 (3%)	44	44	9, 18, 24, 38	7 (3%)
All	All	1687/1752 (96%)	-0.04	34 (2%)	64	63	3, 19, 26, 38	81 (4%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	5.0
1	H	216	GLY	4.7
1	F	2	ALA	3.7
1	E	182[A]	ARG	3.7
1	A	28	GLY	3.5
1	G	60[A]	ASP	3.5
1	A	217	SER	3.2
1	C	23[A]	ARG	3.1
1	H	215	ILE	2.9
1	G	45[A]	ARG	2.9
1	H	137	SER	2.8
1	H	163[A]	GLN	2.6
1	B	79	PHE	2.6
1	B	86	GLU	2.5
1	A	46	LEU	2.5
1	B	66	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	87[A]	ARG	2.5
1	H	150	TYR	2.5
1	A	49[A]	GLU	2.5
1	A	42	ILE	2.3
1	E	158	THR	2.3
1	D	54	GLY	2.3
1	H	170[A]	ASP	2.3
1	B	69[A]	GLN	2.2
1	H	217	SER	2.2
1	C	159	PRO	2.2
1	E	113	SER	2.1
1	H	128	THR	2.1
1	F	123	PRO	2.1
1	E	110[A]	ARG	2.1
1	F	89	CYS	2.1
1	A	45[A]	ARG	2.0
1	F	78	GLY	2.0
1	E	88	VAL	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	ACY	F	2016	4/4	0.57	0.22	61,61,61,62	0
3	ACY	A	2018	4/4	0.60	0.18	61,62,62,62	0
3	ACY	H	2021	4/4	0.61	0.19	64,64,64,64	0
2	SO4	F	2013	5/5	0.63	0.14	88,88,88,88	0
2	SO4	G	2012	5/5	0.65	0.12	80,80,81,81	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACY	C	2019	4/4	0.66	0.23	70,70,70,70	0
2	SO4	A	2006	5/5	0.69	0.17	132,132,133,133	0
2	SO4	H	2010	5/5	0.69	0.25	99,100,100,100	0
2	SO4	H	2008	5/5	0.72	0.18	126,126,126,126	0
2	SO4	A	2007	5/5	0.72	0.22	135,135,135,135	0
2	SO4	G	2011	5/5	0.74	0.21	115,116,116,116	0
2	SO4	H	2005	5/5	0.77	0.11	73,74,74,74	0
4	GOL	D	2022	6/6	0.80	0.24	46,47,48,49	0
3	ACY	F	2014	4/4	0.81	0.16	44,44,44,45	0
2	SO4	D	2009	5/5	0.81	0.14	103,103,103,104	0
3	ACY	C	2015	4/4	0.85	0.17	53,53,53,53	0
3	ACY	B	2017	4/4	0.86	0.17	35,35,36,36	0
3	ACY	G	2020	4/4	0.86	0.18	51,51,51,52	0
2	SO4	D	2002	5/5	0.93	0.09	47,48,50,50	0
2	SO4	C	2001	5/5	0.94	0.10	33,33,33,34	5
2	SO4	C	2004	5/5	0.95	0.11	52,52,53,54	0
2	SO4	A	2003	5/5	0.96	0.09	43,44,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.