



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 05:47 am BST

PDB ID : 1R56  
Title : UNCOMPLEXED URATE OXIDASE FROM ASPERGILLUS FLAVUS  
Authors : Retailleau, P.; Colloc'h, N.; Prange, T.  
Deposited on : 2003-10-09  
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

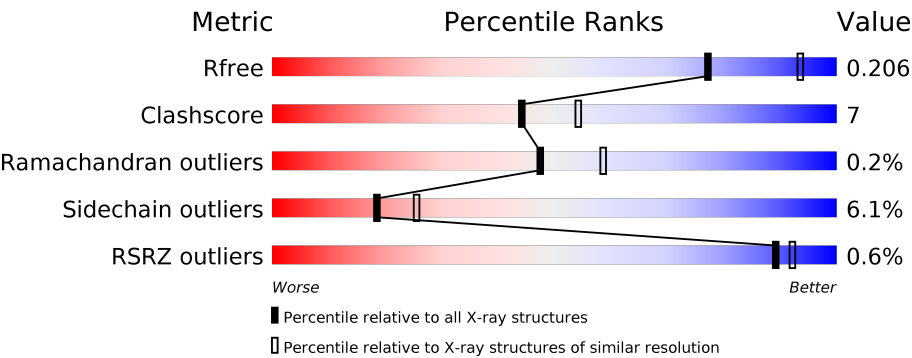
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	301	<div><div></div><div>84%13%..</div></div>
1	B	301	<div><div></div><div>81%15%..</div></div>
1	C	301	<div><div>%</div><div>82%15%..</div></div>
1	D	301	<div><div>%</div><div>80%17%..</div></div>
1	E	301	<div><div>%</div><div>79%17%..</div></div>
1	F	301	<div><div></div><div>78%18%..</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	301	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>..</div> </div> </div>
1	H	301	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>...</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	A	3126	-	-	X	-
2	PEG	B	4126	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19240 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 Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2359	1491	409	452	7			
1	B	295	Total	C	N	O	S	0	0	0
			2357	1490	409	451	7			
1	C	299	Total	C	N	O	S	0	0	0
			2388	1509	414	458	7			
1	D	295	Total	C	N	O	S	0	0	0
			2362	1493	409	453	7			
1	E	295	Total	C	N	O	S	0	0	0
			2359	1491	409	452	7			
1	F	295	Total	C	N	O	S	0	0	0
			2354	1488	409	450	7			
1	G	296	Total	C	N	O	S	0	0	1
			2360	1491	410	452	7			
1	H	295	Total	C	N	O	S	0	0	0
			2359	1491	409	452	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
B	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
C	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
D	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
E	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
F	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
G	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
H	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

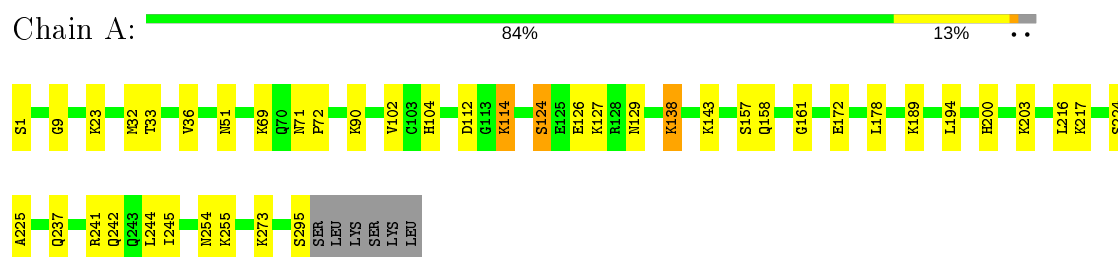
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	45	Total	O	0	0
			45	45		
3	C	50	Total	O	0	0
			50	50		
3	D	41	Total	O	0	0
			41	41		
3	E	29	Total	O	0	0
			29	29		
3	F	34	Total	O	0	0
			34	34		
3	G	31	Total	O	0	0
			31	31		
3	H	35	Total	O	0	0
			35	35		

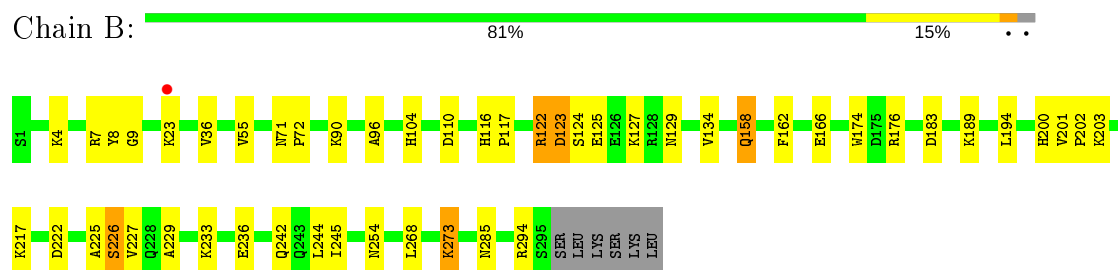
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

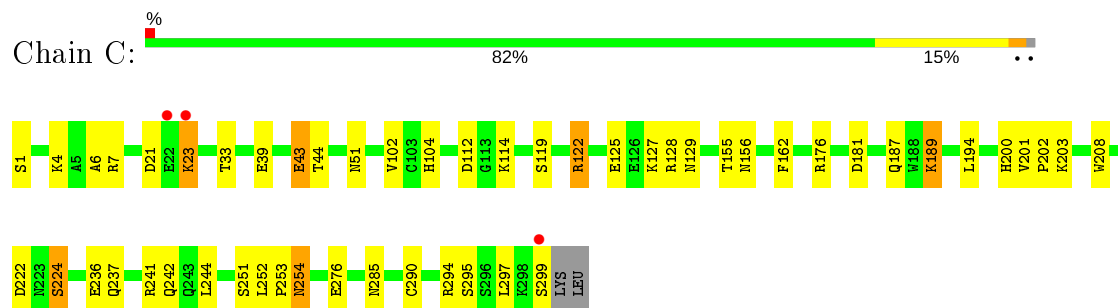
#### • Molecule 1: Uricase



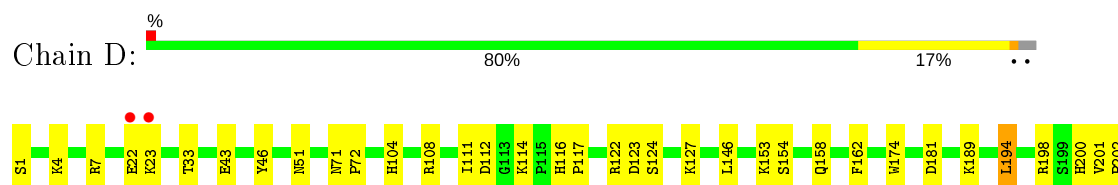
#### • Molecule 1: Uricase

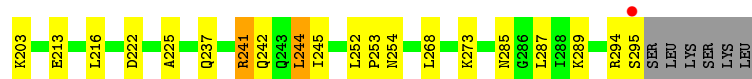


#### • Molecule 1: Uricase

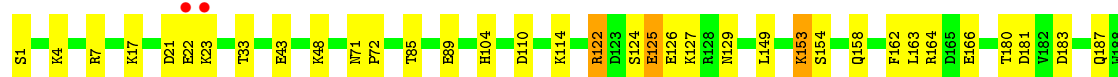
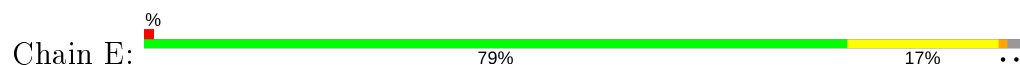


#### • Molecule 1: Uricase

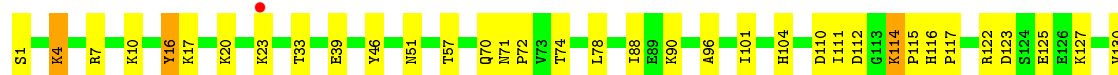
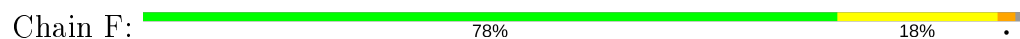




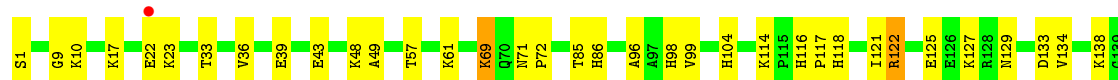
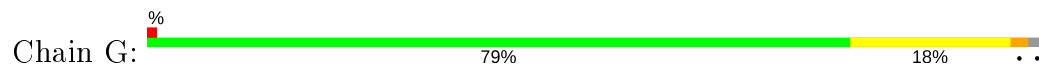
• Molecule 1: Uricase



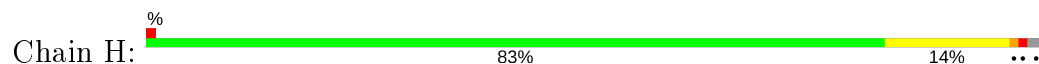
• Molecule 1: Uricase



• Molecule 1: Uricase



• Molecule 1: Uricase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.59Å 141.84Å 134.96Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 31.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 99.2 (31.80-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.50 (at 2.29Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.162 , 0.214 0.155 , 0.206	Depositor DCC
$R_{free}$ test set	13644 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	19240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: SAC, PEG

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	0.75	0/2406	0.78	0/3265
1	B	0.71	0/2401	0.78	0/3258
1	C	0.72	0/2435	0.81	0/3303
1	D	0.69	0/2406	0.75	0/3265
1	E	0.66	0/2406	0.75	0/3265
1	F	0.65	0/2401	0.76	0/3258
1	G	0.64	0/2407	0.79	3/3267 (0.1%)
1	H	0.71	1/2406 (0.0%)	0.81	2/3265 (0.1%)
All	All	0.69	1/19268 (0.0%)	0.78	5/26146 (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	C	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	124	SER	CA-C	5.48	1.67	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	123	ASP	O-C-N	-7.96	109.96	122.70
1	H	124	SER	N-CA-C	7.08	130.10	111.00
1	G	268	LEU	CA-CB-CG	6.56	130.38	115.30
1	G	163	LEU	CA-CB-CG	5.81	128.66	115.30
1	G	163	LEU	CB-CG-CD1	-5.05	102.41	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	SAC	Mainchain
1	F	1	SAC	Mainchain
1	G	1	SAC	Mainchain
1	H	123	ASP	Mainchain

## 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	2359	0	2320	32	0
1	B	2357	0	2319	34	0
1	C	2388	0	2354	33	0
1	D	2362	0	2324	32	0
1	E	2359	0	2320	40	0
1	F	2354	0	2315	37	0
1	G	2360	0	2320	37	0
1	H	2359	0	2320	29	0
2	A	4	0	5	4	0
2	B	4	0	5	5	0
3	A	69	0	0	2	0
3	B	45	0	0	0	0
3	C	50	0	0	1	0
3	D	41	0	0	0	0
3	E	29	0	0	1	0
3	F	34	0	0	1	0
3	G	31	0	0	0	0
3	H	35	0	0	0	0
All	All	19240	0	18602	246	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 7.

All (246) 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:C:189:LYS:HE2	1:C:244:LEU:HD12	1.40	1.01
1:C:43:GLU:CD	1:C:43:GLU:H	1.68	0.96
1:A:112:ASP:HB2	1:A:114:LYS:HE2	1.48	0.93
1:D:108:ARG:HD3	1:D:116:HIS:O	1.70	0.91
1:A:224:SER:HB3	2:A:3126:PEG:C1	2.11	0.80
1:H:200:HIS:HD2	1:H:203:LYS:NZ	1.80	0.79
1:G:294:ARG:HH11	1:G:294:ARG:HG2	1.48	0.78
1:A:112:ASP:CB	1:A:114:LYS:HE2	2.13	0.78
1:A:69:LYS:NZ	1:C:276:GLU:OE1	2.14	0.78
1:E:104:HIS:HD2	1:E:127:LYS:NZ	1.84	0.76
1:A:224:SER:HB3	2:A:3126:PEG:H12	1.68	0.75
1:B:200:HIS:HD2	1:B:203:LYS:NZ	1.87	0.73
1:A:138:LYS:HB3	1:A:138:LYS:HZ2	1.55	0.72
1:B:227:VAL:HG23	2:B:4126:PEG:H11	1.74	0.70
1:D:71:ASN:HB3	1:D:72:PRO:HD2	1.73	0.69
1:A:138:LYS:HB3	1:A:138:LYS:NZ	2.07	0.69
1:E:194:LEU:O	1:E:198:ARG:HG3	1.92	0.69
1:C:181:ASP:O	1:C:253:PRO:HD2	1.92	0.68
1:E:294:ARG:HG2	1:E:294:ARG:HH11	1.59	0.68
1:F:104:HIS:HD2	1:F:127:LYS:NZ	1.92	0.67
1:B:104:HIS:HD2	1:B:127:LYS:NZ	1.93	0.67
1:C:43:GLU:CD	1:C:43:GLU:N	2.44	0.67
1:A:200:HIS:HD2	1:A:203:LYS:NZ	1.92	0.66
1:B:227:VAL:H	2:B:4126:PEG:C1	2.08	0.66
1:B:176:ARG:HH22	2:B:4126:PEG:H22	1.59	0.66
1:G:36:VAL:HG22	1:G:99:VAL:HG22	1.76	0.66
1:H:200:HIS:HD2	1:H:203:LYS:HZ2	1.43	0.66
1:D:294:ARG:HH11	1:D:294:ARG:HG2	1.60	0.65
1:G:39:GLU:HB2	1:G:96:ALA:HB3	1.77	0.65
1:D:242:GLN:HG3	1:D:245:ILE:HG12	1.79	0.65
1:A:104:HIS:HD2	1:A:127:LYS:NZ	1.96	0.64
1:C:200:HIS:HD2	1:C:203:LYS:NZ	1.96	0.62
1:E:162:PHE:HA	1:F:51:ASN:O	1.99	0.62
1:B:294:ARG:HG2	1:B:294:ARG:HH11	1.65	0.61
1:G:294:ARG:HH11	1:G:294:ARG:CG	2.14	0.61
1:B:227:VAL:H	2:B:4126:PEG:H11	1.66	0.61
1:D:200:HIS:HD2	1:D:203:LYS:NZ	1.99	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:GLN:O	1:E:225:ALA:HA	2.01	0.61
1:F:116:HIS:CG	1:F:117:PRO:HD2	2.36	0.60
1:H:4:LYS:HB3	1:H:4:LYS:NZ	2.16	0.60
1:C:222:ASP:OD2	1:C:224:SER:HB2	2.00	0.60
1:C:294:ARG:HH11	1:C:294:ARG:HG2	1.66	0.60
1:E:149:LEU:CD1	1:G:121:ILE:HD11	2.31	0.60
1:D:181:ASP:O	1:D:253:PRO:HD2	2.01	0.60
1:F:176:ARG:NH2	3:F:302:HOH:O	2.34	0.60
1:C:21:ASP:OD2	1:C:23:LYS:HG3	2.03	0.59
1:F:78:LEU:HD22	1:F:201:VAL:CG2	2.33	0.58
1:D:237:GLN:O	1:D:241:ARG:HG3	2.03	0.58
1:G:71:ASN:HB3	1:G:72:PRO:CD	2.33	0.58
1:H:226:SER:HB3	1:H:229:ALA:HB3	1.86	0.58
1:A:71:ASN:HB3	1:A:72:PRO:HD2	1.84	0.58
1:G:17:LYS:NZ	1:G:71:ASN:O	2.37	0.58
1:F:78:LEU:HD22	1:F:201:VAL:HG21	1.86	0.57
1:A:112:ASP:HB2	1:A:114:LYS:CE	2.29	0.57
1:B:201:VAL:HG12	1:B:202:PRO:HD3	1.85	0.57
1:H:254:ASN:O	1:H:285:ASN:HB2	2.05	0.57
1:A:157:SER:OG	2:A:3126:PEG:H21	2.03	0.57
1:C:33:THR:OG1	1:C:104:HIS:HE1	1.87	0.57
1:F:104:HIS:HD2	1:F:127:LYS:HZ1	1.52	0.57
1:G:10:LYS:HD2	1:G:57:THR:HB	1.86	0.57
1:B:200:HIS:HD2	1:B:203:LYS:HZ3	1.53	0.57
1:F:10:LYS:HD3	1:F:57:THR:HB	1.86	0.57
1:C:189:LYS:CE	1:C:244:LEU:HD12	2.25	0.56
1:A:161:GLY:N	1:A:172:GLU:OE2	2.32	0.56
1:F:123:ASP:O	1:H:124:SER:N	2.37	0.56
1:H:237:GLN:O	1:H:241:ARG:HG3	2.05	0.56
1:H:200:HIS:HD2	1:H:203:LYS:HZ3	1.54	0.56
1:B:71:ASN:HB3	1:B:72:PRO:CD	2.35	0.56
1:A:33:THR:OG1	1:A:104:HIS:HE1	1.88	0.56
1:D:294:ARG:HG2	1:D:294:ARG:NH1	2.21	0.56
1:C:189:LYS:HE2	1:C:244:LEU:CD1	2.25	0.55
1:C:242:GLN:OE1	1:C:244:LEU:HD23	2.06	0.55
1:F:111:ILE:CG2	1:H:217:LYS:HG3	2.36	0.55
1:B:71:ASN:HB3	1:B:72:PRO:HD2	1.88	0.55
1:A:138:LYS:CB	1:A:138:LYS:NZ	2.66	0.54
1:D:146:LEU:HD12	1:D:146:LEU:C	2.28	0.54
1:E:104:HIS:HD2	1:E:127:LYS:HZ1	1.55	0.54
1:E:181:ASP:O	1:E:253:PRO:HD2	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:LYS:HB3	1:H:4:LYS:HZ3	1.72	0.54
1:C:104:HIS:HD2	1:C:127:LYS:NZ	2.05	0.54
1:B:294:ARG:HG2	1:B:294:ARG:NH1	2.23	0.54
1:E:277:VAL:HG22	1:G:17:LYS:HG3	1.89	0.54
1:B:254:ASN:O	1:B:285:ASN:HB2	2.08	0.53
1:D:104:HIS:HD2	1:D:127:LYS:NZ	2.06	0.53
1:G:104:HIS:HD2	1:G:127:LYS:NZ	2.07	0.53
1:G:33:THR:OG1	1:G:104:HIS:HE1	1.91	0.53
1:E:180:THR:HG21	1:E:252:LEU:HD13	1.90	0.53
1:D:158:GLN:O	1:D:225:ALA:HA	2.09	0.53
1:H:104:HIS:HD2	1:H:127:LYS:NZ	2.08	0.52
1:C:254:ASN:O	1:C:285:ASN:HB2	2.10	0.52
1:C:51:ASN:O	1:D:162:PHE:HA	2.10	0.52
1:G:231:MET:CE	1:G:290:CYS:HB2	2.40	0.52
1:A:242:GLN:HG3	1:A:245:ILE:HG12	1.92	0.51
1:D:254:ASN:O	1:D:285:ASN:HB2	2.10	0.51
1:F:111:ILE:HG23	1:H:217:LYS:HG3	1.92	0.51
1:E:270:ASN:OD1	1:G:69:LYS:HE2	2.09	0.51
1:E:33:THR:OG1	1:E:104:HIS:HE1	1.93	0.51
1:E:254:ASN:O	1:E:285:ASN:HB2	2.10	0.51
1:F:101:ILE:HB	1:F:130:VAL:HG22	1.93	0.51
1:D:111:ILE:O	1:D:112:ASP:HB2	2.09	0.51
1:F:237:GLN:O	1:F:241:ARG:HG3	2.10	0.51
1:A:124:SER:HB3	1:A:126:GLU:H	1.76	0.51
1:B:217:LYS:NZ	1:D:112:ASP:OD2	2.44	0.51
1:B:104:HIS:HD2	1:B:127:LYS:HZ1	1.59	0.50
1:B:242:GLN:HG3	1:B:245:ILE:HG12	1.93	0.50
1:A:200:HIS:HD2	1:A:203:LYS:HZ2	1.57	0.50
1:A:255:LYS:HE2	3:A:3141:HOH:O	2.11	0.50
1:G:244:LEU:CD2	1:G:244:LEU:N	2.74	0.50
1:A:254:ASN:ND2	3:A:3195:HOH:O	2.39	0.50
1:D:153:LYS:NZ	1:D:222:ASP:O	2.45	0.50
1:A:178:LEU:HD22	2:A:3126:PEG:H22	1.94	0.50
1:E:4:LYS:HD2	1:F:293:GLY:HA3	1.93	0.50
1:F:116:HIS:ND1	1:F:117:PRO:HD2	2.27	0.50
1:D:287:LEU:HD21	1:D:289:LYS:HE2	1.93	0.49
1:A:158:GLN:O	1:A:225:ALA:HA	2.11	0.49
1:F:71:ASN:HB3	1:F:72:PRO:CD	2.43	0.49
1:B:227:VAL:CG2	2:B:4126:PEG:H11	2.41	0.49
1:C:237:GLN:O	1:C:241:ARG:HG3	2.11	0.49
1:E:104:HIS:HD2	1:E:127:LYS:HZ2	1.57	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:GLU:H	1:H:43:GLU:CD	2.17	0.49
1:B:200:HIS:CD2	1:B:203:LYS:HZ3	2.30	0.48
1:H:242:GLN:HG3	1:H:245:ILE:HG12	1.96	0.48
1:F:70:GLN:HE21	1:H:268:LEU:HD11	1.77	0.48
1:C:200:HIS:HD2	1:C:203:LYS:HZ3	1.61	0.48
1:G:146:LEU:C	1:G:146:LEU:HD12	2.34	0.48
1:E:1:SAC:OG	1:F:236:GLU:HG2	2.13	0.48
1:F:242:GLN:HG3	1:F:245:ILE:HG12	1.96	0.48
1:F:39:GLU:HB2	1:F:96:ALA:HB3	1.94	0.48
1:E:288:ILE:N	1:E:288:ILE:HD12	2.28	0.48
1:E:21:ASP:C	1:E:21:ASP:OD2	2.52	0.48
1:C:201:VAL:N	1:C:202:PRO:CD	2.76	0.48
1:E:43:GLU:H	1:E:43:GLU:CD	2.16	0.48
1:G:48:LYS:O	1:G:49:ALA:HB3	2.13	0.48
1:C:128:ARG:HD2	1:C:208:TRP:CD1	2.49	0.47
1:E:166:GLU:OE2	1:F:90:LYS:NZ	2.36	0.47
1:G:134:VAL:HG22	1:G:140:ILE:HG12	1.95	0.47
1:G:85:THR:O	1:G:86:HIS:C	2.52	0.47
1:D:33:THR:OG1	1:D:104:HIS:HE1	1.97	0.47
1:F:88:ILE:HD13	1:F:134:VAL:HG12	1.97	0.47
1:F:242:GLN:CG	1:F:245:ILE:HG12	2.45	0.47
1:G:116:HIS:CG	1:G:117:PRO:HD2	2.49	0.47
1:B:158:GLN:O	1:B:225:ALA:HA	2.15	0.46
1:A:138:LYS:CB	1:A:138:LYS:HZ2	2.23	0.46
1:H:33:THR:OG1	1:H:104:HIS:HE1	1.98	0.46
1:F:16:TYR:C	1:F:16:TYR:CD1	2.88	0.46
1:A:51:ASN:O	1:B:162:PHE:HA	2.15	0.46
1:G:294:ARG:CG	1:G:294:ARG:NH1	2.73	0.46
1:A:90:LYS:NZ	1:B:166:GLU:OE2	2.47	0.46
1:C:4:LYS:HE2	1:C:4:LYS:HB3	1.71	0.46
1:E:4:LYS:HB3	1:E:4:LYS:HE2	1.77	0.46
1:H:233:LYS:O	1:H:237:GLN:HG3	2.15	0.46
1:B:122:ARG:O	1:B:123:ASP:O	2.33	0.46
1:A:217:LYS:NZ	1:C:112:ASP:OD2	2.48	0.46
1:F:189:LYS:HD3	1:F:244:LEU:HD12	1.98	0.46
1:H:200:HIS:CD2	1:H:203:LYS:HZ3	2.34	0.46
1:G:71:ASN:HB3	1:G:72:PRO:HD2	1.98	0.46
1:B:122:ARG:O	1:B:122:ARG:HG3	2.15	0.46
1:H:158:GLN:NE2	1:H:223:ASN:OD1	2.48	0.46
1:G:231:MET:HE3	1:G:290:CYS:HB2	1.98	0.45
1:H:229:ALA:O	1:H:233:LYS:HG3	2.15	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:GLU:OE1	1:G:69:LYS:NZ	2.40	0.45
1:F:153:LYS:NZ	1:F:222:ASP:O	2.50	0.45
1:B:226:SER:HB3	1:B:229:ALA:H	1.82	0.45
1:C:162:PHE:HA	1:D:51:ASN:O	2.16	0.45
1:E:17:LYS:NZ	1:E:71:ASN:O	2.50	0.45
1:B:268:LEU:HA	1:B:268:LEU:HD12	1.71	0.45
1:G:236:GLU:HG2	1:H:1:SAC:OG	2.17	0.44
1:G:244:LEU:HD23	1:G:244:LEU:N	2.32	0.44
1:A:102:VAL:HA	1:A:129:ASN:HD22	1.82	0.44
1:D:237:GLN:O	1:D:241:ARG:CG	2.65	0.44
1:C:244:LEU:N	1:C:244:LEU:HD22	2.33	0.44
1:G:157:SER:C	1:G:158:GLN:HG3	2.37	0.44
1:H:123:ASP:O	1:H:124:SER:O	2.35	0.44
1:F:244:LEU:HA	1:F:244:LEU:HD12	1.88	0.44
1:H:10:LYS:HD3	1:H:57:THR:HB	1.99	0.44
1:F:186:TRP:CZ2	1:F:208:TRP:HA	2.52	0.44
1:C:6:ALA:O	1:C:39:GLU:HG2	2.18	0.44
1:E:124:SER:OG	1:E:126:GLU:N	2.35	0.44
1:E:259:GLU:HG2	3:E:316:HOH:O	2.17	0.44
1:A:1:SAC:OG	1:B:236:GLU:HG2	2.18	0.43
1:D:201:VAL:N	1:D:202:PRO:CD	2.81	0.43
1:C:102:VAL:HA	1:C:129:ASN:HD22	1.84	0.43
1:G:153:LYS:NZ	1:G:222:ASP:O	2.52	0.43
1:F:17:LYS:HA	1:H:276:GLU:O	2.19	0.43
1:C:294:ARG:HG2	1:C:294:ARG:NH1	2.33	0.43
1:E:270:ASN:O	1:E:275:ALA:HA	2.17	0.43
1:E:71:ASN:HB3	1:E:72:PRO:HD2	2.01	0.43
1:F:4:LYS:HE2	1:F:4:LYS:HB3	1.24	0.43
1:D:200:HIS:HD2	1:D:203:LYS:HZ3	1.66	0.43
1:E:290:CYS:HB3	1:F:46:TYR:CE2	2.54	0.43
1:C:251:SER:O	1:C:252:LEU:HD23	2.19	0.43
1:G:122:ARG:O	1:G:122:ARG:HG3	2.18	0.43
1:E:163:LEU:HD23	1:E:164:ARG:N	2.34	0.43
1:G:283:ASP:HB2	1:G:284:PRO:HA	2.00	0.43
1:H:146:LEU:C	1:H:146:LEU:HD12	2.39	0.43
1:B:116:HIS:CG	1:B:117:PRO:HD2	2.54	0.42
1:C:236:GLU:HG2	1:D:1:SAC:OG	2.18	0.42
1:E:154:SER:OG	1:G:118:HIS:HB2	2.18	0.42
1:F:33:THR:OG1	1:F:104:HIS:HE1	2.02	0.42
1:E:163:LEU:HD23	1:E:163:LEU:C	2.40	0.42
1:E:85:THR:O	1:E:89:GLU:HG3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:GLN:OE1	1:F:244:LEU:HB2	2.19	0.42
1:B:222:ASP:OD1	1:B:233:LYS:NZ	2.50	0.42
1:G:142:ILE:HD12	1:G:191:PHE:CE2	2.54	0.42
1:B:158:GLN:HB3	1:B:174:TRP:HA	2.01	0.42
1:B:200:HIS:CD2	1:B:203:LYS:NZ	2.76	0.42
1:D:111:ILE:O	1:D:114:LYS:HG2	2.20	0.42
1:C:290:CYS:HB3	1:D:46:TYR:CE2	2.55	0.42
1:C:176:ARG:NH2	3:C:306:HOH:O	2.52	0.42
1:E:198:ARG:HA	1:E:201:VAL:HG23	2.01	0.42
1:B:273:LYS:HB3	1:B:273:LYS:HE2	1.82	0.42
1:G:98:HIS:ND1	1:G:133:ASP:OD1	2.42	0.42
1:B:8:TYR:OH	1:B:55:VAL:O	2.24	0.42
1:A:104:HIS:HD2	1:A:127:LYS:HZ2	1.67	0.41
1:B:9:GLY:HA3	1:B:36:VAL:O	2.20	0.41
1:H:158:GLN:HG2	1:H:174:TRP:O	2.20	0.41
1:A:237:GLN:O	1:A:241:ARG:HG3	2.21	0.41
1:D:104:HIS:HD2	1:D:127:LYS:HZ1	1.67	0.41
1:E:104:HIS:CD2	1:E:127:LYS:HZ2	2.37	0.41
1:E:122:ARG:O	1:E:122:ARG:HG3	2.20	0.41
1:F:114:LYS:HA	1:F:115:PRO:HD3	1.80	0.41
1:H:4:LYS:CB	1:H:4:LYS:NZ	2.81	0.41
1:B:96:ALA:HA	1:B:134:VAL:O	2.21	0.41
1:G:9:GLY:HA3	1:G:36:VAL:O	2.21	0.41
1:D:244:LEU:HD12	1:D:244:LEU:HA	1.95	0.41
1:F:132:VAL:HG22	1:F:142:ILE:HG12	2.02	0.41
1:A:104:HIS:HD2	1:A:127:LYS:HZ1	1.67	0.41
1:D:194:LEU:O	1:D:198:ARG:HG3	2.21	0.41
1:E:149:LEU:HD13	1:G:121:ILE:HD11	2.00	0.41
1:D:123:ASP:O	1:D:124:SER:HB2	2.20	0.41
1:E:124:SER:OG	1:E:125:GLU:N	2.53	0.41
1:E:153:LYS:HE2	1:E:153:LYS:HB2	1.67	0.41
1:C:155:THR:O	1:C:156:ASN:HB2	2.21	0.40
1:G:116:HIS:CD2	1:G:117:PRO:HD2	2.56	0.40
1:G:61:LYS:HE3	1:G:61:LYS:HB3	1.79	0.40
1:C:122:ARG:O	1:C:122:ARG:HG3	2.20	0.40
1:D:158:GLN:HB2	1:D:225:ALA:HB2	2.04	0.40
1:D:158:GLN:HG2	1:D:174:TRP:O	2.21	0.40
1:H:263:SER:O	1:H:267:GLY:HA2	2.21	0.40
1:A:9:GLY:HA3	1:A:36:VAL:O	2.21	0.40
1:D:116:HIS:CG	1:D:117:PRO:HD2	2.57	0.40
1:E:294:ARG:HG2	1:E:294:ARG:NH1	2.31	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:LEU:C	1:F:288:ILE:HG13	2.41	0.40
1:E:228:GLN:OE1	1:E:228:GLN:N	2.48	0.40
1:F:111:ILE:O	1:F:112:ASP:HB2	2.21	0.40
1:G:166:GLU:OE2	1:H:90:LYS:NZ	2.44	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	293/301 (97%)	288 (98%)	5 (2%)	0	100	100
1	B	293/301 (97%)	283 (97%)	8 (3%)	2 (1%)	22	26
1	C	297/301 (99%)	289 (97%)	8 (3%)	0	100	100
1	D	293/301 (97%)	282 (96%)	11 (4%)	0	100	100
1	E	293/301 (97%)	282 (96%)	11 (4%)	0	100	100
1	F	293/301 (97%)	281 (96%)	12 (4%)	0	100	100
1	G	294/301 (98%)	285 (97%)	9 (3%)	0	100	100
1	H	293/301 (97%)	281 (96%)	9 (3%)	3 (1%)	15	17
All	All	2349/2408 (98%)	2271 (97%)	73 (3%)	5 (0%)	47	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	ASP
1	H	124	SER
1	H	23	LYS
1	B	23	LYS
1	H	253	PRO

### 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	260/266 (98%)	248 (95%)	12 (5%)	27	38
1	B	259/266 (97%)	244 (94%)	15 (6%)	20	27
1	C	264/266 (99%)	248 (94%)	16 (6%)	18	25
1	D	260/266 (98%)	243 (94%)	17 (6%)	17	23
1	E	260/266 (98%)	243 (94%)	17 (6%)	17	23
1	F	259/266 (97%)	242 (93%)	17 (7%)	16	22
1	G	260/266 (98%)	241 (93%)	19 (7%)	14	18
1	H	260/266 (98%)	246 (95%)	14 (5%)	22	30
All	All	2082/2128 (98%)	1955 (94%)	127 (6%)	18	25

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	32	MET
1	A	114	LYS
1	A	124	SER
1	A	138	LYS
1	A	143	LYS
1	A	189	LYS
1	A	194	LEU
1	A	216	LEU
1	A	244	LEU
1	A	273	LYS
1	A	295	SER
1	B	4	LYS
1	B	7	ARG
1	B	90	LYS
1	B	110	ASP
1	B	122	ARG
1	B	124	SER
1	B	125	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	129	ASN
1	B	158	GLN
1	B	183	ASP
1	B	189	LYS
1	B	194	LEU
1	B	226	SER
1	B	244	LEU
1	B	273	LYS
1	C	7	ARG
1	C	23	LYS
1	C	43	GLU
1	C	44	THR
1	C	114	LYS
1	C	119	SER
1	C	122	ARG
1	C	125	GLU
1	C	187	GLN
1	C	189	LYS
1	C	194	LEU
1	C	224	SER
1	C	254	ASN
1	C	295	SER
1	C	297	LEU
1	C	299	SER
1	D	4	LYS
1	D	7	ARG
1	D	22	GLU
1	D	23	LYS
1	D	43	GLU
1	D	122	ARG
1	D	154	SER
1	D	189	LYS
1	D	194	LEU
1	D	213	GLU
1	D	216	LEU
1	D	241	ARG
1	D	244	LEU
1	D	252	LEU
1	D	268	LEU
1	D	273	LYS
1	D	295	SER
1	E	7	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	22	GLU
1	E	23	LYS
1	E	48	LYS
1	E	110	ASP
1	E	114	LYS
1	E	122	ARG
1	E	125	GLU
1	E	129	ASN
1	E	153	LYS
1	E	183	ASP
1	E	187	GLN
1	E	189	LYS
1	E	194	LEU
1	E	216	LEU
1	E	244	LEU
1	E	273	LYS
1	F	4	LYS
1	F	7	ARG
1	F	16	TYR
1	F	20	LYS
1	F	23	LYS
1	F	74	THR
1	F	110	ASP
1	F	114	LYS
1	F	122	ARG
1	F	125	GLU
1	F	138	LYS
1	F	183	ASP
1	F	189	LYS
1	F	213	GLU
1	F	216	LEU
1	F	244	LEU
1	F	273	LYS
1	G	22	GLU
1	G	23	LYS
1	G	43	GLU
1	G	69	LYS
1	G	114	LYS
1	G	122	ARG
1	G	125	GLU
1	G	129	ASN
1	G	138	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	158	GLN
1	G	183	ASP
1	G	187	GLN
1	G	194	LEU
1	G	216	LEU
1	G	243	GLN
1	G	244	LEU
1	G	290	CYS
1	G	294	ARG
1	G	295	SER
1	H	4	LYS
1	H	7	ARG
1	H	16	TYR
1	H	48	LYS
1	H	110	ASP
1	H	114	LYS
1	H	122	ARG
1	H	171	LYS
1	H	183	ASP
1	H	189	LYS
1	H	216	LEU
1	H	244	LEU
1	H	268	LEU
1	H	273	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	129	ASN
1	A	200	HIS
1	B	104	HIS
1	B	131	GLN
1	B	200	HIS
1	C	104	HIS
1	C	129	ASN
1	C	200	HIS
1	D	104	HIS
1	D	131	GLN
1	D	200	HIS
1	D	243	GLN
1	D	254	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	104	HIS
1	E	129	ASN
1	E	200	HIS
1	F	70	GLN
1	F	86	HIS
1	F	104	HIS
1	F	129	ASN
1	G	104	HIS
1	G	129	ASN
1	G	243	GLN
1	H	104	HIS
1	H	129	ASN
1	H	200	HIS
1	H	243	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	SAC	G	1	1	4,5,9	0.59	0	0,5,11	0.00	-
1	SAC	A	1	1	4,5,9	0.65	0	0,5,11	0.00	-
1	SAC	B	1	1	7,8,9	1.05	0	8,9,11	1.93	3 (37%)
1	SAC	C	1	1	4,5,9	0.56	0	0,5,11	0.00	-
1	SAC	D	1	1	7,8,9	0.85	0	8,9,11	1.48	1 (12%)
1	SAC	E	1	1	4,5,9	0.65	0	0,5,11	0.00	-
1	SAC	F	1	1	4,5,9	0.69	0	0,5,11	0.00	-
1	SAC	H	1	1	4,5,9	0.70	0	0,5,11	0.00	-

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
1	SAC	G	1	1	-	2/2/4/10	-
1	SAC	A	1	1	-	2/2/4/10	-
1	SAC	B	1	1	-	0/7/8/10	-
1	SAC	C	1	1	-	2/2/4/10	-
1	SAC	D	1	1	-	1/7/8/10	-
1	SAC	E	1	1	-	0/2/4/10	-
1	SAC	F	1	1	-	0/2/4/10	-
1	SAC	H	1	1	-	2/2/4/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	SAC	CA-N-C1A	-3.51	116.67	123.15
1	B	1	SAC	C-CA-N	2.64	114.50	109.73
1	B	1	SAC	O-C-CA	-2.36	118.60	124.78
1	D	1	SAC	O-C-CA	-2.32	118.70	124.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	1	SAC	N-CA-CB-OG
1	G	1	SAC	C-CA-CB-OG
1	A	1	SAC	C-CA-CB-OG
1	C	1	SAC	C-CA-CB-OG
1	H	1	SAC	C-CA-CB-OG
1	C	1	SAC	N-CA-CB-OG
1	H	1	SAC	N-CA-CB-OG
1	D	1	SAC	N-CA-CB-OG
1	A	1	SAC	N-CA-CB-OG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	SAC	1	0
1	D	1	SAC	1	0
1	E	1	SAC	1	0
1	H	1	SAC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	PEG	B	4126	-	3,3,6	0.65	0	2,2,5	0.96	0
2	PEG	A	3126	-	3,3,6	1.07	0	2,2,5	1.08	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	PEG	B	4126	-	-	0/1/1/4	-
2	PEG	A	3126	-	-	1/1/1/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	A	3126	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4126	PEG	5	0
2	A	3126	PEG	4	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	294/301 (97%)	-0.86	0 100 100	15, 27, 55, 63	0
1	B	294/301 (97%)	-0.74	1 (0%) 94 96	19, 32, 56, 86	0
1	C	298/301 (99%)	-0.67	3 (1%) 82 86	16, 30, 59, 88	0
1	D	294/301 (97%)	-0.65	3 (1%) 82 86	18, 34, 60, 94	0
1	E	294/301 (97%)	-0.56	2 (0%) 87 91	21, 37, 61, 91	0
1	F	294/301 (97%)	-0.60	1 (0%) 94 96	22, 38, 67, 100	0
1	G	295/301 (98%)	-0.57	2 (0%) 87 91	20, 40, 69, 99	0
1	H	294/301 (97%)	-0.60	2 (0%) 87 91	19, 35, 61, 90	0
All	All	2357/2408 (97%)	-0.66	14 (0%) 89 92	15, 34, 61, 100	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	23	LYS	4.0
1	G	22	GLU	3.4
1	C	23	LYS	2.7
1	H	22	GLU	2.7
1	E	23	LYS	2.6
1	C	299	SER	2.4
1	H	23	LYS	2.4
1	D	295	SER	2.3
1	C	22	GLU	2.2
1	B	23	LYS	2.2
1	G	243	GLN	2.2
1	E	22	GLU	2.2
1	D	23	LYS	2.2
1	D	22	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SAC	C	1	6/10	0.81	0.17	48,63,63,63	0
1	SAC	E	1	6/10	0.91	0.14	51,53,54,71	0
1	SAC	A	1	6/10	0.92	0.20	53,56,59,69	0
1	SAC	F	1	6/10	0.93	0.18	50,65,65,66	0
1	SAC	H	1	6/10	0.93	0.12	58,59,59,82	0
1	SAC	D	1	9/10	0.94	0.16	39,43,56,66	0
1	SAC	G	1	6/10	0.94	0.16	51,57,59,73	0
1	SAC	B	1	9/10	0.95	0.19	37,46,61,72	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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
2	PEG	B	4126	4/7	0.79	0.31	50,52,63,72	0
2	PEG	A	3126	4/7	0.95	0.19	28,35,36,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.