



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:34 am GMT

PDB ID : 4PIR  
Title : X-ray structure of the mouse serotonin 5-HT3 receptor  
Authors : Hassaine, G.; Deluz, C.; Grasso, L.; Wyss, R.; Tol, M.B.; Hovius, R.; Graff, A.; Stahlberg, H.; Tomizaki, T.; Desmyter, A.; Moreau, C.; Li, X.-D.; Poitevin, F.; Vogel, H.; Nury, H.  
Deposited on : 2014-05-09  
Resolution : 3.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

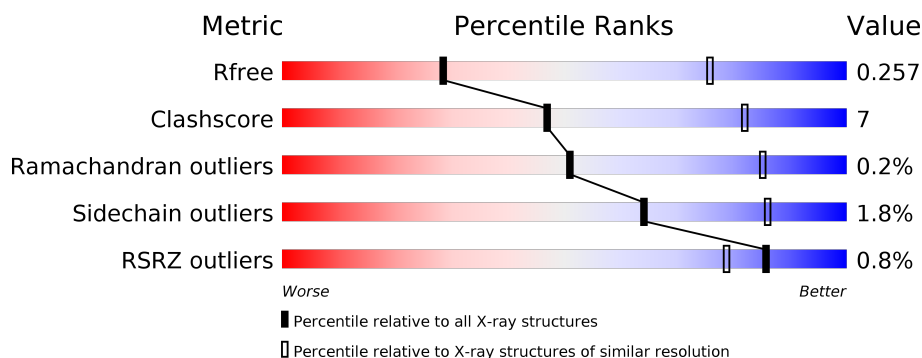
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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. 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	456	
1	B	456	
1	C	456	
1	D	456	
1	E	456	
2	F	124	

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Mol	Chain	Length	Quality of chain
2	G	124	<div><div>%</div><div><div></div></div><div>90%10%</div></div>
2	H	124	<div><div></div><div>82%18%</div></div>
2	I	124	<div><div>%</div><div><div></div></div><div>89%11%</div></div>
2	J	124	<div><div></div><div>85%15%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20739 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 5-hydroxytryptamine receptor 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			3108	2045	507	547	9			
1	B	383	Total	C	N	O	S	0	0	0
			3111	2046	507	549	9			
1	C	384	Total	C	N	O	S	0	0	0
			3125	2057	509	550	9			
1	D	384	Total	C	N	O	S	0	0	0
			3125	2057	509	550	9			
1	E	383	Total	C	N	O	S	0	0	0
			3111	2046	507	549	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ALA	GLU	conflict	UNP P23979
A	5	ARG	-	insertion	UNP P23979
A	277	ALA	-	insertion	UNP P23979
A	461	SER	TYR	conflict	UNP P23979
B	4	ALA	GLU	conflict	UNP P23979
B	5	ARG	-	insertion	UNP P23979
B	277	ALA	-	insertion	UNP P23979
B	461	SER	TYR	conflict	UNP P23979
C	4	ALA	GLU	conflict	UNP P23979
C	5	ARG	-	insertion	UNP P23979
C	277	ALA	-	insertion	UNP P23979
C	461	SER	TYR	conflict	UNP P23979
D	4	ALA	GLU	conflict	UNP P23979
D	5	ARG	-	insertion	UNP P23979
D	277	ALA	-	insertion	UNP P23979
D	461	SER	TYR	conflict	UNP P23979
E	4	ALA	GLU	conflict	UNP P23979
E	5	ARG	-	insertion	UNP P23979
E	277	ALA	-	insertion	UNP P23979

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Chain	Residue	Modelled	Actual	Comment	Reference
E	461	SER	TYR	conflict	UNP P23979

- Molecule 2 is a protein called VHH15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	122	Total	C	N	O	S	0	0	0
			920	572	162	182	4			
2	G	124	Total	C	N	O	S	0	0	0
			936	579	164	189	4			
2	H	124	Total	C	N	O	S	0	0	0
			936	579	164	189	4			
2	I	124	Total	C	N	O	S	0	0	0
			936	579	164	189	4			
2	J	124	Total	C	N	O	S	0	0	0
			936	579	164	189	4			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	D	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		

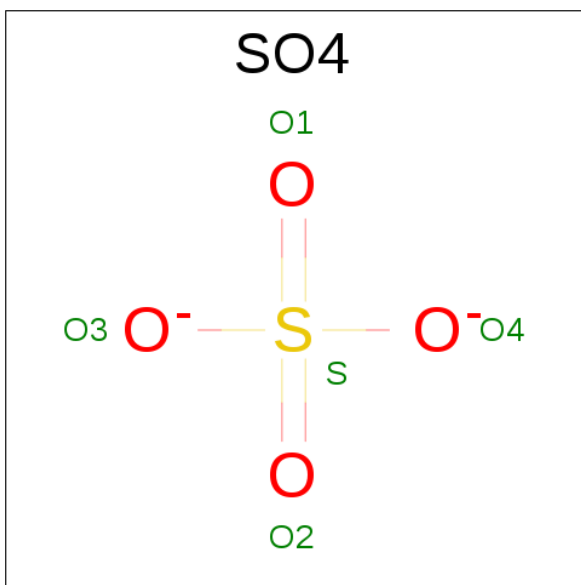
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	E	1	Total	Cl	0	0
			1	1		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

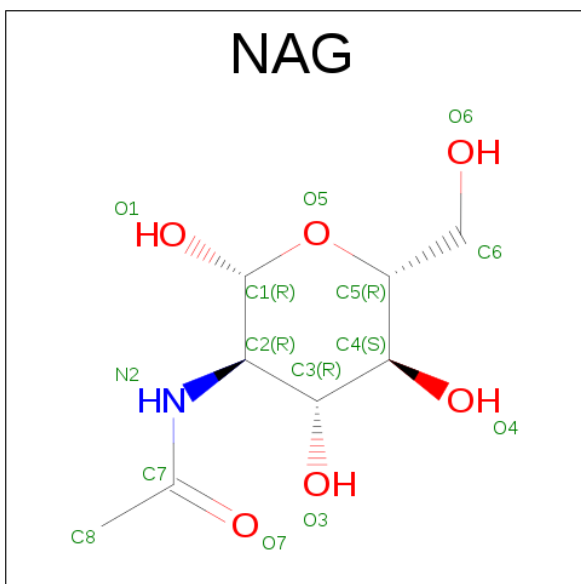
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



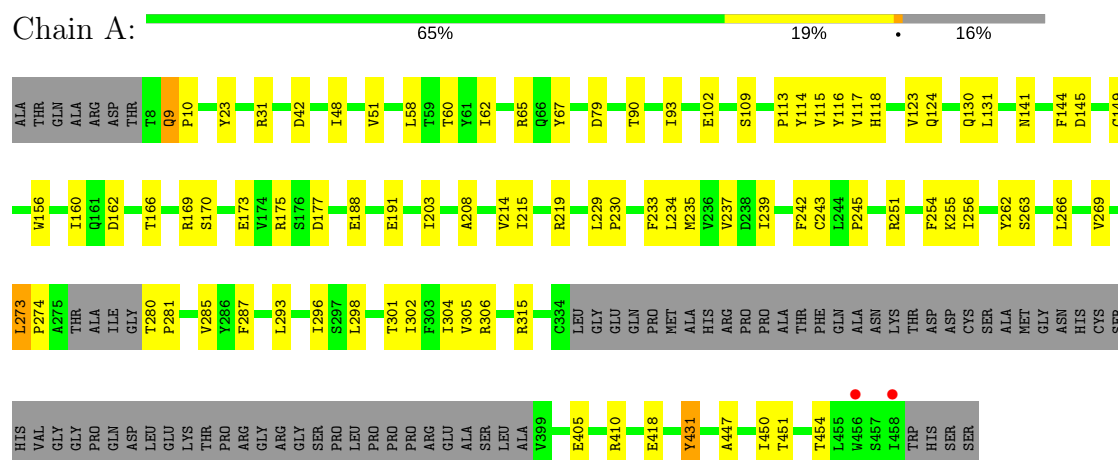
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		



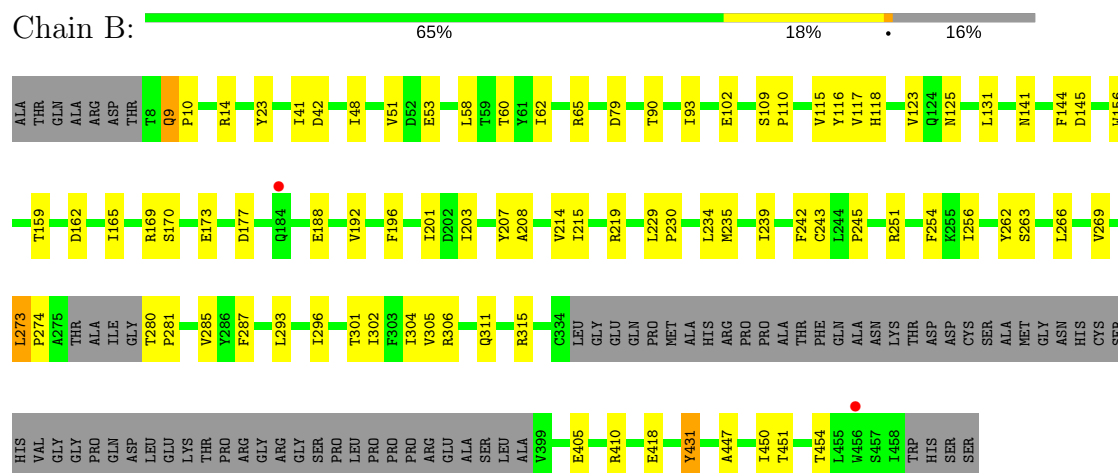
### 3 Residue-property plots

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.

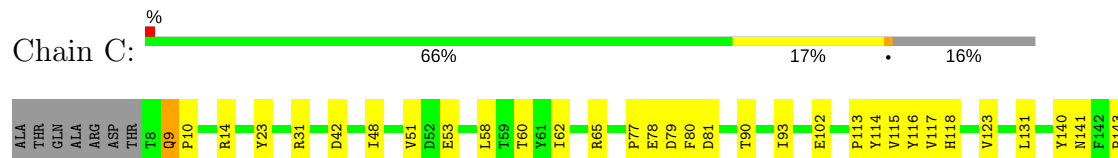
#### • Molecule 1: 5-hydroxytryptamine receptor 3A

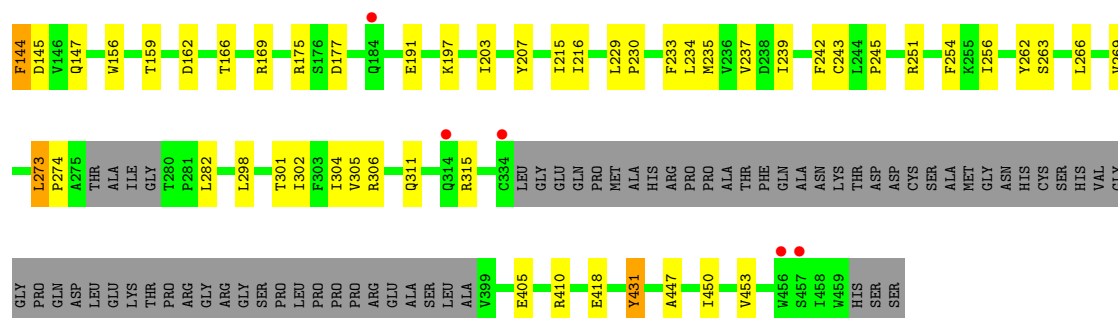


#### • Molecule 1: 5-hydroxytryptamine receptor 3A



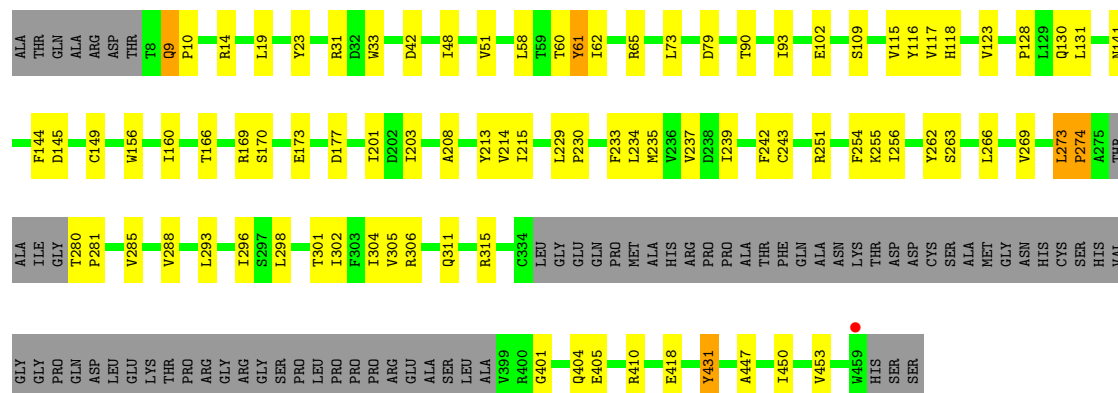
#### • Molecule 1: 5-hydroxytryptamine receptor 3A





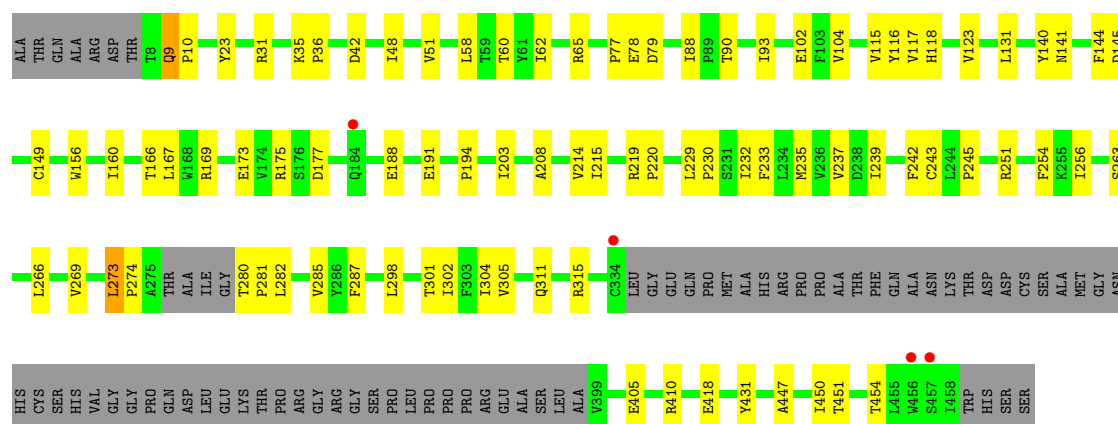
- Molecule 1: 5-hydroxytryptamine receptor 3A

Chain D: 65% 18% 16%



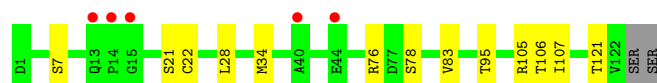
- Molecule 1: 5-hydroxytryptamine receptor 3A

Chain E: 65% 19% 16%

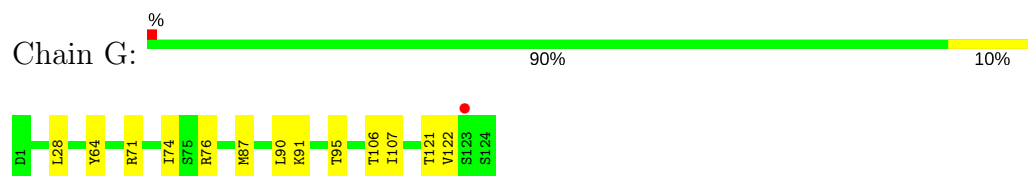


- Molecule 2: VHH15

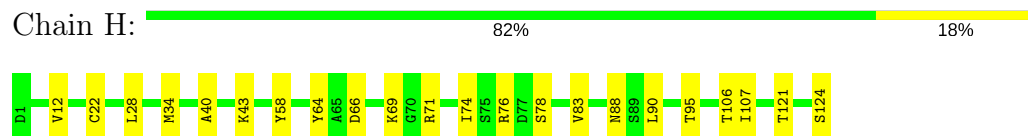
Chain F: 4% 88% 10%



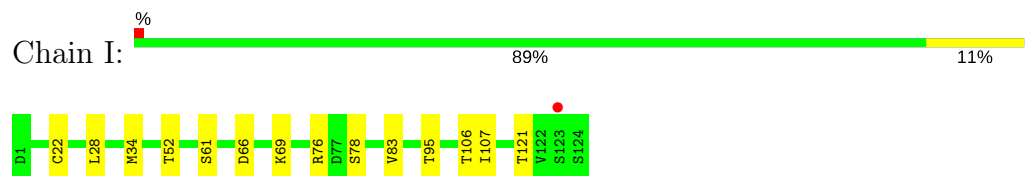
- Molecule 2: VHH15



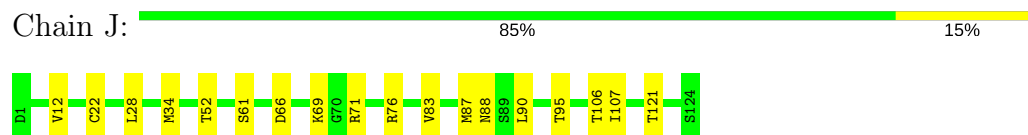
- Molecule 2: VHH15



- Molecule 2: VHH15



- Molecule 2: VHH15



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.54Å 187.09Å 240.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.50) 99.8 (20.00-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 3.52Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1685)	Depositor
R, $R_{free}$	0.217 , 0.257 0.218 , 0.257	Depositor DCC
$R_{free}$ test set	3503 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.1	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 86.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: CL, BMA, SO4, NAG

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	0.22	0/3190	0.40	0/4358
1	B	0.22	0/3193	0.41	0/4362
1	C	0.23	0/3209	0.40	0/4385
1	D	0.23	0/3209	0.41	0/4385
1	E	0.22	0/3193	0.40	0/4362
2	F	0.20	0/936	0.36	0/1269
2	G	0.20	0/952	0.37	0/1289
2	H	0.21	0/952	0.37	0/1289
2	I	0.20	0/952	0.36	0/1289
2	J	0.20	0/952	0.36	0/1289
All	All	0.22	0/20738	0.40	0/28277

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3108	0	3087	55	0
1	B	3111	0	3089	55	0
1	C	3125	0	3099	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3125	0	3099	59	0
1	E	3111	0	3089	55	0
2	F	920	0	886	10	0
2	G	936	0	898	9	0
2	H	936	0	898	15	0
2	I	936	0	898	9	0
2	J	936	0	900	11	0
3	A	56	0	50	1	0
3	B	56	0	50	1	0
3	C	56	0	50	1	0
3	D	56	0	50	2	0
3	E	28	0	25	1	0
4	A	39	0	34	1	0
4	C	39	0	34	1	0
4	D	39	0	34	1	0
4	E	39	0	34	2	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
5	C	1	0	0	1	0
5	D	1	0	0	1	0
5	E	1	0	0	1	0
6	B	39	0	34	1	0
7	D	5	0	0	0	0
7	H	10	0	0	1	0
8	E	28	0	26	0	0
All	All	20739	0	20364	293	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 (293) 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:E:31:ARG:NH1	5:E:508:CL:CL	2.35	0.95
1:C:31:ARG:NH1	5:C:508:CL:CL	2.50	0.81
1:B:90:THR:HG22	1:B:115:VAL:HG13	1.64	0.80
1:D:90:THR:HG22	1:D:115:VAL:HG13	1.69	0.74
1:E:90:THR:HG22	1:E:115:VAL:HG13	1.69	0.73
1:C:215:ILE:HG12	3:C:507:NAG:H82	1.72	0.72
1:E:215:ILE:HG12	3:E:507:NAG:H82	1.72	0.72
1:A:215:ILE:HG12	3:A:506:NAG:H82	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:THR:HG22	1:C:115:VAL:HG13	1.72	0.70
1:D:215:ILE:HG12	3:D:507:NAG:H82	1.73	0.69
1:A:90:THR:HG22	1:A:115:VAL:HG13	1.73	0.69
1:E:117:VAL:HG22	1:E:123:VAL:HG22	1.76	0.68
1:B:215:ILE:HG12	3:B:507:NAG:H82	1.77	0.67
1:D:42:ASP:OD1	1:D:169:ARG:NH1	2.29	0.66
1:B:42:ASP:OD1	1:B:169:ARG:NH1	2.30	0.64
1:A:31:ARG:NH1	5:A:508:CL:CL	2.62	0.64
2:H:95:THR:HG23	2:H:121:THR:HA	1.80	0.64
1:C:42:ASP:OD1	1:C:169:ARG:NH1	2.31	0.63
1:D:117:VAL:HG22	1:D:123:VAL:HG22	1.81	0.62
2:J:34:MET:HG2	2:J:83:VAL:HG11	1.81	0.62
1:A:203:ILE:HG23	2:F:76:ARG:NH1	2.13	0.62
2:H:34:MET:HG2	2:H:83:VAL:HG11	1.82	0.61
2:I:34:MET:HG2	2:I:83:VAL:HG11	1.82	0.61
1:C:117:VAL:HG22	1:C:123:VAL:HG22	1.83	0.61
1:A:67:TYR:HE1	1:A:124:GLN:HG3	1.65	0.61
2:I:95:THR:HG23	2:I:121:THR:HA	1.82	0.60
1:A:42:ASP:OD1	1:A:169:ARG:NH1	2.34	0.60
1:C:42:ASP:HB3	1:C:65:ARG:HB2	1.82	0.60
2:J:95:THR:HG23	2:J:121:THR:HA	1.84	0.60
1:E:42:ASP:OD1	1:E:169:ARG:NH1	2.35	0.59
1:A:117:VAL:HG22	1:A:123:VAL:HG22	1.83	0.59
1:A:306:ARG:HG3	1:E:245:PRO:HD3	1.84	0.59
1:B:117:VAL:HG22	1:B:123:VAL:HG22	1.84	0.58
1:C:410:ARG:NH1	1:D:405:GLU:OE1	2.37	0.58
1:A:405:GLU:OE1	1:E:410:ARG:NH1	2.36	0.58
1:D:42:ASP:HB3	1:D:65:ARG:HB2	1.85	0.58
2:G:95:THR:HG23	2:G:121:THR:HA	1.85	0.58
1:C:203:ILE:HG23	2:H:76:ARG:NH1	2.18	0.58
1:D:203:ILE:HG23	2:I:76:ARG:NH1	2.19	0.57
1:E:42:ASP:HB3	1:E:65:ARG:HB2	1.84	0.57
1:C:48:ILE:HA	1:C:60:THR:HG22	1.87	0.57
2:F:76:ARG:HH12	2:F:78:SER:HB3	1.69	0.57
2:F:95:THR:HG23	2:F:121:THR:HA	1.86	0.57
1:C:251:ARG:NH1	1:C:304:ILE:HD11	2.20	0.56
1:D:48:ILE:HA	1:D:60:THR:HG22	1.86	0.56
1:E:315:ARG:NH2	1:E:418:GLU:OE2	2.36	0.56
1:A:23:TYR:HE1	1:A:93:ILE:HA	1.71	0.56
1:D:255:LYS:NZ	1:D:301:THR:OG1	2.35	0.56
1:A:315:ARG:NH2	1:A:418:GLU:OE2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:CYS:HB2	1:C:302:ILE:HD13	1.88	0.55
1:B:410:ARG:NH1	1:C:405:GLU:OE1	2.38	0.55
1:D:315:ARG:NH2	1:D:418:GLU:OE2	2.37	0.55
1:A:255:LYS:NZ	1:A:301:THR:OG1	2.35	0.55
1:B:245:PRO:HD3	1:C:306:ARG:HG3	1.89	0.55
1:C:169:ARG:NH2	1:C:177:ASP:OD2	2.40	0.55
1:A:175:ARG:NE	1:A:191:GLU:OE2	2.39	0.55
1:D:234:LEU:HD13	1:D:262:TYR:HD1	1.72	0.55
1:D:51:VAL:HG12	1:D:58:LEU:HD13	1.89	0.55
1:C:245:PRO:HD3	1:D:306:ARG:HG3	1.88	0.55
1:E:203:ILE:HG23	2:J:76:ARG:HD2	1.89	0.55
2:I:22:CYS:HB3	2:I:83:VAL:HG13	1.89	0.54
1:B:42:ASP:HB3	1:B:65:ARG:HB2	1.88	0.54
1:A:302:ILE:HD13	1:E:243:CYS:HB2	1.88	0.54
2:F:34:MET:HG2	2:F:83:VAL:HG11	1.89	0.54
2:H:22:CYS:HB3	2:H:83:VAL:HG13	1.88	0.54
1:D:31:ARG:NH1	5:D:509:CL:CL	2.75	0.54
1:B:254:PHE:CE2	1:C:256:ILE:HD11	2.42	0.54
1:B:234:LEU:HD13	1:B:262:TYR:HD1	1.73	0.53
2:J:22:CYS:HB3	2:J:83:VAL:HG13	1.90	0.53
1:E:188:GLU:HB2	1:E:219:ARG:HD3	1.91	0.53
1:A:256:ILE:HD11	1:E:254:PHE:CE2	2.43	0.53
1:D:42:ASP:CG	1:D:169:ARG:HH11	2.13	0.52
1:C:23:TYR:HE1	1:C:93:ILE:HA	1.75	0.52
1:D:243:CYS:HB2	1:E:302:ILE:HD13	1.92	0.52
1:B:203:ILE:HG23	2:G:76:ARG:HD2	1.91	0.52
1:D:251:ARG:HH11	1:D:301:THR:HG23	1.75	0.51
1:A:234:LEU:HD13	1:A:262:TYR:HD1	1.75	0.51
1:B:48:ILE:HA	1:B:60:THR:HG22	1.91	0.51
1:B:266:LEU:HA	1:B:269:VAL:HG12	1.93	0.51
1:C:254:PHE:CE2	1:D:256:ILE:HD11	2.45	0.51
1:C:243:CYS:HB2	1:D:302:ILE:HD13	1.91	0.51
1:E:251:ARG:NH1	1:E:304:ILE:HD11	2.25	0.51
1:B:23:TYR:HE2	1:B:93:ILE:HA	1.76	0.51
1:B:192:VAL:HG22	1:B:214:VAL:HG12	1.93	0.51
1:D:254:PHE:CE2	1:E:256:ILE:HD11	2.45	0.51
1:A:251:ARG:HH11	1:A:301:THR:HG23	1.76	0.51
1:D:23:TYR:HE2	1:D:93:ILE:HA	1.75	0.50
1:D:273:LEU:HD13	1:D:274:PRO:HD2	1.92	0.50
1:B:10:PRO:HD2	1:B:14:ARG:HD3	1.94	0.50
1:A:243:CYS:HB2	1:B:302:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:TYR:OH	1:B:311:GLN:OE1	2.27	0.50
1:A:410:ARG:NH1	1:B:405:GLU:OE1	2.44	0.50
1:B:51:VAL:HG12	1:B:58:LEU:HD13	1.92	0.50
2:F:7:SER:OG	2:F:21:SER:OG	2.27	0.50
1:A:254:PHE:CE2	1:B:256:ILE:HD11	2.46	0.50
1:B:41:ILE:HD13	1:B:165:ILE:HD11	1.92	0.50
1:B:169:ARG:NH2	1:B:177:ASP:OD2	2.45	0.50
1:E:239:ILE:HA	1:E:242:PHE:HD2	1.77	0.49
1:C:175:ARG:NE	1:C:191:GLU:OE1	2.45	0.49
1:C:42:ASP:CG	1:C:169:ARG:HH11	2.16	0.49
1:A:166:THR:HG22	4:A:505:NAG:H62	1.94	0.49
1:C:266:LEU:HA	1:C:269:VAL:HG12	1.95	0.49
2:F:22:CYS:HB3	2:F:83:VAL:HG13	1.94	0.49
2:J:106:THR:OG1	2:J:107:ILE:N	2.46	0.49
1:E:48:ILE:HA	1:E:60:THR:HG22	1.94	0.49
1:E:23:TYR:HE2	1:E:93:ILE:HA	1.77	0.49
2:I:106:THR:OG1	2:I:107:ILE:N	2.45	0.49
1:B:239:ILE:HA	1:B:242:PHE:HD2	1.78	0.49
1:B:118:HIS:CE1	2:H:28:LEU:HD12	2.48	0.49
1:A:48:ILE:HA	1:A:60:THR:HG22	1.94	0.48
1:B:42:ASP:CG	1:B:169:ARG:HH11	2.16	0.48
1:C:51:VAL:HG12	1:C:58:LEU:HD13	1.95	0.48
1:E:149:CYS:HB2	1:E:214:VAL:HG13	1.95	0.48
2:G:106:THR:OG1	2:G:107:ILE:N	2.46	0.48
1:A:251:ARG:NH1	1:A:304:ILE:HD11	2.29	0.48
1:E:169:ARG:NH2	1:E:177:ASP:OD2	2.47	0.48
1:E:118:HIS:CE1	2:F:28:LEU:HD12	2.49	0.48
2:F:106:THR:OG1	2:F:107:ILE:N	2.47	0.48
1:B:141:ASN:O	1:B:145:ASP:HB3	2.13	0.47
1:A:141:ASN:O	1:A:145:ASP:HB3	2.13	0.47
1:A:239:ILE:HA	1:A:242:PHE:HD2	1.80	0.47
1:D:141:ASN:O	1:D:145:ASP:HB3	2.14	0.47
1:D:160:ILE:HG13	1:D:208:ALA:HB2	1.97	0.47
1:B:102:GLU:N	1:B:102:GLU:OE2	2.48	0.47
2:G:90:LEU:HB3	2:G:122:VAL:HG21	1.95	0.47
1:A:266:LEU:HA	1:A:269:VAL:HG12	1.97	0.47
1:D:10:PRO:HD2	1:D:14:ARG:HD3	1.96	0.47
2:H:106:THR:OG1	2:H:107:ILE:N	2.48	0.47
1:C:141:ASN:O	1:C:145:ASP:HB3	2.15	0.47
1:C:234:LEU:HD13	1:C:262:TYR:HD1	1.79	0.47
1:D:239:ILE:HA	1:D:242:PHE:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:76:ARG:HH12	2:H:78:SER:HB3	1.80	0.47
1:A:109:SER:HG	1:A:130:GLN:H	1.62	0.46
1:D:266:LEU:HA	1:D:269:VAL:HG12	1.95	0.46
1:C:431:TYR:OH	1:D:311:GLN:OE1	2.27	0.46
1:E:266:LEU:HA	1:E:269:VAL:HG12	1.97	0.46
1:D:251:ARG:NH1	1:D:304:ILE:HD11	2.31	0.46
2:H:66:ASP:HA	2:H:69:LYS:HD3	1.97	0.46
1:A:51:VAL:HG12	1:A:58:LEU:HD13	1.96	0.46
1:E:273:LEU:HD13	1:E:274:PRO:HD2	1.98	0.46
1:B:251:ARG:NH1	1:B:304:ILE:HD11	2.31	0.46
1:A:42:ASP:HB3	1:A:65:ARG:HB2	1.97	0.46
1:C:273:LEU:HD13	1:C:274:PRO:HD2	1.98	0.46
2:H:12:VAL:HG21	2:H:90:LEU:HD13	1.97	0.45
1:A:188:GLU:HB2	1:A:219:ARG:HD3	1.98	0.45
1:A:273:LEU:HD13	1:A:274:PRO:HD2	1.98	0.45
1:E:141:ASN:O	1:E:145:ASP:HB3	2.16	0.45
1:E:280:THR:HA	1:E:281:PRO:HD3	1.84	0.45
1:C:239:ILE:HA	1:C:242:PHE:HD2	1.81	0.45
2:I:52:THR:O	2:I:61:SER:OG	2.28	0.45
2:J:52:THR:O	2:J:61:SER:OG	2.27	0.45
1:C:118:HIS:CE1	2:I:28:LEU:HD12	2.50	0.45
1:C:102:GLU:N	1:C:102:GLU:OE2	2.49	0.45
1:D:169:ARG:NH2	1:D:177:ASP:OD2	2.49	0.45
1:E:42:ASP:CG	1:E:169:ARG:HH11	2.20	0.45
1:A:160:ILE:HG13	1:A:208:ALA:HB2	1.99	0.45
1:A:280:THR:HA	1:A:281:PRO:HD3	1.83	0.45
1:D:61:TYR:HE1	1:D:128:PRO:HB2	1.82	0.45
1:D:62:ILE:HD13	1:D:131:LEU:HD12	1.99	0.45
1:B:203:ILE:HG23	2:G:76:ARG:NH1	2.31	0.45
1:B:451:THR:O	1:B:454:THR:HG22	2.17	0.45
1:E:160:ILE:HG13	1:E:208:ALA:HB2	1.98	0.44
1:E:51:VAL:HG12	1:E:58:LEU:HD13	1.98	0.44
1:B:196:PHE:CE2	6:B:501:NAG:H5	2.52	0.44
1:B:53:GLU:HG2	1:B:273:LEU:HD11	1.99	0.44
1:A:451:THR:O	1:A:454:THR:HG22	2.16	0.44
1:E:251:ARG:HH11	1:E:301:THR:HG23	1.81	0.44
1:B:159:THR:HG22	1:B:207:TYR:HE1	1.83	0.44
1:D:61:TYR:CE1	1:D:128:PRO:HB2	2.53	0.44
1:E:88:ILE:HD11	1:E:117:VAL:HG21	2.00	0.44
1:A:102:GLU:N	1:A:102:GLU:OE2	2.50	0.44
1:D:431:TYR:OH	1:E:311:GLN:OE1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:PRO:HG2	1:E:78:GLU:OE2	2.17	0.44
1:B:263:SER:O	1:B:266:LEU:HG	2.17	0.44
1:C:203:ILE:HG23	2:H:76:ARG:HD2	2.00	0.44
1:D:102:GLU:N	1:D:102:GLU:OE2	2.48	0.43
1:E:447:ALA:O	1:E:450:ILE:HG22	2.18	0.43
1:D:118:HIS:CE1	2:J:28:LEU:HD12	2.53	0.43
1:A:42:ASP:CG	1:A:169:ARG:HH11	2.21	0.43
1:B:235:MET:O	1:B:239:ILE:HG12	2.19	0.43
1:B:251:ARG:HH11	1:B:301:THR:HG23	1.81	0.43
1:D:170:SER:HB3	1:D:173:GLU:HG3	2.00	0.43
1:D:251:ARG:HD3	1:D:301:THR:HG23	2.00	0.43
1:E:173:GLU:OE1	2:F:105:ARG:NH2	2.52	0.43
1:B:188:GLU:HB2	1:B:219:ARG:HD3	2.00	0.43
1:C:235:MET:O	1:C:239:ILE:HG12	2.19	0.43
1:D:61:TYR:CD2	1:E:104:VAL:HA	2.53	0.43
1:E:451:THR:O	1:E:454:THR:HG22	2.19	0.43
4:E:502:NAG:HN2	4:E:503:NAG:H61	1.82	0.43
1:B:280:THR:HA	1:B:281:PRO:HD3	1.85	0.43
1:E:35:LYS:HA	1:E:36:PRO:HD3	1.87	0.43
1:C:81:ASP:OD2	1:D:33:TRP:NE1	2.48	0.43
1:D:166:THR:HG22	4:D:503:NAG:H62	1.98	0.43
1:E:102:GLU:N	1:E:102:GLU:OE2	2.49	0.43
1:E:235:MET:O	1:E:239:ILE:HG12	2.18	0.43
1:A:203:ILE:HG23	2:F:76:ARG:HH11	1.84	0.43
1:D:410:ARG:NH1	1:E:405:GLU:OE1	2.49	0.43
2:G:64:TYR:CZ	2:G:74:ILE:HG22	2.54	0.43
1:A:118:HIS:CE1	2:G:28:LEU:HD12	2.53	0.43
1:A:169:ARG:NH2	1:A:177:ASP:OD2	2.52	0.43
1:C:263:SER:O	1:C:266:LEU:HG	2.19	0.43
1:E:62:ILE:HD13	1:E:131:LEU:HD12	1.99	0.43
1:E:263:SER:O	1:E:266:LEU:HG	2.18	0.43
1:C:77:PRO:HG2	1:C:78:GLU:OE2	2.19	0.43
1:D:149:CYS:HB2	1:D:214:VAL:HG13	2.00	0.43
1:A:447:ALA:O	1:A:450:ILE:HG22	2.19	0.43
1:B:62:ILE:HD13	1:B:131:LEU:HD12	2.01	0.43
1:C:62:ILE:HD13	1:C:131:LEU:HD12	2.00	0.43
1:D:229:LEU:HB3	1:D:230:PRO:HD3	2.01	0.43
1:A:229:LEU:HB3	1:A:230:PRO:HD3	1.99	0.43
1:D:280:THR:HA	1:D:281:PRO:HD3	1.85	0.43
2:G:87:MET:HB3	2:G:90:LEU:HD21	2.01	0.43
1:A:298:LEU:HD21	1:E:254:PHE:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:71:ARG:NH1	2:G:91:LYS:HE3	2.34	0.42
1:B:273:LEU:HD13	1:B:274:PRO:HD2	2.00	0.42
1:C:197:LYS:HD3	2:H:58:TYR:CZ	2.54	0.42
1:C:447:ALA:O	1:C:450:ILE:HG22	2.19	0.42
1:B:447:ALA:O	1:B:450:ILE:HG22	2.20	0.42
1:E:229:LEU:HB3	1:E:230:PRO:HD3	2.01	0.42
2:I:76:ARG:HH12	2:I:78:SER:HB3	1.85	0.42
1:C:254:PHE:HE2	1:D:298:LEU:HD21	1.84	0.42
1:E:167:LEU:HD11	1:E:194:PRO:HB2	2.02	0.42
1:B:115:VAL:HG12	1:B:125:ASN:HA	2.01	0.42
1:C:147:GLN:HB2	1:C:216:ILE:HG13	2.02	0.42
1:C:159:THR:HG22	1:C:207:TYR:HE1	1.85	0.42
1:D:447:ALA:O	1:D:450:ILE:HG22	2.19	0.42
1:E:166:THR:HG22	4:E:503:NAG:H62	2.00	0.42
1:A:235:MET:O	1:A:239:ILE:HG12	2.19	0.42
1:A:245:PRO:HD3	1:B:306:ARG:HG3	2.02	0.42
2:J:71:ARG:HB3	2:J:88:ASN:O	2.19	0.42
1:A:113:PRO:HG2	1:A:114:TYR:CD2	2.55	0.42
1:C:166:THR:HG22	4:C:503:NAG:H62	2.02	0.42
1:A:293:LEU:O	1:A:296:ILE:HG13	2.19	0.42
1:B:201:ILE:HD12	1:B:201:ILE:HA	1.94	0.42
1:B:165:ILE:HG22	1:B:208:ALA:HB1	2.02	0.42
1:C:315:ARG:NH2	1:C:418:GLU:OE2	2.51	0.42
1:C:450:ILE:HA	1:C:453:VAL:HG22	2.02	0.42
1:E:219:ARG:HA	1:E:220:PRO:HD3	1.86	0.42
1:C:251:ARG:HH11	1:C:301:THR:HG23	1.84	0.42
1:D:235:MET:O	1:D:239:ILE:HG12	2.18	0.42
1:D:293:LEU:O	1:D:296:ILE:HG13	2.20	0.42
1:D:9:GLN:N	1:D:10:PRO:HD3	2.35	0.42
1:B:229:LEU:HB3	1:B:230:PRO:HD3	2.01	0.41
1:B:315:ARG:NH2	1:B:418:GLU:OE2	2.51	0.41
1:E:175:ARG:NE	1:E:191:GLU:OE1	2.52	0.41
1:E:140:TYR:CZ	1:E:282:LEU:HD22	2.55	0.41
2:H:124:SER:OG	7:H:302:SO4:O2	2.37	0.41
2:H:71:ARG:HB3	2:H:88:ASN:O	2.19	0.41
1:C:53:GLU:HG2	1:C:273:LEU:HD11	2.02	0.41
1:E:229:LEU:O	1:E:232:ILE:HG13	2.20	0.41
2:I:66:ASP:HA	2:I:69:LYS:HD3	2.02	0.41
2:J:66:ASP:HA	2:J:69:LYS:HD3	2.01	0.41
1:D:109:SER:OG	1:D:130:GLN:N	2.49	0.41
1:B:293:LEU:O	1:B:296:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:PHE:O	1:C:237:VAL:HG23	2.20	0.41
1:D:263:SER:O	1:D:266:LEU:HG	2.19	0.41
1:A:9:GLN:N	1:A:10:PRO:HD3	2.34	0.41
1:D:201:ILE:HD12	1:D:201:ILE:HA	1.94	0.41
1:D:19:LEU:HD23	1:D:73:LEU:HD22	2.02	0.41
2:J:87:MET:HB3	2:J:90:LEU:HD21	2.02	0.41
1:E:285:VAL:C	1:E:287:PHE:H	2.24	0.41
2:H:64:TYR:CZ	2:H:74:ILE:HG22	2.56	0.41
1:A:263:SER:O	1:A:266:LEU:HG	2.20	0.41
1:B:109:SER:HA	1:B:110:PRO:HD3	1.93	0.41
1:C:9:GLN:N	1:C:10:PRO:HD3	2.35	0.41
1:A:233:PHE:O	1:A:237:VAL:HG23	2.20	0.41
1:B:285:VAL:C	1:B:287:PHE:H	2.24	0.41
1:C:256:ILE:HD13	1:C:298:LEU:HD11	2.03	0.41
1:A:170:SER:HB3	1:A:173:GLU:HG3	2.03	0.41
1:D:233:PHE:O	1:D:237:VAL:HG23	2.20	0.41
1:E:9:GLN:N	1:E:10:PRO:HD3	2.35	0.41
1:E:256:ILE:HD13	1:E:298:LEU:HD11	2.03	0.41
1:C:113:PRO:HG2	1:C:114:TYR:CD2	2.56	0.41
1:C:143:PRO:HG2	1:C:144:PHE:CE1	2.56	0.41
1:D:213:TYR:CE1	3:D:507:NAG:H5	2.56	0.41
1:A:149:CYS:HB2	1:A:214:VAL:HG13	2.02	0.41
1:B:9:GLN:N	1:B:10:PRO:HD3	2.36	0.41
1:E:233:PHE:O	1:E:237:VAL:HG23	2.21	0.41
1:B:170:SER:HB3	1:B:173:GLU:HG3	2.03	0.40
1:C:140:TYR:CZ	1:C:282:LEU:HD22	2.57	0.40
1:D:450:ILE:HA	1:D:453:VAL:HG22	2.02	0.40
1:A:62:ILE:HD13	1:A:131:LEU:HD12	2.02	0.40
1:B:254:PHE:HE2	1:C:298:LEU:HD21	1.86	0.40
1:B:431:TYR:OH	1:C:311:GLN:OE1	2.31	0.40
1:A:285:VAL:C	1:A:287:PHE:H	2.23	0.40
1:C:78:GLU:C	1:C:80:PHE:H	2.24	0.40
1:D:401:GLY:O	1:D:404:GLN:HG2	2.22	0.40
2:J:12:VAL:HG21	2:J:90:LEU:HD13	2.03	0.40
1:C:10:PRO:HD2	1:C:14:ARG:HD3	2.03	0.40
1:A:109:SER:OG	1:A:130:GLN:N	2.46	0.40
1:C:229:LEU:HB3	1:C:230:PRO:HD3	2.03	0.40
1:D:285:VAL:HA	1:D:288:VAL:HG12	2.04	0.40
2:H:40:ALA:HB3	2:H:43:LYS:HB2	2.04	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	377/456 (83%)	352 (93%)	24 (6%)	1 (0%)	44	80
1	B	377/456 (83%)	352 (93%)	24 (6%)	1 (0%)	44	80
1	C	378/456 (83%)	353 (93%)	24 (6%)	1 (0%)	44	80
1	D	378/456 (83%)	352 (93%)	24 (6%)	2 (0%)	32	73
1	E	377/456 (83%)	352 (93%)	24 (6%)	1 (0%)	44	80
2	F	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
2	G	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
2	H	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
2	I	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
2	J	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
All	All	2495/2900 (86%)	2347 (94%)	142 (6%)	6 (0%)	51	85

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	79	ASP
1	A	79	ASP
1	B	79	ASP
1	D	79	ASP
1	E	79	ASP
1	D	274	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	341/417 (82%)	333 (98%)	8 (2%)	56	82
1	B	342/417 (82%)	334 (98%)	8 (2%)	56	82
1	C	343/417 (82%)	335 (98%)	8 (2%)	56	82
1	D	343/417 (82%)	335 (98%)	8 (2%)	56	82
1	E	342/417 (82%)	335 (98%)	7 (2%)	60	84
2	F	94/99 (95%)	94 (100%)	0	100	100
2	G	97/99 (98%)	97 (100%)	0	100	100
2	H	97/99 (98%)	97 (100%)	0	100	100
2	I	97/99 (98%)	97 (100%)	0	100	100
2	J	97/99 (98%)	97 (100%)	0	100	100
All	All	2193/2580 (85%)	2154 (98%)	39 (2%)	64	86

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	116	TYR
1	A	144	PHE
1	A	156	TRP
1	A	162	ASP
1	A	273	LEU
1	A	305	VAL
1	A	431	TYR
1	B	9	GLN
1	B	116	TYR
1	B	144	PHE
1	B	156	TRP
1	B	162	ASP
1	B	273	LEU
1	B	305	VAL
1	B	431	TYR
1	C	9	GLN
1	C	116	TYR
1	C	144	PHE
1	C	156	TRP
1	C	162	ASP
1	C	273	LEU
1	C	305	VAL
1	C	431	TYR

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Mol	Chain	Res	Type
1	D	9	GLN
1	D	61	TYR
1	D	116	TYR
1	D	144	PHE
1	D	156	TRP
1	D	273	LEU
1	D	305	VAL
1	D	431	TYR
1	E	9	GLN
1	E	116	TYR
1	E	144	PHE
1	E	156	TRP
1	E	273	LEU
1	E	305	VAL
1	E	431	TYR

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 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 ⓘ

33 carbohydrates 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	$\# Z  > 2$
3	NAG	A	501	1,3	14,14,15	0.25	0	15,19,21	0.51	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	502	3	14,14,15	0.73	1 (7%)	15,19,21	1.07	1 (6%)
4	BMA	A	503	4	11,11,12	0.62	0	13,15,17	0.77	0
4	NAG	A	504	4	14,14,15	0.23	0	15,19,21	0.40	0
4	NAG	A	505	1,4	14,14,15	0.24	0	15,19,21	0.42	0
3	NAG	A	506	1,3	14,14,15	0.28	0	15,19,21	0.51	0
3	NAG	A	507	3	14,14,15	0.23	0	15,19,21	0.48	0
6	NAG	B	501	1,6	14,14,15	0.21	0	15,19,21	0.56	0
6	NAG	B	502	6	14,14,15	0.22	0	15,19,21	0.46	0
6	BMA	B	503	6	11,11,12	0.60	0	13,15,17	0.78	0
3	NAG	B	504	3	14,14,15	0.71	1 (7%)	15,19,21	1.06	1 (6%)
3	NAG	B	505	1,3	14,14,15	0.24	0	15,19,21	0.49	0
3	NAG	B	506	3	14,14,15	0.26	0	15,19,21	0.48	0
3	NAG	B	507	1,3	14,14,15	0.32	0	15,19,21	0.53	0
4	BMA	C	501	4	11,11,12	0.60	0	13,15,17	0.75	0
4	NAG	C	502	4	14,14,15	0.20	0	15,19,21	0.43	0
4	NAG	C	503	1,4	14,14,15	0.25	0	15,19,21	0.42	0
3	NAG	C	504	3	14,14,15	0.71	1 (7%)	15,19,21	1.07	1 (6%)
3	NAG	C	505	1,3	14,14,15	0.24	0	15,19,21	0.47	0
3	NAG	C	506	3	14,14,15	0.23	0	15,19,21	0.48	0
3	NAG	C	507	1,3	14,14,15	0.30	0	15,19,21	0.50	0
4	BMA	D	501	4	11,11,12	0.88	1 (9%)	13,15,17	1.47	3 (23%)
4	NAG	D	502	4	14,14,15	0.18	0	15,19,21	0.47	0
4	NAG	D	503	1,4	14,14,15	0.25	0	15,19,21	0.38	0
3	NAG	D	504	3	14,14,15	0.73	1 (7%)	15,19,21	1.07	1 (6%)
3	NAG	D	505	1,3	14,14,15	0.29	0	15,19,21	0.50	0
3	NAG	D	506	3	14,14,15	0.24	0	15,19,21	0.47	0
3	NAG	D	507	1,3	14,14,15	0.32	0	15,19,21	0.53	0
4	BMA	E	501	4	11,11,12	1.42	3 (27%)	13,15,17	1.48	2 (15%)
4	NAG	E	502	4	14,14,15	0.20	0	15,19,21	0.46	0
4	NAG	E	503	1,4	14,14,15	0.25	0	15,19,21	0.44	0
3	NAG	E	506	3	14,14,15	0.24	0	15,19,21	0.49	0
3	NAG	E	507	1,3	14,14,15	0.28	0	15,19,21	0.55	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
3	NAG	A	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	A	503	4	-	0/2/19/22	0/1/1/1
4	NAG	A	504	4	-	0/6/23/26	0/1/1/1
4	NAG	A	505	1,4	-	0/6/23/26	0/1/1/1
3	NAG	A	506	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	507	3	-	0/6/23/26	0/1/1/1
6	NAG	B	501	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	502	6	-	0/6/23/26	0/1/1/1
6	BMA	B	503	6	-	0/2/19/22	0/1/1/1
3	NAG	B	504	3	-	0/6/23/26	0/1/1/1
3	NAG	B	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	506	3	-	0/6/23/26	0/1/1/1
3	NAG	B	507	1,3	-	0/6/23/26	0/1/1/1
4	BMA	C	501	4	-	0/2/19/22	0/1/1/1
4	NAG	C	502	4	-	0/6/23/26	0/1/1/1
4	NAG	C	503	1,4	-	0/6/23/26	0/1/1/1
3	NAG	C	504	3	-	0/6/23/26	0/1/1/1
3	NAG	C	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	506	3	-	0/6/23/26	0/1/1/1
3	NAG	C	507	1,3	-	0/6/23/26	0/1/1/1
4	BMA	D	501	4	-	0/2/19/22	0/1/1/1
4	NAG	D	502	4	-	0/6/23/26	0/1/1/1
4	NAG	D	503	1,4	-	0/6/23/26	0/1/1/1
3	NAG	D	504	3	-	0/6/23/26	0/1/1/1
3	NAG	D	505	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	506	3	-	0/6/23/26	0/1/1/1
3	NAG	D	507	1,3	-	0/6/23/26	0/1/1/1
4	BMA	E	501	4	-	0/2/19/22	0/1/1/1
4	NAG	E	502	4	-	0/6/23/26	0/1/1/1
4	NAG	E	503	1,4	-	0/6/23/26	0/1/1/1
3	NAG	E	506	3	-	0/6/23/26	0/1/1/1
3	NAG	E	507	1,3	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	501	BMA	O5-C1	-2.64	1.39	1.43
4	D	501	BMA	C2-C3	2.01	1.55	1.52
4	E	501	BMA	C2-C3	2.14	1.55	1.52
3	C	504	NAG	O5-C1	2.49	1.47	1.43
3	B	504	NAG	O5-C1	2.50	1.47	1.43
4	E	501	BMA	C4-C3	2.53	1.58	1.52
3	A	502	NAG	O5-C1	2.56	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	504	NAG	O5-C1	2.58	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	BMA	C1-C2-C3	2.42	112.72	109.65
4	D	501	BMA	C1-O5-C5	2.54	115.67	112.17
4	D	501	BMA	O5-C1-C2	2.95	115.41	110.79
4	E	501	BMA	C3-C4-C5	3.20	115.85	110.22
4	E	501	BMA	C2-C3-C4	3.35	116.72	110.88
3	B	504	NAG	C1-O5-C5	3.80	117.41	112.17
3	C	504	NAG	C1-O5-C5	3.85	117.47	112.17
3	D	504	NAG	C1-O5-C5	3.86	117.49	112.17
3	A	502	NAG	C1-O5-C5	3.86	117.49	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	NAG	1	0
3	A	506	NAG	1	0
6	B	501	NAG	1	0
3	B	507	NAG	1	0
4	C	503	NAG	1	0
3	C	507	NAG	1	0
4	D	503	NAG	1	0
3	D	507	NAG	2	0
4	E	502	NAG	1	0
4	E	503	NAG	2	0
3	E	507	NAG	1	0

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	SO4	D	508	-	4,4,4	0.14	0	6,6,6	0.06	0
8	NAG	E	504	-	14,14,15	0.20	0	15,19,21	0.46	0
8	NAG	E	505	1	14,14,15	0.20	0	15,19,21	0.43	0
7	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.06	0
7	SO4	H	302	-	4,4,4	0.14	0	6,6,6	0.06	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
7	SO4	D	508	-	-	0/0/0/0	0/0/0/0
8	NAG	E	504	-	-	0/6/23/26	0/1/1/1
8	NAG	E	505	1	-	0/6/23/26	0/1/1/1
7	SO4	H	301	-	-	0/0/0/0	0/0/0/0
7	SO4	H	302	-	-	0/0/0/0	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	302	SO4	1	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	383/456 (83%)	-0.63	2 (0%) 90 86	66, 108, 158, 186	0
1	B	383/456 (83%)	-0.68	2 (0%) 90 86	63, 102, 152, 189	0
1	C	384/456 (84%)	-0.65	5 (1%) 77 69	62, 103, 155, 184	0
1	D	384/456 (84%)	-0.69	1 (0%) 93 90	62, 103, 161, 189	0
1	E	383/456 (83%)	-0.63	4 (1%) 82 75	60, 103, 157, 195	0
2	F	122/124 (98%)	-0.06	5 (4%) 38 31	75, 120, 153, 178	1 (0%)
2	G	124/124 (100%)	-0.37	1 (0%) 86 79	86, 108, 140, 156	1 (0%)
2	H	124/124 (100%)	-0.51	0 100 100	71, 95, 125, 147	1 (0%)
2	I	124/124 (100%)	-0.43	1 (0%) 86 79	74, 119, 160, 178	1 (0%)
2	J	124/124 (100%)	-0.44	0 100 100	73, 98, 135, 156	1 (0%)
All	All	2535/2900 (87%)	-0.58	21 (0%) 86 79	60, 105, 156, 195	5 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	457	SER	4.5
1	E	456	TRP	3.7
2	F	15	GLY	3.0
1	C	456	TRP	2.8
2	I	123	SER	2.6
2	F	40	ALA	2.5
1	C	314	GLN	2.5
1	D	459	TRP	2.5
1	C	184	GLN	2.5
1	E	184	GLN	2.4
1	B	456	TRP	2.4
1	B	184	GLN	2.3
1	A	456	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	458	ILE	2.3
2	F	14	PRO	2.2
1	C	457	SER	2.1
2	F	13	GLN	2.1
2	F	44	GLU	2.1
1	C	334	CYS	2.0
1	E	334	CYS	2.0
2	G	123	SER	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](#)

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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	506	14/15	0.93	0.23	0.52	86,107,126,148	0
6	NAG	B	501	14/15	0.92	0.23	0.19	78,101,135,149	0
3	NAG	C	507	14/15	0.95	0.19	-0.04	63,97,134,147	0
3	NAG	E	507	14/15	0.96	0.19	-0.14	77,94,120,134	0
3	NAG	D	507	14/15	0.96	0.18	-0.17	76,105,125,143	0
3	NAG	B	507	14/15	0.94	0.15	-0.77	82,99,136,163	0
4	NAG	E	503	14/15	0.94	0.16	-	73,113,121,132	0
3	NAG	D	504	14/15	0.79	0.50	-	126,137,167,187	0
3	NAG	B	504	14/15	0.88	0.52	-	116,132,167,172	0
3	NAG	A	502	14/15	0.77	0.58	-	131,161,174,178	0
4	NAG	A	505	14/15	0.95	0.21	-	81,107,150,152	0
4	BMA	C	501	11/12	0.61	0.41	-	122,145,162,174	0
6	NAG	B	502	14/15	0.85	0.33	-	86,107,138,140	0
4	BMA	E	501	11/12	0.39	0.48	-	128,165,179,194	0
4	NAG	A	504	14/15	0.92	0.35	-	93,136,146,151	0
4	NAG	D	502	14/15	0.84	0.38	-	88,120,157,163	0
6	BMA	B	503	11/12	0.74	0.37	-	107,129,155,168	0
3	NAG	B	505	14/15	0.88	0.28	-	112,123,142,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	501	14/15	0.89	0.28	-	109,140,165,167	0
3	NAG	C	505	14/15	0.86	0.36	-	132,144,160,165	0
4	NAG	E	502	14/15	0.88	0.40	-	76,108,139,156	0
3	NAG	E	506	14/15	0.92	0.36	-	103,125,145,149	0
4	NAG	C	502	14/15	0.92	0.34	-	86,106,135,149	0
4	NAG	C	503	14/15	0.92	0.21	-	77,105,133,141	0
4	BMA	A	503	11/12	0.72	0.38	-	130,154,169,170	0
4	BMA	D	501	11/12	0.70	0.42	-	109,159,179,197	0
3	NAG	D	505	14/15	0.89	0.28	-	105,127,139,152	0
3	NAG	A	507	14/15	0.87	0.32	-	97,143,159,161	0
3	NAG	C	504	14/15	0.75	0.60	-	140,171,185,192	0
3	NAG	D	506	14/15	0.89	0.36	-	107,130,143,150	0
3	NAG	B	506	14/15	0.88	0.46	-	124,151,174,180	0
3	NAG	C	506	14/15	0.92	0.34	-	111,139,151,157	0
4	NAG	D	503	14/15	0.92	0.24	-	89,110,145,147	0

## 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. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	H	302	5/5	0.86	0.23	-0.70	125,141,156,163	0
5	CL	D	509	1/1	0.89	0.14	-	88,88,88,88	0
7	SO4	H	301	5/5	0.81	0.48	-	154,161,191,193	0
8	NAG	E	504	14/15	0.69	0.97	-	136,174,190,191	0
5	CL	E	508	1/1	0.89	0.19	-	87,87,87,87	0
8	NAG	E	505	14/15	0.87	0.32	-	117,132,149,151	0
5	CL	A	508	1/1	0.87	0.23	-	114,114,114,114	0
5	CL	B	508	1/1	0.94	0.08	-	84,84,84,84	0
5	CL	C	508	1/1	0.96	0.14	-	70,70,70,70	0
7	SO4	D	508	5/5	0.88	0.15	-	169,186,200,203	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.