



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2017 – 12:19 PM EDT

PDB ID : 1YYM  
Title : crystal structure of F23, a scorpion-toxin mimic of CD4, in complex with HIV-1 YU2 gp120 envelope glycoprotein and anti-HIV-1 antibody 17b  
Authors : Huang, C.C.; Stricher, F.; Martin, L.; Decker, J.M.; Majeed, S.; Barthe, P.; Hendrickson, W.A.; Robinson, J.; Roumestand, C.; Sodroski, J.; Wyatt, R.; Shaw, G.M.; Vita, C.; Kwong, P.D.  
Deposited on : 2005-02-25  
Resolution : 2.20 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 : rb-20029077  
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) : rb-20029077

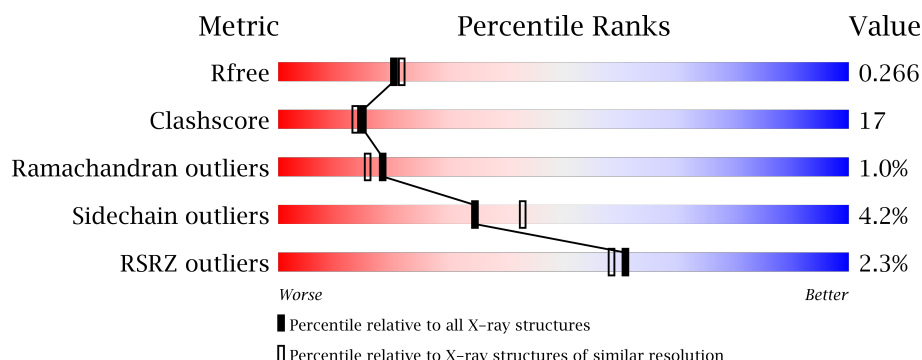
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	G	313	<div> <div>2%</div> <div>67%</div> <div>27%</div> <div>• •</div> </div>
1	P	313	<div> <div>4%</div> <div>60%</div> <div>34%</div> <div>• •</div> </div>
2	L	214	<div> <div>71%</div> <div>26%</div> <div>•</div> </div>
2	Q	214	<div> <div>2%</div> <div>67%</div> <div>29%</div> <div>•</div> </div>
3	H	229	<div> <div>3%</div> <div>72%</div> <div>25%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	R	229	
4	M	27	
4	S	27	

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
5	NAG	G	886	-	-	-	X
5	NAG	P	1734	-	-	-	X
7	EDO	G	903	-	-	-	X
8	IPA	G	901	-	-	-	X
8	IPA	P	902	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12823 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 Exterior membrane glycoprotein(GP120),Exterior membrane glycoprotein(GP120),Exterior membrane glycoprotein(GP120).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	301	Total	C	N	O	S	0	0	0
			2341	1468	407	446	20			
1	P	299	Total	C	N	O	S	0	0	0
			2325	1460	404	441	20			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	79	GLY	-	expression tag	UNP P35961
G	80	ALA	-	expression tag	UNP P35961
G	81	ARG	-	expression tag	UNP P35961
G	82	SER	-	expression tag	UNP P35961
G	128	GLY	-	linker	UNP P35961
G	129	ALA	-	linker	UNP P35961
G	194	GLY	-	linker	UNP P35961
G	298	GLY	-	linker	UNP P35961
G	299	ALA	-	linker	UNP P35961
G	329	GLY	-	linker	UNP P35961
P	1079	GLY	-	expression tag	UNP P35961
P	1080	ALA	-	expression tag	UNP P35961
P	1081	ARG	-	expression tag	UNP P35961
P	1082	SER	-	expression tag	UNP P35961
P	1128	GLY	-	linker	UNP P35961
P	1129	ALA	-	linker	UNP P35961
P	1194	GLY	-	linker	UNP P35961
P	1298	GLY	-	linker	UNP P35961
P	1299	ALA	-	linker	UNP P35961
P	1329	GLY	-	linker	UNP P35961

- Molecule 2 is a protein called antibody 17b light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1647	1028	282	332	5			
2	Q	214	Total	C	N	O	S	0	0	0
			1647	1028	282	332	5			

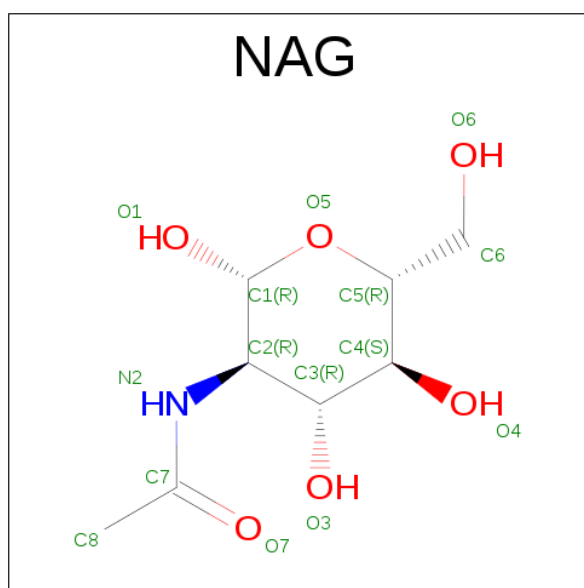
- Molecule 3 is a protein called antibody 17b heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	229	Total	C	N	O	S	0	0	0
			1722	1086	289	342	5			
3	R	229	Total	C	N	O	S	0	0	0
			1722	1086	289	342	5			

- Molecule 4 is a protein called F23, scorpion-toxin mimic of CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	27	Total	C	N	O	S	0	0	0
			195	122	36	31	6			
4	S	27	Total	C	N	O	S	0	0	0
			195	122	36	31	6			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



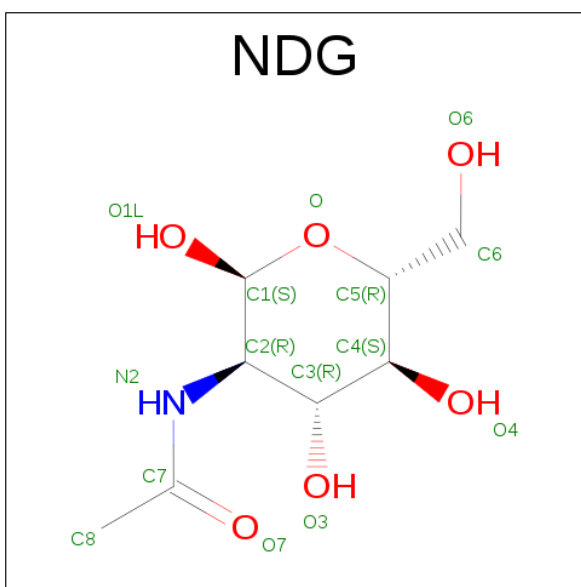
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

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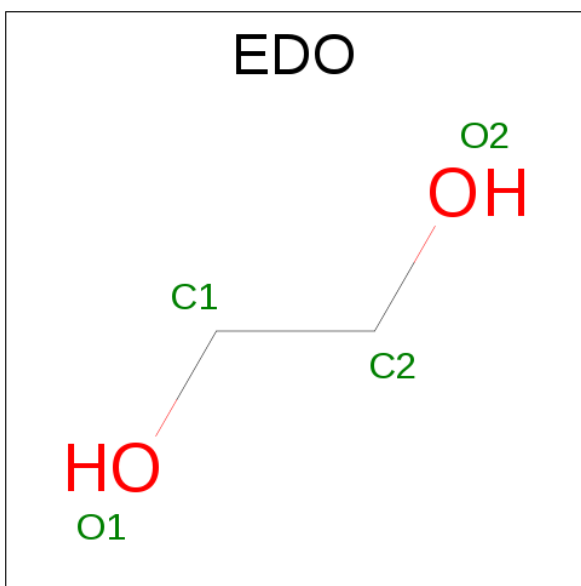
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1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

- Molecule 6 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



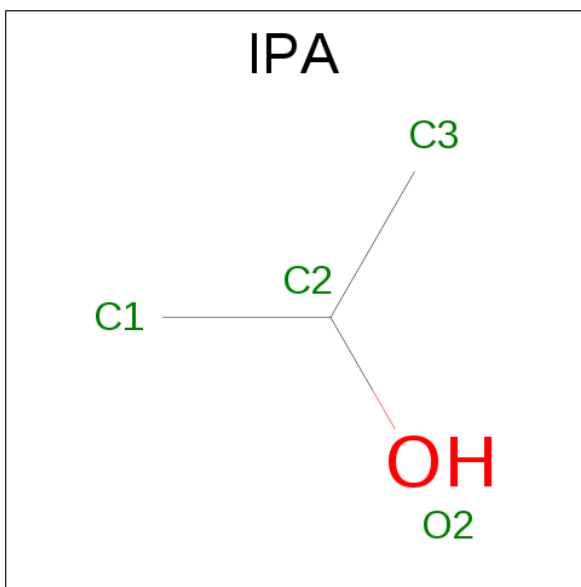
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	O	0	0
			4	2	2		
7	M	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula:  $C_3H_8O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			4	3	1		
8	P	1	Total	C	O	0	0
			4	3	1		

- Molecule 9 is water.

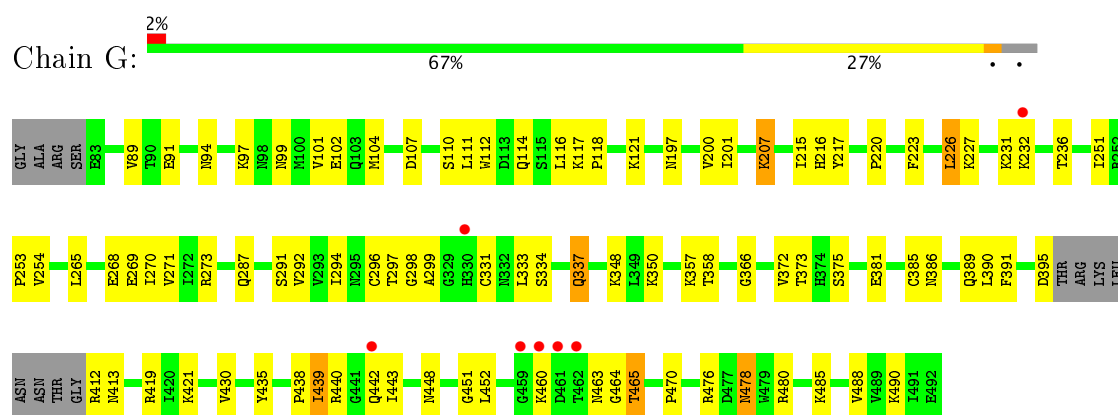
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	134	Total	O	0	0
			134	134		
9	L	135	Total	O	0	0
			135	135		
9	H	146	Total	O	0	0
			146	146		
9	M	9	Total	O	0	0
			9	9		
9	P	124	Total	O	0	0
			124	124		
9	Q	101	Total	O	0	0
			101	101		
9	R	129	Total	O	0	0
			129	129		
9	S	11	Total	O	0	0
			11	11		



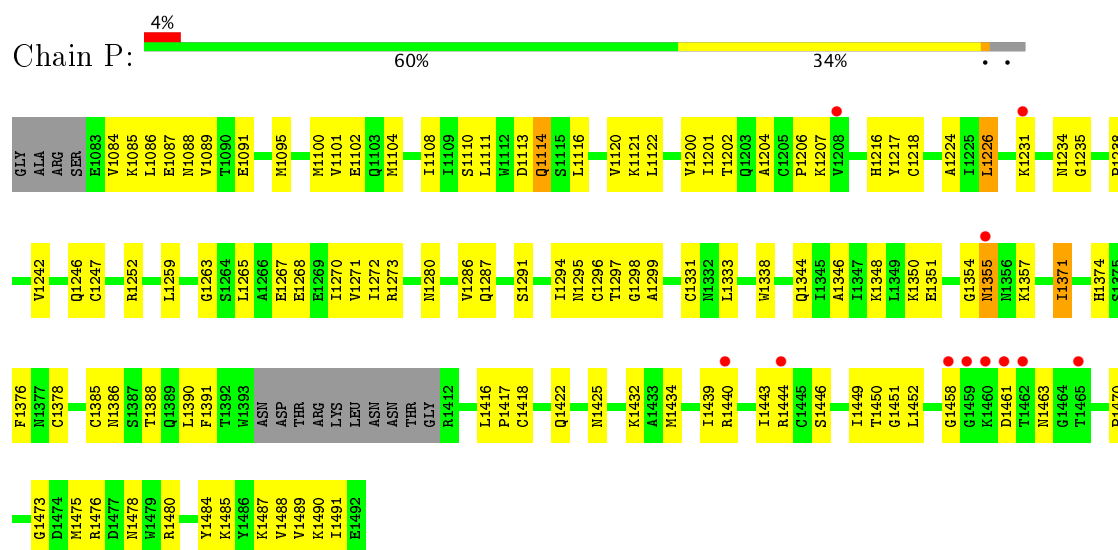
### 3 Residue-property plots

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: Exterior membrane glycoprotein(GP120),Exterior membrane glycoprotein(GP120), Exterior membrane glycoprotein(GP120)

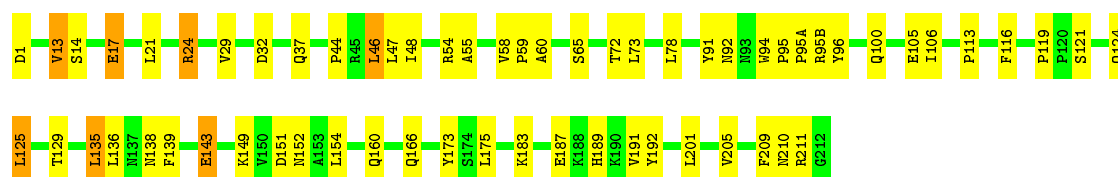


- Molecule 1: Exterior membrane glycoprotein(GP120),Exterior membrane glycoprotein(GP120), Exterior membrane glycoprotein(GP120)

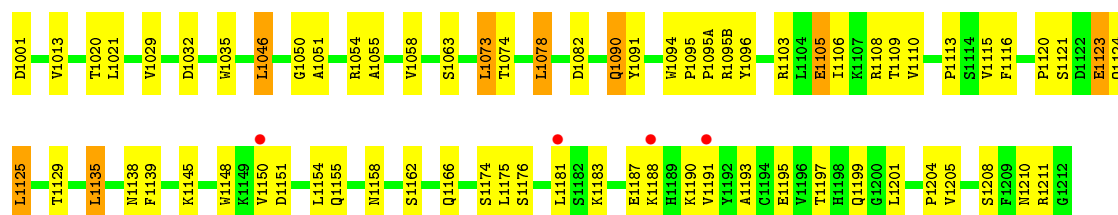


- Molecule 2: antibody 17b light chain

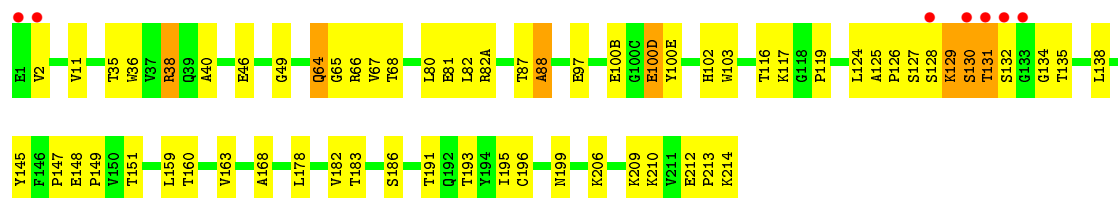




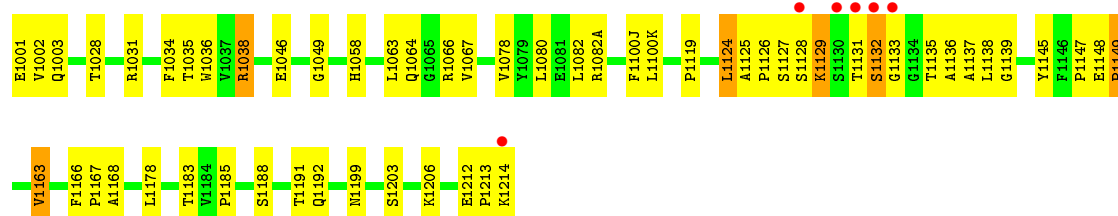
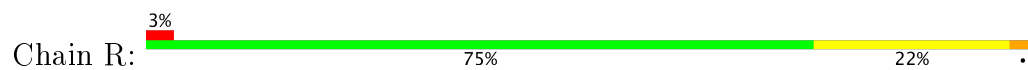
- Molecule 2: antibody 17b light chain



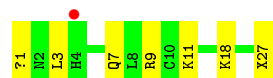
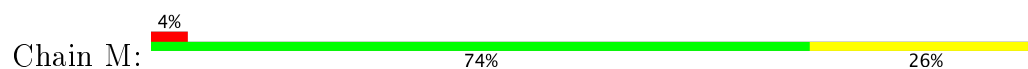
- Molecule 3: antibody 17b heavy chain



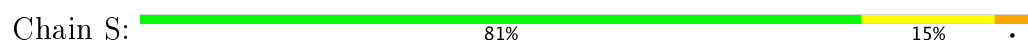
- Molecule 3: antibody 17b heavy chain



- Molecule 4: F23, scorpion-toxin mimic of CD4



- Molecule 4: F23, scorpion-toxin mimic of CD4



Z1001	N1002	L1003	H1004	F1005	C1006	Q1007	K1018	X1027
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.62Å 157.04Å 108.93Å 90.00° 93.45° 90.00°	Depositor
Resolution (Å)	19.99 – 2.20 44.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.6 (19.99-2.20) 72.3 (44.70-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.209 , 0.268 0.206 , 0.266	Depositor DCC
$R_{free}$ test set	7773 reflections (11.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, VLM, NAG, EDO, NDG, MPT

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	G	0.33	0/2386	0.61	0/3234
1	P	0.33	0/2370	0.59	0/3212
2	L	0.37	0/1684	0.67	0/2288
2	Q	0.36	0/1684	0.64	0/2288
3	H	0.38	0/1762	0.67	0/2399
3	R	0.37	0/1762	0.65	0/2399
4	M	0.37	0/184	0.64	0/243
4	S	0.36	0/184	0.62	0/243
All	All	0.36	0/12016	0.64	0/16306

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2341	0	2294	79	0
1	P	2325	0	2284	91	0
2	L	1647	0	1593	56	0
2	Q	1647	0	1590	68	0
3	H	1722	0	1691	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	1722	0	1688	51	0
4	M	195	0	195	6	0
4	S	195	0	195	5	0
5	G	98	0	91	6	0
5	P	112	0	104	9	0
6	G	14	0	13	0	0
7	G	4	0	6	0	0
7	M	4	0	6	0	0
8	G	4	0	8	1	0
8	P	4	0	8	0	0
9	G	134	0	0	9	0
9	H	146	0	0	6	0
9	L	135	0	0	2	0
9	M	9	0	0	0	0
9	P	124	0	0	4	0
9	Q	101	0	0	2	0
9	R	129	0	0	2	0
9	S	11	0	0	0	0
All	All	12823	0	11766	403	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 17.

All (403) 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)
2:Q:1013:VAL:HG11	2:Q:1078:LEU:HD13	1.43	0.99
2:L:24:ARG:HH11	2:L:24:ARG:HB3	1.29	0.96
3:R:1131:THR:HG22	3:R:1132:SER:H	1.35	0.90
3:H:126:PRO:HG3	3:H:138:LEU:HB3	1.54	0.88
3:R:1135:THR:HG23	3:R:1183:THR:HG23	1.56	0.86
1:P:1272:ILE:HG22	1:P:1286:VAL:HG22	1.60	0.83
1:P:1333:LEU:HD21	1:P:1338:TRP:HB2	1.59	0.83
2:Q:1105:GLU:HG2	2:Q:1106:ILE:N	1.92	0.83
2:Q:1106:ILE:H	2:Q:1166:GLN:HE22	1.26	0.82
3:H:199:ASN:HD21	3:H:206:LYS:HE2	1.45	0.81
1:P:1476:ARG:HB3	1:P:1480:ARG:HH12	1.44	0.80
1:G:439:ILE:HG13	1:G:440:ARG:H	1.48	0.77
3:R:1129:LYS:HA	3:R:1129:LYS:HE3	1.67	0.76
1:P:1444:ARG:HB3	1:P:1444:ARG:NH1	2.00	0.75
1:G:207:LYS:HE3	1:G:381:GLU:OE2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:106:ILE:H	2:L:166:GLN:HE22	1.34	0.74
1:P:1120:VAL:HG12	1:P:1434:MET:HB3	1.68	0.74
2:L:94:TRP:HA	2:L:95:PRO:C	2.06	0.74
1:P:1371:ILE:HD11	1:P:1473:GLY:CA	2.19	0.73
2:Q:1078:LEU:HD23	2:Q:1082:ASP:HB2	1.71	0.73
3:H:135:THR:HG23	3:H:183:THR:HG23	1.71	0.72
2:L:24:ARG:HB3	2:L:24:ARG:NH1	2.03	0.72
1:G:107:ASP:O	1:G:111:LEU:HD13	1.90	0.71
3:R:1126:PRO:HG3	3:R:1138:LEU:HG	1.71	0.71
3:H:193:THR:HG23	3:H:210:LYS:NZ	2.05	0.71
2:L:105:GLU:HG2	2:L:106:ILE:N	2.05	0.71
1:P:1439:ILE:HG13	1:P:1440:ARG:H	1.55	0.71
2:Q:1013:VAL:CG1	2:Q:1078:LEU:HD13	2.20	0.71
3:R:1131:THR:HG22	3:R:1132:SER:N	2.06	0.71
1:P:1121:LYS:HE3	1:P:1201:ILE:HD12	1.73	0.71
1:P:1095:MET:HE1	1:P:1273:ARG:HD2	1.73	0.70
3:H:127:SER:H	3:H:129:LYS:HE2	1.57	0.70
2:Q:1013:VAL:HG11	2:Q:1078:LEU:CD1	2.20	0.70
3:R:1127:SER:HB3	3:R:1129:LYS:NZ	2.05	0.70
1:P:1122:LEU:CD2	1:P:1200:VAL:HG22	2.21	0.70
1:P:1439:ILE:HG13	1:P:1440:ARG:N	2.06	0.70
2:L:116:PHE:CD2	3:H:129:LYS:HA	2.27	0.70
1:P:1371:ILE:HD11	1:P:1473:GLY:HA2	1.74	0.69
3:H:134:GLY:H	3:H:186:SER:HB3	1.55	0.69
2:Q:1094:TRP:HA	2:Q:1095:PRO:C	2.14	0.67
1:G:337:GLN:HE21	1:G:337:GLN:C	1.98	0.67
2:L:65:SER:HB3	2:L:72:THR:CG2	2.24	0.67
1:P:1386:ASN:ND2	5:P:1886:NAG:H82	2.10	0.67
2:L:1:ASP:HB2	9:L:252:HOH:O	1.93	0.67
1:G:412:ARG:HG2	1:G:413:ASN:H	1.60	0.67
2:Q:1046:LEU:HD13	2:Q:1055:ALA:HB2	1.77	0.67
3:R:1063:LEU:HD13	3:R:1067:VAL:HG21	1.76	0.66
1:G:333:LEU:HD23	1:G:390:LEU:HD21	1.77	0.66
3:H:68:THR:OG1	3:H:82(A):ARG:NH2	2.27	0.66
1:P:1120:VAL:CG1	1:P:1434:MET:HB3	2.25	0.66
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.78	0.66
3:R:1148:GLU:HG3	3:R:1149:PRO:HA	1.78	0.66
2:L:135:LEU:HD22	2:L:136:LEU:N	2.11	0.65
1:G:350:LYS:HE2	1:G:357:LYS:O	1.96	0.65
2:L:48:ILE:HD13	2:L:54:ARG:HA	1.78	0.65
1:P:1476:ARG:HB3	1:P:1480:ARG:NH1	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:VAL:O	1:G:89:VAL:HG13	1.96	0.65
2:Q:1120:PRO:HB2	2:Q:1125:LEU:HD11	1.79	0.64
2:Q:1125:LEU:O	2:Q:1183:LYS:HD2	1.97	0.64
1:P:1086:LEU:HD23	1:P:1087:GLU:N	2.13	0.63
2:Q:1001:ASP:OD2	2:Q:1095(B):ARG:NE	2.27	0.63
2:L:65:SER:HB3	2:L:72:THR:HG23	1.81	0.63
1:G:251:ILE:O	1:G:253:PRO:HD3	1.99	0.63
2:Q:1188:LYS:HG2	2:Q:1188:LYS:O	1.99	0.63
1:P:1297:THR:HG23	1:P:1299:ALA:H	1.65	0.62
3:H:87:THR:O	3:H:88:ALA:HB2	1.97	0.62
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.80	0.62
3:H:160:THR:O	3:H:163:VAL:HG22	2.00	0.61
2:Q:1145:LYS:HB3	2:Q:1197:THR:OG1	2.00	0.61
5:P:1762:NAG:H83	9:P:785:HOH:O	2.01	0.60
3:R:1128:SER:HA	9:R:799:HOH:O	2.01	0.60
2:L:116:PHE:HD2	3:H:129:LYS:HA	1.65	0.60
2:L:46:LEU:HD13	2:L:55:ALA:HB2	1.82	0.60
3:H:38:ARG:HD2	3:H:46:GLU:OE2	2.02	0.60
1:G:118:PRO:HG3	1:G:435:TYR:CZ	2.37	0.60
3:R:1185:PRO:HG2	3:R:1188:SER:OG	2.01	0.60
1:G:430:VAL:HG22	4:M:1:MPT:HA2	1.83	0.59
3:H:65:GLY:HA2	9:H:332:HOH:O	2.02	0.59
1:P:1271:VAL:HG11	1:P:1273:ARG:NH1	2.17	0.59
1:P:1297:THR:C	1:P:1299:ALA:H	2.05	0.59
1:P:1207:LYS:HD3	1:P:1439:ILE:HG23	1.83	0.59
9:Q:137:HOH:O	3:R:1058:HIS:HB3	2.02	0.59
3:R:1178:LEU:C	3:R:1178:LEU:HD12	2.23	0.59
1:G:121:LYS:HE3	1:G:201:ILE:HD12	1.84	0.59
1:G:254:VAL:HG22	5:G:762:NAG:H83	1.84	0.59
2:Q:1175:LEU:HD23	2:Q:1176:SER:N	2.17	0.59
3:R:1127:SER:HB3	3:R:1129:LYS:HZ3	1.66	0.59
4:S:1002:ASN:CB	4:S:1005:PHE:HD2	2.16	0.58
1:G:273:ARG:NH2	1:G:287:GLN:OE1	2.34	0.58
3:H:195:ILE:HD13	3:H:210:LYS:HA	1.85	0.58
1:P:1224:ALA:HB2	1:P:1491:ILE:HD11	1.84	0.58
1:P:1391:PHE:CG	1:P:1470:PRO:HG3	2.38	0.58
1:G:430:VAL:CG2	4:M:1:MPT:HA2	2.32	0.58
2:L:32:ASP:HB2	2:L:92:ASN:HB2	1.85	0.57
2:L:95(B):ARG:NH1	9:L:251:HOH:O	2.34	0.57
3:H:193:THR:HG23	3:H:210:LYS:HZ3	1.69	0.57
2:Q:1108:ARG:NH1	2:Q:1109:THR:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:1150:VAL:HB	2:Q:1155:GLN:NE2	2.19	0.57
1:G:334:SER:OG	1:G:337:GLN:HB2	2.04	0.57
2:L:100:GLN:HA	2:L:100:GLN:NE2	2.18	0.57
1:P:1095:MET:HE1	1:P:1234:ASN:O	2.04	0.57
1:G:102:GLU:OE2	1:G:476:ARG:HD2	2.05	0.57
1:P:1440:ARG:HG3	1:P:1440:ARG:HH11	1.69	0.57
1:P:1295:ASN:ND2	5:P:1795:NAG:H82	2.19	0.57
2:Q:1032:ASP:HB3	2:Q:1091:TYR:CD1	2.40	0.57
1:P:1425:ASN:OD1	1:P:1432:LYS:HE3	2.04	0.57
1:G:269:GLU:HB3	5:G:789:NAG:H61	1.86	0.57
1:G:358:THR:HG23	1:G:395:ASP:OD1	2.05	0.57
1:G:439:ILE:HG13	1:G:440:ARG:N	2.17	0.57
1:G:215:ILE:HD12	1:G:215:ILE:C	2.24	0.57
1:P:1270:ILE:HD12	1:P:1344:GLN:HB3	1.87	0.56
4:S:1018:LYS:HB3	4:S:1018:LYS:NZ	2.19	0.56
1:G:91:GLU:HG3	1:G:226:LEU:HD23	1.88	0.56
2:L:32:ASP:OD2	2:L:92:ASN:ND2	2.35	0.56
1:P:1444:ARG:CZ	1:P:1444:ARG:HB3	2.35	0.56
1:G:110:SER:O	1:G:114:GLN:HG2	2.05	0.56
1:G:94:ASN:ND2	1:G:97:LYS:HD2	2.20	0.56
1:P:1489:VAL:HG22	1:P:1490:LYS:N	2.21	0.56
2:Q:1193:ALA:HB2	2:Q:1208:SER:HB3	1.88	0.56
2:L:91:TYR:HA	2:L:96:TYR:CD1	2.41	0.55
2:Q:1029:VAL:HG13	2:Q:1090:GLN:HG2	1.88	0.55
1:G:270:ILE:HD11	9:G:980:HOH:O	2.05	0.55
1:G:478:ASN:H	1:G:478:ASN:HD22	1.54	0.55
3:H:193:THR:HG23	3:H:210:LYS:HZ2	1.71	0.55
2:Q:1091:TYR:HA	2:Q:1096:TYR:CD1	2.41	0.55
2:Q:1211:ARG:HB3	2:Q:1211:ARG:HH11	1.71	0.55
1:P:1089:VAL:HG13	1:P:1089:VAL:O	2.07	0.55
3:R:1131:THR:CG2	3:R:1132:SER:H	2.15	0.55
1:G:333:LEU:CD2	1:G:390:LEU:HD21	2.37	0.55
2:L:189:HIS:HB2	2:L:192:TYR:OH	2.07	0.54
3:R:1129:LYS:HG2	3:R:1136:ALA:HA	1.90	0.54
1:G:271:VAL:HG11	1:G:273:ARG:NH1	2.22	0.54
1:P:1091:GLU:O	1:P:1238:PRO:HA	2.06	0.54
1:P:1446:SER:O	5:P:1762:NAG:H3	2.07	0.54
1:G:254:VAL:CG2	5:G:762:NAG:H83	2.38	0.54
1:G:478:ASN:N	1:G:478:ASN:HD22	2.06	0.54
1:G:297:THR:HG23	1:G:299:ALA:HB3	1.90	0.54
3:H:126:PRO:HA	3:H:129:LYS:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:1110:VAL:HG11	2:Q:1199:GLN:HG2	1.89	0.54
1:P:1298:GLY:HA3	1:P:1443:ILE:O	2.07	0.54
2:Q:1124:GLN:HG2	2:Q:1129:THR:O	2.08	0.54
1:P:1346:ALA:O	1:P:1350:LYS:HG2	2.08	0.53
1:P:1204:ALA:C	1:P:1206:PRO:HD3	2.29	0.53
1:P:1451:GLY:C	1:P:1452:LEU:HD12	2.28	0.53
2:Q:1029:VAL:HG12	2:Q:1029:VAL:O	2.07	0.53
2:Q:1120:PRO:HB2	2:Q:1125:LEU:CD1	2.39	0.53
3:R:1036:TRP:CE2	3:R:1080:LEU:HB2	2.43	0.53
3:R:1129:LYS:HE3	3:R:1129:LYS:CA	2.37	0.53
1:P:1390:LEU:HD11	1:P:1416:LEU:HD11	1.91	0.53
1:P:1371:ILE:HD11	1:P:1473:GLY:HA3	1.91	0.53
2:Q:1201:LEU:HD13	2:Q:1205:VAL:HG23	1.90	0.53
3:H:135:THR:HG23	3:H:183:THR:CG2	2.37	0.53
1:P:1110:SER:O	1:P:1114:GLN:HG3	2.09	0.53
3:R:1135:THR:HG23	3:R:1183:THR:CG2	2.32	0.53
3:R:1148:GLU:HG3	3:R:1149:PRO:CA	2.38	0.53
2:Q:1151:ASP:HA	2:Q:1191:VAL:CG1	2.39	0.52
3:H:38:ARG:HG3	3:H:46:GLU:HB3	1.91	0.52
1:P:1231:LYS:HG3	5:P:1741:NAG:H62	1.92	0.52
2:L:94:TRP:CE3	2:L:95(A):PRO:HD3	2.44	0.52
1:G:337:GLN:CA	1:G:337:GLN:HE21	2.21	0.52
2:L:100:GLN:HA	2:L:100:GLN:HE21	1.74	0.52
4:M:9:ARG:HH11	4:M:9:ARG:HA	1.74	0.52
1:P:1259:LEU:HD13	1:P:1449:ILE:HD13	1.91	0.52
1:P:1265:LEU:HD11	1:P:1291:SER:OG	2.10	0.52
2:Q:1054:ARG:HG2	2:Q:1058:VAL:HB	1.90	0.52
2:Q:1105:GLU:HG2	2:Q:1106:ILE:H	1.69	0.52
1:G:463:ASN:O	1:G:465:THR:HG22	2.10	0.52
1:P:1488:VAL:HG12	9:P:127:HOH:O	2.09	0.52
4:S:1003:LEU:O	4:S:1007:GLN:HG3	2.09	0.52
3:H:196:CYS:SG	3:H:209:LYS:HB3	2.50	0.52
2:L:151:ASP:HA	2:L:191:VAL:HG13	1.91	0.52
2:L:135:LEU:HD22	2:L:136:LEU:H	1.73	0.51
3:R:1119:PRO:HB3	3:R:1145:TYR:HB3	1.92	0.51
1:P:1095:MET:CE	1:P:1235:GLY:HA3	2.39	0.51
1:P:1386:ASN:HD22	5:P:1886:NAG:H82	1.75	0.51
1:G:298:GLY:N	1:G:443:ILE:O	2.44	0.51
4:M:7:GLN:O	4:M:11:LYS:HB2	2.10	0.51
1:P:1202:THR:HG22	2:Q:1095:PRO:HG3	1.93	0.51
2:Q:1183:LYS:O	2:Q:1187:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1294:ILE:HG23	1:P:1294:ILE:O	2.11	0.51
1:G:357:LYS:HA	1:G:464:GLY:O	2.11	0.51
1:P:1087:GLU:HG2	1:P:1088:ASN:O	2.11	0.51
2:L:143:GLU:CD	2:L:143:GLU:H	2.14	0.50
2:L:143:GLU:N	2:L:143:GLU:CD	2.65	0.50
2:L:175:LEU:HD23	2:L:175:LEU:C	2.31	0.50
2:L:32:ASP:HB3	2:L:91:TYR:CD1	2.45	0.50
1:G:251:ILE:C	1:G:253:PRO:HD3	2.32	0.50
1:G:490:LYS:HG3	9:G:1009:HOH:O	2.11	0.50
3:R:1126:PRO:CG	3:R:1138:LEU:HG	2.40	0.50
3:H:97:GLU:HG3	3:H:100(E):TYR:CZ	2.46	0.50
3:H:40:ALA:HA	3:H:88:ALA:HB2	1.94	0.50
2:L:121:SER:O	2:L:125:LEU:HD22	2.12	0.50
3:R:1001:GLU:O	3:R:1003:GLN:HG2	2.11	0.50
2:L:119:PRO:HB3	2:L:209:PHE:CZ	2.47	0.49
1:P:1246:GLN:HA	1:P:1246:GLN:NE2	2.27	0.49
1:P:1091:GLU:HG3	1:P:1226:LEU:HD23	1.94	0.49
2:Q:1195:GLU:OE2	2:Q:1204:PRO:HB3	2.12	0.49
1:G:292:VAL:HG11	1:G:333:LEU:HD11	1.94	0.49
3:R:1199:ASN:HD21	3:R:1206:LYS:HD3	1.77	0.49
4:S:1002:ASN:HB3	4:S:1005:PHE:HD2	1.76	0.49
3:H:36:TRP:CE2	3:H:80:LEU:HB2	2.48	0.48
2:Q:1123:GLU:H	2:Q:1123:GLU:CD	2.16	0.48
1:G:412:ARG:CG	1:G:413:ASN:H	2.25	0.48
3:H:214:LYS:HD3	3:H:214:LYS:O	2.13	0.48
1:P:1476:ARG:CB	1:P:1480:ARG:HH12	2.22	0.48
3:H:178:LEU:C	3:H:178:LEU:HD12	2.34	0.48
1:P:1095:MET:CE	1:P:1273:ARG:HD2	2.41	0.48
1:P:1297:THR:C	1:P:1299:ALA:N	2.67	0.48
1:P:1101:VAL:HG21	1:P:1480:ARG:HG2	1.95	0.48
2:L:24:ARG:HH11	2:L:24:ARG:CB	2.15	0.48
1:G:412:ARG:HG2	1:G:413:ASN:N	2.26	0.48
2:L:124:GLN:HG2	2:L:129:THR:O	2.14	0.48
2:Q:1021:LEU:HD12	2:Q:1021:LEU:N	2.29	0.48
2:L:29:VAL:O	2:L:29:VAL:CG1	2.62	0.48
3:R:1137:ALA:C	3:R:1138:LEU:HD12	2.34	0.48
2:Q:1116:PHE:HD1	2:Q:1135:LEU:HD13	1.78	0.48
3:R:1127:SER:HB3	3:R:1129:LYS:HZ2	1.75	0.48
3:R:1212:GLU:HG2	3:R:1213:PRO:CD	2.43	0.48
2:L:21:LEU:HD12	2:L:21:LEU:N	2.29	0.47
1:G:265:LEU:HD11	1:G:291:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:1115:VAL:HA	2:Q:1135:LEU:O	2.14	0.47
1:G:220:PRO:HD2	1:G:223:PHE:HB2	1.95	0.47
1:G:232:LYS:HD2	1:G:271:VAL:HG22	1.97	0.47
1:P:1461:ASP:OD1	1:P:1463:ASN:ND2	2.47	0.47
1:P:1489:VAL:HG22	1:P:1490:LYS:H	1.78	0.47
1:G:200:VAL:HG12	9:G:922:HOH:O	2.14	0.47
1:G:101:VAL:HG21	1:G:480:ARG:HG2	1.97	0.47
2:Q:1029:VAL:CG1	2:Q:1090:GLN:HG2	2.44	0.47
1:G:118:PRO:HG3	1:G:435:TYR:OH	2.15	0.47
1:P:1089:VAL:O	1:P:1242:VAL:HG11	2.14	0.47
1:P:1386:ASN:O	1:P:1416:LEU:HD22	2.15	0.47
2:Q:1001:ASP:CG	2:Q:1095(B):ARG:HE	2.15	0.47
1:G:439:ILE:CG1	1:G:440:ARG:H	2.14	0.47
3:H:2:VAL:HG22	3:H:102:HIS:CG	2.50	0.47
1:P:1084:VAL:HG22	1:P:1085:LYS:N	2.30	0.47
1:P:1440:ARG:HG3	1:P:1440:ARG:NH1	2.30	0.47
3:H:117:LYS:HD2	9:H:313:HOH:O	2.15	0.46
1:P:1348:LYS:O	1:P:1351:GLU:HB3	2.14	0.46
3:R:1148:GLU:CG	3:R:1149:PRO:HA	2.45	0.46
1:G:448:ASN:ND2	9:G:940:HOH:O	2.48	0.46
3:H:64:GLN:HG3	3:H:64:GLN:O	2.16	0.46
1:P:1267:GLU:HG2	1:P:1267:GLU:H	1.57	0.46
3:R:1034:PHE:CG	3:R:1078:VAL:HG21	2.50	0.46
3:H:100(D):GLU:HB3	9:H:331:HOH:O	2.13	0.46
2:Q:1148:TRP:HB2	2:Q:1155:GLN:HB2	1.98	0.46
3:R:1066:ARG:O	3:R:1082(A):ARG:HG2	2.15	0.46
2:Q:1190:LYS:O	2:Q:1210:ASN:HA	2.16	0.46
1:G:232:LYS:HG3	1:G:232:LYS:O	2.16	0.46
1:P:1386:ASN:HB3	1:P:1417:PRO:HD2	1.97	0.46
1:P:1444:ARG:HH11	1:P:1444:ARG:HB3	1.76	0.46
1:P:1280:ASN:HD22	1:P:1458:GLY:H	1.64	0.46
2:Q:1046:LEU:HD13	2:Q:1055:ALA:CB	2.45	0.46
3:R:1125:ALA:HA	3:R:1126:PRO:HD3	1.79	0.46
1:G:421:LYS:HE2	3:H:100(B):GLU:O	2.16	0.46
2:L:13:VAL:CG2	2:L:78:LEU:HD22	2.46	0.46
1:P:1478:ASN:N	1:P:1478:ASN:HD22	2.13	0.46
3:H:127:SER:N	3:H:129:LYS:HE2	2.26	0.46
3:H:80:LEU:C	3:H:80:LEU:HD13	2.35	0.46
2:Q:1029:VAL:CG2	2:Q:1090:GLN:HG3	2.45	0.46
3:H:130:SER:HB2	3:H:135:THR:O	2.16	0.45
3:H:199:ASN:HD21	3:H:206:LYS:CE	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:1038:ARG:HG3	3:R:1046:GLU:HB3	1.98	0.45
1:P:1095:MET:HE1	1:P:1273:ARG:CD	2.45	0.45
5:P:1776:NAG:H83	5:P:1776:NAG:O3	2.17	0.45
3:H:134:GLY:N	3:H:186:SER:HB3	2.26	0.45
1:P:1331:CYS:SG	1:P:1385:CYS:SG	3.14	0.45
2:Q:1162:SER:OG	3:R:1167:PRO:HD2	2.17	0.45
1:G:254:VAL:HG22	5:G:762:NAG:C8	2.47	0.45
1:G:488:VAL:HG12	9:G:945:HOH:O	2.16	0.45
2:Q:1029:VAL:CG1	2:Q:1029:VAL:O	2.64	0.45
1:G:386:ASN:HB3	5:G:886:NAG:H83	1.98	0.45
3:R:1129:LYS:HG3	3:R:1137:ALA:H	1.81	0.45
4:S:1002:ASN:HB3	4:S:1005:PHE:CD2	2.51	0.45
1:G:200:VAL:HG13	1:G:200:VAL:O	2.17	0.45
1:G:112:TRP:CE3	1:G:116:LEU:HD23	2.52	0.45
3:H:11:VAL:HG23	3:H:11:VAL:O	2.17	0.45
3:H:129:LYS:HD3	3:H:129:LYS:N	2.32	0.45
2:L:151:ASP:HA	2:L:191:VAL:CG1	2.47	0.45
2:L:94:TRP:CA	2:L:95:PRO:C	2.83	0.45
1:P:1296:CYS:HA	1:P:1331:CYS:HA	1.99	0.45
2:Q:1063:SER:OG	2:Q:1074:THR:HG23	2.16	0.45
3:R:1131:THR:O	3:R:1133:GLY:N	2.45	0.45
2:Q:1116:PHE:CD1	2:Q:1135:LEU:HD13	2.52	0.45
2:Q:1103:ARG:HH11	2:Q:1103:ARG:HG3	1.82	0.45
2:Q:1105:GLU:HG2	2:Q:1166:GLN:HE22	1.81	0.45
2:Q:1193:ALA:CB	2:Q:1208:SER:HB3	2.47	0.45
5:P:1734:NAG:O3	5:P:1734:NAG:H82	2.17	0.45
2:Q:1094:TRP:CE3	2:Q:1095(A):PRO:HD3	2.51	0.45
1:G:451:GLY:C	1:G:452:LEU:HD12	2.37	0.44
1:G:91:GLU:HG3	1:G:226:LEU:CD2	2.47	0.44
3:H:64:GLN:HA	9:H:273:HOH:O	2.17	0.44
1:P:1263:GLY:O	1:P:1450:THR:HG21	2.18	0.44
1:P:1297:THR:HG23	1:P:1299:ALA:HB3	1.98	0.44
1:P:1355:ASN:O	1:P:1355:ASN:ND2	2.50	0.44
3:R:1100(J):PHE:O	3:R:1100(K):LEU:HD23	2.16	0.44
1:G:297:THR:CG2	1:G:299:ALA:HB3	2.46	0.44
1:G:89:VAL:CG1	1:G:89:VAL:O	2.65	0.44
1:G:375:SER:OG	8:G:901:IPA:H13	2.17	0.44
1:G:438:PRO:HB3	1:G:443:ILE:HD11	1.99	0.44
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.52	0.44
2:Q:1175:LEU:C	2:Q:1175:LEU:HD23	2.37	0.44
2:L:116:PHE:CE2	3:H:129:LYS:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:87:THR:O	3:H:88:ALA:CB	2.64	0.44
2:L:29:VAL:O	2:L:29:VAL:HG12	2.17	0.44
2:Q:1020:THR:C	2:Q:1021:LEU:HD12	2.38	0.44
1:P:1224:ALA:HA	9:P:94:HOH:O	2.18	0.43
2:Q:1029:VAL:HG22	2:Q:1090:GLN:HG3	2.00	0.43
1:G:366:GLY:HA2	1:G:372:VAL:HG22	1.99	0.43
3:H:35:THR:HG23	3:H:49:GLY:O	2.18	0.43
2:Q:1116:PHE:HD2	3:R:1129:LYS:HE3	1.83	0.43
3:R:1135:THR:CG2	3:R:1183:THR:HG23	2.40	0.43
2:L:210:ASN:O	2:L:211:ARG:C	2.57	0.43
2:Q:1121:SER:O	2:Q:1125:LEU:HD13	2.18	0.43
3:H:116:THR:HB	3:R:1203:SER:HA	2.00	0.43
1:P:1252:ARG:HH11	1:P:1252:ARG:HG3	1.82	0.43
1:G:460:LYS:HA	1:G:460:LYS:HD2	1.77	0.43
3:H:40:ALA:HA	3:H:88:ALA:CB	2.48	0.43
3:H:66:ARG:HD2	3:H:82(A):ARG:O	2.19	0.43
3:R:1163:VAL:HG22	9:R:246:HOH:O	2.17	0.43
1:G:232:LYS:HG3	9:G:920:HOH:O	2.17	0.43
2:L:105:GLU:HG3	2:L:166:GLN:NE2	2.33	0.43
1:P:1100:MET:HE1	1:P:1487:LYS:N	2.33	0.43
2:Q:1123:GLU:OE1	2:Q:1123:GLU:N	2.51	0.43
3:R:1199:ASN:ND2	3:R:1206:LYS:HD3	2.33	0.43
1:P:1376:PHE:HE2	1:P:1378:CYS:HB2	1.83	0.43
2:Q:1108:ARG:HH11	2:Q:1108:ARG:HG3	1.83	0.43
1:G:287:GLN:NE2	9:G:955:HOH:O	2.52	0.43
1:G:373:THR:HB	1:G:385:CYS:O	2.18	0.43
3:H:67:VAL:HA	3:H:81:GLU:O	2.18	0.43
3:H:159:LEU:HD21	3:H:182:VAL:HG21	2.00	0.43
1:P:1354:GLY:O	1:P:1357:LYS:HB2	2.19	0.43
2:L:151:ASP:O	2:L:152:ASN:HB2	2.19	0.43
2:L:54:ARG:HD2	2:L:58:VAL:O	2.19	0.43
3:R:1124:LEU:HB2	3:R:1139:GLY:C	2.39	0.43
1:G:294:ILE:O	1:G:294:ILE:HG23	2.19	0.42
1:P:1218:CYS:HA	1:P:1247:CYS:HA	2.01	0.42
2:Q:1211:ARG:HB3	2:Q:1211:ARG:NH1	2.32	0.42
1:G:104:MET:HA	1:G:217:TYR:OH	2.20	0.42
3:R:1063:LEU:HB3	3:R:1067:VAL:HG23	2.01	0.42
2:L:183:LYS:O	2:L:187:GLU:HG2	2.20	0.42
1:P:1104:MET:O	1:P:1108:ILE:HG12	2.19	0.42
1:P:1478:ASN:HD22	1:P:1478:ASN:H	1.67	0.42
1:P:1422:GLN:O	1:P:1434:MET:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1259:LEU:HD13	1:P:1449:ILE:CD1	2.50	0.42
3:R:1028:THR:HB	3:R:1031:ARG:HD2	2.00	0.42
3:R:1127:SER:H	3:R:1129:LYS:HD3	1.85	0.42
1:G:197:ASN:ND2	9:G:996:HOH:O	2.53	0.42
1:G:463:ASN:OD1	1:G:465:THR:HG23	2.19	0.42
2:L:149:LYS:HG2	2:L:154:LEU:HD13	2.00	0.42
2:Q:1158:ASN:HD22	2:Q:1181:LEU:HD21	1.84	0.42
3:R:1035:THR:HG23	3:R:1049:GLY:O	2.19	0.42
2:L:201:LEU:HD13	2:L:205:VAL:HG23	2.02	0.42
1:P:1391:PHE:CD2	1:P:1470:PRO:HG3	2.55	0.42
1:P:1484:TYR:CZ	1:P:1485:LYS:HD2	2.55	0.42
2:Q:1074:THR:HG22	9:Q:516:HOH:O	2.19	0.42
2:Q:1113:PRO:HB3	2:Q:1139:PHE:HB3	2.00	0.42
2:L:13:VAL:HG21	2:L:78:LEU:HD22	2.02	0.42
3:H:130:SER:O	3:H:131:THR:O	2.38	0.42
2:Q:1054:ARG:CG	2:Q:1058:VAL:HB	2.50	0.42
4:M:18:LYS:HE2	4:M:27:VLM:CG2	2.50	0.41
1:G:296:CYS:HA	1:G:331:CYS:HA	2.03	0.41
1:G:227:LYS:HE3	1:G:485:LYS:HE3	2.02	0.41
1:G:389:GLN:HG3	5:G:886:NAG:H81	2.01	0.41
1:P:1104:MET:HA	1:P:1217:TYR:OH	2.20	0.41
1:P:1287:GLN:HB2	9:P:689:HOH:O	2.20	0.41
3:R:1138:LEU:HD12	3:R:1138:LEU:N	2.35	0.41
3:H:168:ALA:HA	3:H:178:LEU:HB3	2.01	0.41
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.02	0.41
1:P:1246:GLN:HA	1:P:1246:GLN:HE21	1.86	0.41
1:P:1388:THR:HG21	5:P:1886:NAG:H5	2.02	0.41
3:R:1129:LYS:CG	3:R:1136:ALA:HA	2.50	0.41
1:G:270:ILE:O	1:G:348:LYS:HE3	2.20	0.41
1:G:391:PHE:CD1	1:G:470:PRO:HG3	2.55	0.41
3:H:210:LYS:HE3	3:H:212:GLU:HG2	2.01	0.41
1:P:1390:LEU:HG	1:P:1416:LEU:HD21	2.02	0.41
1:P:1476:ARG:O	1:P:1480:ARG:HG3	2.21	0.41
3:R:1212:GLU:HG2	3:R:1213:PRO:HD2	2.02	0.41
3:H:148:GLU:HB2	9:H:242:HOH:O	2.21	0.41
3:H:151:THR:HG22	9:H:239:HOH:O	2.20	0.41
2:L:105:GLU:HG3	2:L:173:TYR:OH	2.20	0.41
3:R:1191:THR:HG23	3:R:1192:GLN:HG3	2.03	0.41
2:Q:1050:GLY:O	2:Q:1051:ALA:HB3	2.21	0.41
1:G:117:LYS:HA	1:G:118:PRO:HD3	1.82	0.40
2:L:160:GLN:HB2	2:L:160:GLN:HE21	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1086:LEU:C	1:P:1086:LEU:HD23	2.41	0.40
2:Q:1032:ASP:HB3	2:Q:1091:TYR:CE1	2.56	0.40
3:R:1168:ALA:HA	3:R:1178:LEU:HB3	2.03	0.40
1:G:232:LYS:CE	9:G:990:HOH:O	2.68	0.40
3:H:125:ALA:HA	3:H:126:PRO:HD3	1.83	0.40
2:L:54:ARG:CZ	2:L:60:ALA:HA	2.51	0.40
2:L:58:VAL:HA	2:L:59:PRO:HD3	1.94	0.40
2:Q:1035:TRP:CE2	2:Q:1073:LEU:HB2	2.56	0.40
1:G:231:LYS:HE3	1:G:268:GLU:OE1	2.21	0.40
1:G:337:GLN:CA	1:G:337:GLN:NE2	2.84	0.40
3:H:193:THR:CG2	3:H:210:LYS:HZ3	2.33	0.40
3:H:214:LYS:C	3:H:214:LYS:HD3	2.42	0.40
2:L:116:PHE:HD2	3:H:129:LYS:HD3	1.86	0.40
2:L:14:SER:O	2:L:17:GLU:HB2	2.21	0.40
4:M:3:LEU:O	4:M:7:GLN:HG3	2.21	0.40
2:Q:1187:GLU:O	2:Q:1211:ARG:NH2	2.54	0.40
2:L:44:PRO:HD2	3:H:103:TRP:CE3	2.56	0.40
2:Q:1135:LEU:C	2:Q:1135:LEU:CD2	2.90	0.40
2:Q:1174:SER:O	3:R:1166:PHE:HE2	2.04	0.40

There are no symmetry-related clashes.

## 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	G	297/313 (95%)	280 (94%)	16 (5%)	1 (0%)	44	49
1	P	295/313 (94%)	277 (94%)	17 (6%)	1 (0%)	44	49
2	L	212/214 (99%)	204 (96%)	7 (3%)	1 (0%)	32	34
2	Q	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	32	34
3	H	227/229 (99%)	208 (92%)	11 (5%)	8 (4%)	4	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	227/229 (99%)	212 (93%)	12 (5%)	3 (1%)	14	11
4	M	25/27 (93%)	25 (100%)	0	0	100	100
4	S	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
All	All	1520/1566 (97%)	1433 (94%)	72 (5%)	15 (1%)	18	16

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	131	THR
1	P	1268	GLU
1	G	439	ILE
3	H	64	GLN
3	H	129	LYS
3	R	1064	GLN
3	H	88	ALA
3	H	130	SER
3	H	132	SER
3	R	1132	SER
2	L	138	ASN
3	H	128	SER
2	Q	1138	ASN
3	H	213	PRO
3	R	1002	VAL

### 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	G	266/276 (96%)	256 (96%)	10 (4%)	38	47
1	P	264/276 (96%)	252 (96%)	12 (4%)	32	39
2	L	184/184 (100%)	176 (96%)	8 (4%)	33	41
2	Q	184/184 (100%)	175 (95%)	9 (5%)	29	35
3	H	193/193 (100%)	186 (96%)	7 (4%)	40	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R	193/193 (100%)	185 (96%)	8 (4%)	35	44
4	M	20/20 (100%)	20 (100%)	0	100	100
4	S	20/20 (100%)	19 (95%)	1 (5%)	28	34
All	All	1324/1346 (98%)	1269 (96%)	55 (4%)	34	43

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	99	ASN
1	G	207	LYS
1	G	216	HIS
1	G	226	LEU
1	G	236	THR
1	G	337	GLN
1	G	419	ARG
1	G	442	GLN
1	G	465	THR
1	G	478	ASN
2	L	13	VAL
2	L	17	GLU
2	L	24	ARG
2	L	46	LEU
2	L	73	LEU
2	L	125	LEU
2	L	135	LEU
2	L	143	GLU
3	H	38	ARG
3	H	82	LEU
3	H	100(D)	GLU
3	H	124	LEU
3	H	147	PRO
3	H	149	PRO
3	H	191	THR
1	P	1102	GLU
1	P	1111	LEU
1	P	1113	ASP
1	P	1114	GLN
1	P	1116	LEU
1	P	1216	HIS
1	P	1226	LEU
1	P	1355	ASN

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Mol	Chain	Res	Type
1	P	1371	ILE
1	P	1374	HIS
1	P	1418	CYS
1	P	1475	MET
2	Q	1046	LEU
2	Q	1073	LEU
2	Q	1078	LEU
2	Q	1090	GLN
2	Q	1105	GLU
2	Q	1123	GLU
2	Q	1125	LEU
2	Q	1135	LEU
2	Q	1154	LEU
3	R	1038	ARG
3	R	1082	LEU
3	R	1124	LEU
3	R	1129	LYS
3	R	1147	PRO
3	R	1149	PRO
3	R	1163	VAL
3	R	1214	LYS
4	S	1018	LYS

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

Mol	Chain	Res	Type
1	G	114	GLN
1	G	216	HIS
1	G	337	GLN
1	G	413	ASN
1	G	442	GLN
1	G	448	ASN
1	G	478	ASN
2	L	100	GLN
2	L	166	GLN
2	L	210	ASN
3	H	64	GLN
3	H	164	HIS
3	H	192	GLN
3	H	199	ASN
1	P	1099	ASN
1	P	1197	ASN

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Mol	Chain	Res	Type
1	P	1203	GLN
1	P	1246	GLN
1	P	1340	ASN
1	P	1355	ASN
1	P	1356	ASN
1	P	1389	GLN
1	P	1463	ASN
1	P	1478	ASN
2	Q	1147	GLN
2	Q	1166	GLN
2	Q	1210	ASN
3	R	1171	GLN
3	R	1199	ASN
4	S	1002	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z  > 2$
4	VLM	M	27	4	5,7,7	1.79	1 (20%)	5,9,9	1.14	0
4	VLM	S	1027	4	5,7,7	1.75	1 (20%)	5,9,9	0.83	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	VLM	M	27	4	-	0/7/8/8	0/0/0/0
4	VLM	S	1027	4	-	0/7/8/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	27	VLM	C-NT	-3.86	1.25	1.32
4	S	1027	VLM	C-NT	-3.79	1.25	1.32

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
4	M	27	VLM	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

20 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	$\# Z  > 2$
5	NAG	G	588	1	14,14,15	0.57	0	15,19,21	0.73	0
6	NDG	G	734	1	14,14,15	0.59	0	15,19,21	0.63	0
5	NAG	G	741	1	14,14,15	0.55	0	15,19,21	0.85	1 (6%)
5	NAG	G	762	1	14,14,15	0.45	0	15,19,21	0.80	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	G	776	1	14,14,15	0.43	0	15,19,21	0.82	1 (6%)
5	NAG	G	789	1	14,14,15	0.48	0	15,19,21	0.71	0
5	NAG	G	795	1	14,14,15	0.52	0	15,19,21	0.71	1 (6%)
5	NAG	G	886	1	14,14,15	0.73	1 (7%)	15,19,21	0.93	1 (6%)
8	IPA	G	901	-	3,3,3	0.62	0	3,3,3	0.34	0
7	EDO	G	903	-	3,3,3	0.44	0	2,2,2	0.46	0
7	EDO	M	904	-	3,3,3	0.45	0	2,2,2	0.44	0
5	NAG	P	1588	1	14,14,15	0.58	0	15,19,21	0.70	0
5	NAG	P	1734	1	14,14,15	0.47	0	15,19,21	0.62	0
5	NAG	P	1741	1	14,14,15	0.63	0	15,19,21	0.65	0
5	NAG	P	1762	1	14,14,15	0.45	0	15,19,21	0.83	0
5	NAG	P	1776	1	14,14,15	0.66	0	15,19,21	0.68	0
5	NAG	P	1789	1	14,14,15	0.54	0	15,19,21	0.88	1 (6%)
5	NAG	P	1795	1	14,14,15	0.54	0	15,19,21	0.83	1 (6%)
5	NAG	P	1886	1	14,14,15	0.50	0	15,19,21	0.88	1 (6%)
8	IPA	P	902	-	3,3,3	0.61	0	3,3,3	0.32	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
5	NAG	G	588	1	-	0/6/23/26	0/1/1/1
6	NDG	G	734	1	-	0/6/23/26	0/1/1/1
5	NAG	G	741	1	-	0/6/23/26	0/1/1/1
5	NAG	G	762	1	-	0/6/23/26	0/1/1/1
5	NAG	G	776	1	-	0/6/23/26	0/1/1/1
5	NAG	G	789	1	-	0/6/23/26	0/1/1/1
5	NAG	G	795	1	-	0/6/23/26	0/1/1/1
5	NAG	G	886	1	-	0/6/23/26	0/1/1/1
8	IPA	G	901	-	-	0/0/0/0	0/0/0/0
7	EDO	G	903	-	-	0/1/1/1	0/0/0/0
7	EDO	M	904	-	-	0/1/1/1	0/0/0/0
5	NAG	P	1588	1	-	0/6/23/26	0/1/1/1
5	NAG	P	1734	1	-	0/6/23/26	0/1/1/1
5	NAG	P	1741	1	-	0/6/23/26	0/1/1/1
5	NAG	P	1762	1	-	0/6/23/26	0/1/1/1
5	NAG	P	1776	1	-	0/6/23/26	0/1/1/1
5	NAG	P	1789	1	-	0/6/23/26	0/1/1/1
5	NAG	P	1795	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	1886	1	-	0/6/23/26	0/1/1/1
8	IPA	P	902	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	886	NAG	C1-C2	2.03	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	1886	NAG	C2-N2-C7	-2.46	119.36	122.94
5	G	776	NAG	C2-N2-C7	-2.41	119.43	122.94
5	P	1795	NAG	C2-N2-C7	-2.39	119.45	122.94
5	P	1789	NAG	C2-N2-C7	-2.26	119.64	122.94
5	G	741	NAG	C2-N2-C7	-2.18	119.76	122.94
5	G	886	NAG	C3-C4-C5	-2.14	106.45	110.22
5	G	795	NAG	C2-N2-C7	-2.10	119.88	122.94
5	G	762	NAG	C2-N2-C7	-2.05	119.95	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	762	NAG	3	0
5	G	789	NAG	1	0
5	G	886	NAG	2	0
8	G	901	IPA	1	0
5	P	1734	NAG	1	0
5	P	1741	NAG	1	0
5	P	1762	NAG	2	0
5	P	1776	NAG	1	0
5	P	1795	NAG	1	0
5	P	1886	NAG	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	G	301/313 (96%)	0.02	7 (2%) 61 58	17, 31, 55, 78	0
1	P	299/313 (95%)	0.14	11 (3%) 42 40	19, 36, 61, 82	0
2	L	214/214 (100%)	-0.32	0 100 100	16, 27, 39, 44	0
2	Q	214/214 (100%)	-0.09	4 (1%) 67 65	16, 31, 51, 59	0
3	H	229/229 (100%)	-0.19	7 (3%) 49 47	14, 24, 50, 82	0
3	R	229/229 (100%)	-0.18	6 (2%) 56 54	18, 27, 50, 79	0
4	M	25/27 (92%)	-0.05	1 (4%) 39 37	23, 32, 40, 49	0
4	S	25/27 (92%)	-0.06	0 100 100	25, 33, 44, 45	0
All	All	1536/1566 (98%)	-0.08	36 (2%) 61 58	14, 29, 53, 82	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	1132	SER	8.0
3	R	1133	GLY	7.7
3	H	131	THR	6.9
1	P	1459	GLY	6.7
1	P	1462	THR	5.5
1	G	459	GLY	5.0
3	H	130	SER	5.0
1	P	1458	GLY	4.9
3	R	1131	THR	4.7
3	H	132	SER	4.7
1	G	462	THR	4.4
2	Q	1150	VAL	4.2
3	R	1130	SER	4.1
1	P	1460	LYS	3.5
1	P	1355	ASN	3.2
1	P	1208	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
3	H	1	GLU	3.1
4	M	4	HIS	3.0
1	P	1461	ASP	2.9
1	G	460	LYS	2.8
3	R	1128	SER	2.8
1	G	232	LYS	2.6
3	H	2	VAL	2.5
1	P	1444	ARG	2.5
1	G	442	GLN	2.5
1	G	330	HIS	2.3
3	H	133	GLY	2.3
3	H	128	SER	2.2
3	R	1214	LYS	2.2
1	P	1465	THR	2.2
1	P	1440	ARG	2.1
1	P	1231	LYS	2.1
2	Q	1191	VAL	2.1
2	Q	1181	LEU	2.1
1	G	461	ASP	2.1
2	Q	1188	LYS	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. 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
4	VLM	S	1027	8/8	0.84	0.20	-	38,39,42,44	0
4	VLM	M	27	8/8	0.95	0.11	-	31,34,35,35	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. 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
8	IPA	G	901	4/4	0.86	0.27	6.26	39,40,41,41	0
8	IPA	P	902	4/4	0.85	0.20	4.91	44,44,45,45	0
7	EDO	G	903	4/4	0.94	0.22	4.47	39,39,39,39	0
5	NAG	P	1734	14/15	0.65	0.29	3.89	65,66,67,68	0
5	NAG	G	886	14/15	0.79	0.19	3.87	43,46,49,51	0
5	NAG	P	1795	14/15	0.77	0.18	0.54	49,51,54,54	0
5	NAG	G	795	14/15	0.89	0.14	0.51	48,50,51,54	0
5	NAG	P	1762	14/15	0.91	0.13	0.18	32,35,38,38	0
5	NAG	P	1789	14/15	0.82	0.18	-0.14	52,58,64,65	0
5	NAG	G	789	14/15	0.89	0.14	-0.19	40,41,46,47	0
5	NAG	G	762	14/15	0.96	0.15	-0.26	25,27,30,30	0
7	EDO	M	904	4/4	0.79	0.20	-	45,45,46,47	0
5	NAG	G	741	14/15	0.70	0.36	-	56,60,62,63	0
5	NAG	P	1886	14/15	0.76	0.20	-	55,58,61,61	0
5	NAG	P	1588	14/15	0.88	0.14	-	39,42,44,45	0
5	NAG	P	1776	14/15	0.63	0.25	-	46,52,54,55	0
6	NDG	G	734	14/15	0.73	0.31	-	57,58,60,60	0
5	NAG	G	776	14/15	0.85	0.17	-	43,45,51,54	0
5	NAG	P	1741	14/15	0.62	0.33	-	60,63,63,65	0
5	NAG	G	588	14/15	0.84	0.23	-	51,53,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.