



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 06:56 pm GMT

PDB ID : 4R4F  
Title : Crystal structure of non-neutralizing, A32-like antibody 2.2c in complex with HIV-1 YU2 gp120  
Authors : Acharya, P.; Kwong, P.D.  
Deposited on : 2014-08-19  
Resolution : 3.51 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

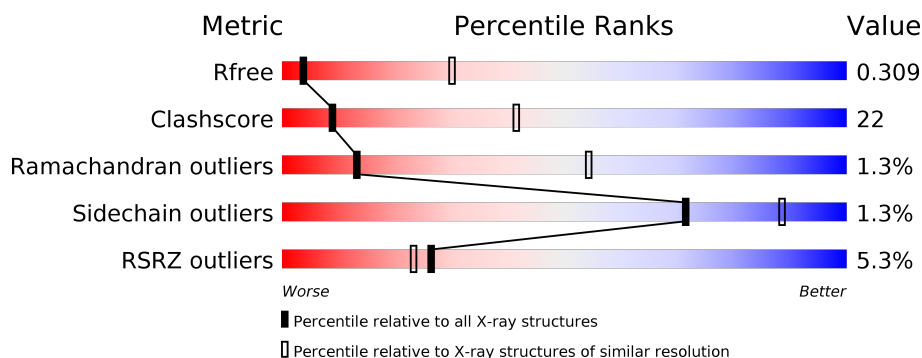
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.51 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))
$R_{free}$	111664	1052 (3.62-3.42)
Clashscore	122126	1048 (3.60-3.44)
Ramachandran outliers	120053	1014 (3.60-3.44)
Sidechain outliers	120020	1015 (3.60-3.44)
RSRZ outliers	108989	1353 (3.64-3.40)

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	376	<div> <div>8%</div> <div> <div></div> <div>63%</div> <div>26%</div> <div>10%</div> </div> </div>
2	L	209	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>33%</div> </div> </div>
3	H	219	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>34%</div> </div> </div>
4	R	28	<div> <div></div> <div> <div></div> <div>82%</div> <div>18%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	H	301	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6316 atoms, of which 30 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 HIV-1 Env gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2669	1672	466	511	20			

- Molecule 2 is a protein called Antibody 2.2c LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	209	Total	C	N	O	S	0	0	0
			1606	1010	271	320	5			

- Molecule 3 is a protein called Antibody 2.2c heavy CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1662	1059	281	317	5			

- Molecule 4 is a protein called M48U1 peptide.

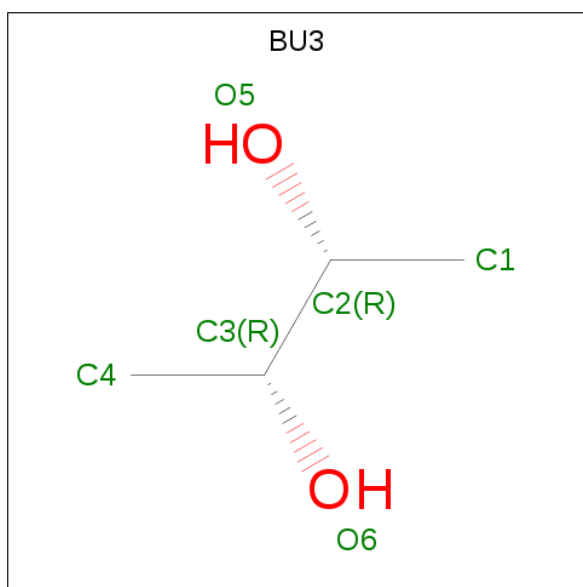
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



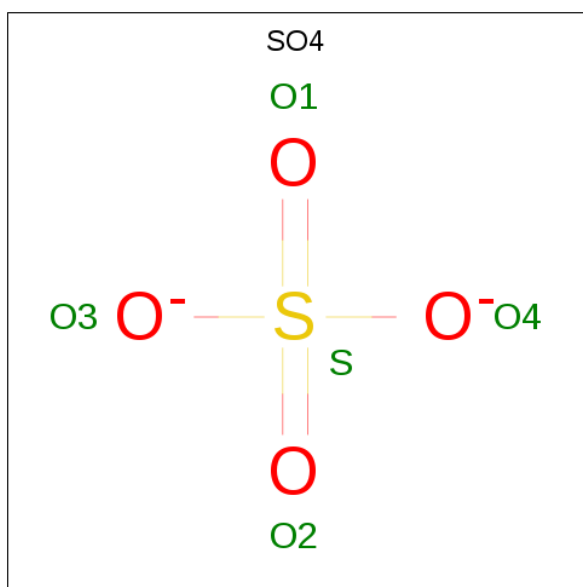
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			16	4	10	2		
6	A	1	Total	C	H	O	0	0
			16	4	10	2		
6	L	1	Total	C	H	O	0	0
			16	4	10	2		

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



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

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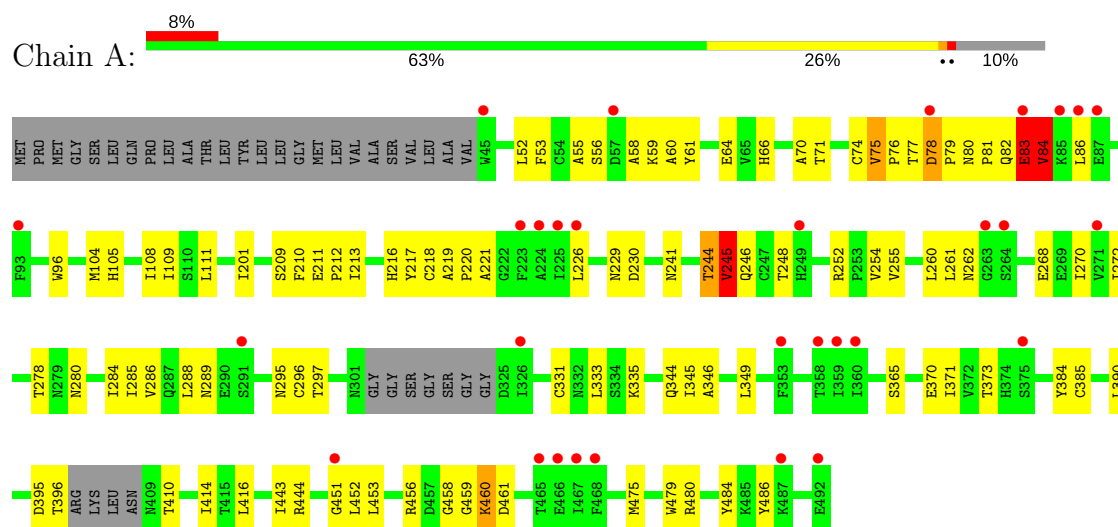
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	O	S	0	0
			5	4	1		

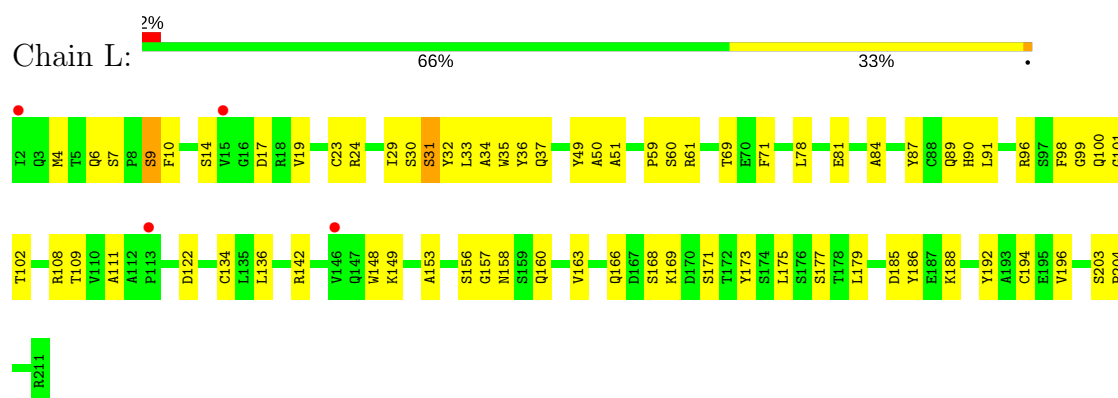
### 3 Residue-property plots

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.

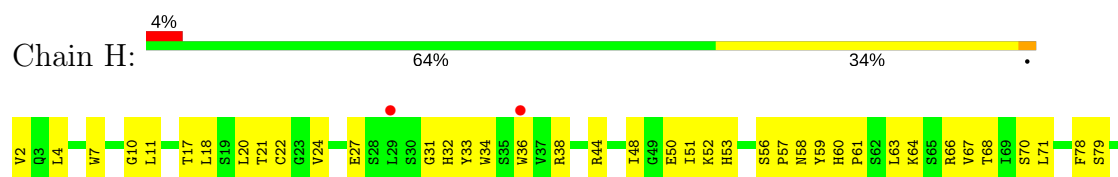
#### • Molecule 1: HIV-1 Env gp120



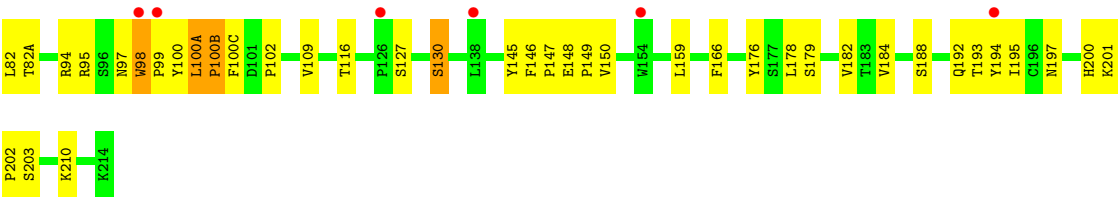
#### • Molecule 2: Antibody 2.2c LIGHT CHAIN



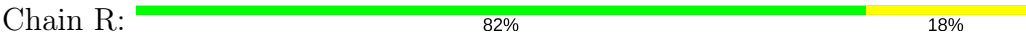
#### • Molecule 3: Antibody 2.2c heavy CHAIN







● Molecule 4: M48U1 peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.32Å 171.23Å 227.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.75 – 3.51 35.75 – 3.51	Depositor EDS
% Data completeness (in resolution range)	82.3 (35.75-3.51) 83.0 (35.75-3.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.251 , 0.295 0.270 , 0.309	Depositor DCC
$R_{free}$ test set	1635 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 178.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6316	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	223.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: DPR, BU3, MPT, OAS, SO4, NH2, U2X, 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	0.34	0/2725	0.51	0/3698
2	L	0.37	0/1630	0.61	0/2209
3	H	0.38	0/1711	0.59	0/2340
4	R	0.32	0/176	0.59	0/231
All	All	0.36	0/6242	0.56	0/8478

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	A	2669	0	2590	121	0
2	L	1606	0	1577	61	0
3	H	1662	0	1636	95	0
4	R	209	0	212	6	0
5	A	98	0	91	5	0
5	H	14	0	13	3	0
6	A	12	20	20	2	0
6	L	6	10	10	3	0
7	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	5	0	0	0	0
All	All	6286	30	6149	269	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 22.

All (269) 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)
3:H:98:TRP:HB3	3:H:100:TYR:H	1.11	1.11
1:A:84:VAL:HB	1:A:244:THR:HG23	1.35	1.08
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.34	1.06
3:H:57:PRO:HB2	3:H:59:TYR:HE1	1.17	1.03
3:H:100(A):LEU:HB3	3:H:100(B):PRO:HA	1.44	0.99
1:A:221:ALA:HB2	3:H:98:TRP:HZ2	1.28	0.97
3:H:57:PRO:HB2	3:H:59:TYR:CE1	2.06	0.90
1:A:272:ILE:HG12	1:A:286:VAL:HG22	1.55	0.89
1:A:80:ASN:HB2	1:A:82:GLN:HB3	1.53	0.89
3:H:178:LEU:HD12	3:H:179:SER:N	1.92	0.85
3:H:98:TRP:HB3	3:H:100:TYR:N	1.90	0.85
3:H:98:TRP:H	3:H:99:PRO:HA	1.42	0.84
3:H:38:ARG:HB3	3:H:48:ILE:HD11	1.61	0.82
3:H:100(A):LEU:HB3	3:H:100(B):PRO:CA	2.10	0.81
1:A:75:VAL:HG22	1:A:76:PRO:HD2	1.64	0.80
1:A:77:THR:HB	1:A:78:ASP:HA	1.65	0.78
3:H:95:ARG:HH21	3:H:100(A):LEU:HD13	1.48	0.78
1:A:55:ALA:HB1	1:A:77:THR:HG21	1.66	0.77
3:H:95:ARG:NH2	3:H:100(A):LEU:HD13	1.99	0.77
1:A:390:LEU:HD11	1:A:416:LEU:HD11	1.67	0.77
2:L:6:GLN:HB2	2:L:100:GLN:HE22	1.51	0.75
1:A:221:ALA:HB2	3:H:98:TRP:CZ2	2.19	0.74
1:A:78:ASP:HB2	1:A:80:ASN:N	2.01	0.74
1:A:52:LEU:HD22	1:A:219:ALA:HA	1.70	0.73
1:A:459:GLY:HA2	1:A:460:LYS:HB2	1.71	0.73
1:A:81:PRO:CD	1:A:82:GLN:HA	2.19	0.72
1:A:371:ILE:HD11	4:R:23:U2X:HB3	1.70	0.72
3:H:148:GLU:HG3	3:H:176:TYR:CE2	2.24	0.72
3:H:98:TRP:N	3:H:99:PRO:HA	2.04	0.72
1:A:460:LYS:CB	1:A:461:ASP:HA	2.19	0.71
1:A:460:LYS:HG2	1:A:461:ASP:HA	1.73	0.71
1:A:60:ALA:HA	1:A:71:THR:HG21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:59:TYR:CE2	3:H:67:VAL:HG12	2.25	0.71
1:A:280:ASN:HD22	1:A:458:GLY:HA3	1.56	0.70
3:H:79:SER:CB	5:H:302:NAG:H81	2.22	0.70
2:L:4:MET:HB2	2:L:99:GLY:HA2	1.73	0.70
3:H:63:LEU:HB3	3:H:67:VAL:CG2	2.22	0.70
3:H:184:VAL:HG11	3:H:194:TYR:CE1	2.26	0.69
2:L:96:ARG:NH2	3:H:50:GLU:OE2	2.26	0.69
1:A:365:SER:HG	4:R:28:NH2:N	1.91	0.69
2:L:29:ILE:HD13	2:L:90:HIS:CD2	2.29	0.68
3:H:178:LEU:HD12	3:H:179:SER:H	1.57	0.68
3:H:100(B):PRO:HB2	3:H:100(C):PHE:CD2	2.29	0.68
2:L:9:SER:OG	2:L:10:PHE:N	2.27	0.68
1:A:335:LYS:NZ	1:A:410:THR:OG1	2.26	0.68
1:A:459:GLY:HA2	1:A:460:LYS:CB	2.24	0.67
2:L:108:ARG:HG2	2:L:109:THR:H	1.59	0.67
1:A:280:ASN:HD22	1:A:458:GLY:CA	2.09	0.66
3:H:2:VAL:HG22	3:H:27:GLU:HB2	1.78	0.65
1:A:297:THR:HG23	1:A:444:ARG:HG3	1.77	0.65
2:L:91:LEU:HD22	3:H:100(B):PRO:HB3	1.79	0.65
2:L:29:ILE:CG2	2:L:32:TYR:HB2	2.27	0.65
3:H:79:SER:HB2	5:H:302:NAG:H81	1.80	0.64
1:A:55:ALA:CB	1:A:77:THR:HG21	2.28	0.64
1:A:66:HIS:CD2	1:A:212:PRO:HA	2.32	0.64
2:L:122:ASP:N	2:L:122:ASP:OD1	2.31	0.63
3:H:148:GLU:HB3	3:H:149:PRO:HA	1.80	0.63
1:A:456:ARG:HH22	6:A:508:BU3:C4	2.10	0.63
1:A:278:THR:O	6:A:508:BU3:H42	1.99	0.63
3:H:2:VAL:HG21	3:H:27:GLU:OE1	1.99	0.63
1:A:268:GLU:O	1:A:289:ASN:ND2	2.28	0.62
1:A:460:LYS:CG	1:A:461:ASP:HA	2.29	0.62
3:H:63:LEU:HB3	3:H:67:VAL:HG23	1.81	0.62
2:L:156:SER:O	2:L:158:ASN:N	2.33	0.62
1:A:79:PRO:HB3	3:H:52:LYS:HE2	1.80	0.62
3:H:195:ILE:HG12	3:H:210:LYS:HG3	1.80	0.62
1:A:81:PRO:CB	1:A:82:GLN:HA	2.28	0.62
2:L:7:SER:O	2:L:9:SER:N	2.30	0.62
1:A:78:ASP:N	1:A:78:ASP:OD1	2.30	0.61
1:A:81:PRO:HD2	1:A:82:GLN:HA	1.81	0.61
3:H:52:LYS:HD2	3:H:53:HIS:H	1.64	0.61
3:H:4:LEU:HD22	3:H:24:VAL:HG22	1.81	0.61
1:A:52:LEU:HD23	1:A:220:PRO:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:31:SER:O	2:L:50:ALA:HA	2.00	0.60
2:L:166:GLN:HG3	2:L:173:TYR:CZ	2.37	0.60
3:H:51:ILE:HG13	3:H:52:LYS:H	1.66	0.60
3:H:193:THR:CG2	3:H:210:LYS:HE2	2.30	0.60
2:L:163:VAL:HG22	2:L:175:LEU:HD12	1.83	0.60
1:A:59:LYS:HD3	1:A:61:TYR:OH	2.02	0.59
1:A:335:LYS:HA	1:A:414:ILE:HG13	1.84	0.59
3:H:33:TYR:HB2	3:H:95:ARG:HB2	1.85	0.59
2:L:148:TRP:CZ3	2:L:194:CYS:HB3	2.38	0.58
3:H:2:VAL:CG2	3:H:27:GLU:HB2	2.32	0.58
3:H:94:ARG:NH2	3:H:102:PRO:HD3	2.19	0.58
3:H:98:TRP:CB	3:H:100:TYR:H	2.02	0.57
1:A:104:MET:HG3	1:A:217:TYR:OH	2.03	0.57
1:A:254:VAL:HG13	5:A:506:NAG:C8	2.34	0.57
1:A:285:ILE:HG12	1:A:453:LEU:CD2	2.35	0.57
2:L:33:LEU:HD22	2:L:71:PHE:CD2	2.40	0.57
3:H:18:LEU:HD11	3:H:20:LEU:HG	1.87	0.57
3:H:57:PRO:CB	3:H:59:TYR:HE1	2.06	0.57
2:L:108:ARG:HH21	2:L:111:ALA:HB2	1.70	0.57
1:A:272:ILE:HG23	1:A:284:ILE:CG2	2.35	0.56
1:A:66:HIS:HB3	1:A:213:ILE:HG12	1.87	0.56
1:A:390:LEU:CD1	1:A:416:LEU:HD11	2.34	0.56
2:L:134:CYS:HB2	2:L:148:TRP:CZ2	2.39	0.56
1:A:335:LYS:HA	1:A:414:ILE:CD1	2.35	0.56
1:A:255:VAL:HG12	4:R:23:U2X:H21	1.87	0.56
2:L:158:ASN:HD21	2:L:179:LEU:CD1	2.19	0.56
3:H:100(A):LEU:CB	3:H:100(B):PRO:CA	2.83	0.56
2:L:19:VAL:HG11	2:L:78:LEU:HD21	1.87	0.56
1:A:451:GLY:C	1:A:452:LEU:HD12	2.26	0.56
3:H:98:TRP:H	3:H:99:PRO:CA	2.17	0.56
1:A:459:GLY:HA3	1:A:460:LYS:O	2.06	0.56
1:A:254:VAL:HG13	5:A:506:NAG:H81	1.88	0.55
3:H:63:LEU:HB3	3:H:67:VAL:HG21	1.87	0.55
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.41	0.55
1:A:346:ALA:HA	1:A:349:LEU:HD12	1.89	0.55
2:L:9:SER:HA	2:L:102:THR:HG23	1.89	0.55
1:A:52:LEU:CD2	1:A:219:ALA:HA	2.37	0.55
3:H:97:ASN:O	3:H:98:TRP:HB2	2.06	0.55
1:A:81:PRO:N	1:A:82:GLN:HA	2.19	0.54
2:L:6:GLN:HB2	2:L:100:GLN:NE2	2.21	0.54
3:H:59:TYR:HE2	3:H:67:VAL:HG12	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:136:LEU:HD21	2:L:196:VAL:CG1	2.38	0.54
1:A:59:LYS:HB3	1:A:61:TYR:CE1	2.42	0.54
3:H:94:ARG:HH21	3:H:102:PRO:HD3	1.73	0.54
3:H:150:VAL:HG12	3:H:200:HIS:HB2	1.89	0.54
3:H:71:LEU:HD23	3:H:78:PHE:HB3	1.90	0.54
3:H:67:VAL:HG22	3:H:82:LEU:HD13	1.90	0.54
1:A:70:ALA:O	1:A:74:CYS:HB2	2.08	0.54
1:A:108:ILE:HD12	1:A:479:TRP:CE2	2.44	0.53
2:L:14:SER:O	2:L:17:ASP:HB2	2.08	0.53
3:H:116:THR:HG22	3:H:203:SER:HB3	1.91	0.53
1:A:84:VAL:HB	1:A:244:THR:CG2	2.23	0.53
1:A:81:PRO:HB2	1:A:82:GLN:HA	1.91	0.53
2:L:136:LEU:HD21	2:L:196:VAL:HG13	1.90	0.53
3:H:59:TYR:CD2	3:H:67:VAL:HG12	2.43	0.52
2:L:156:SER:C	2:L:158:ASN:H	2.12	0.52
1:A:78:ASP:H	1:A:79:PRO:HA	1.75	0.52
3:H:193:THR:HG21	3:H:210:LYS:HE2	1.91	0.52
2:L:9:SER:HB2	2:L:102:THR:HA	1.91	0.52
2:L:166:GLN:NE2	2:L:171:SER:O	2.40	0.52
1:A:460:LYS:HB3	1:A:460:LYS:NZ	2.24	0.52
2:L:158:ASN:HD21	2:L:179:LEU:HD12	1.75	0.52
1:A:395:ASP:OD1	1:A:396:THR:N	2.42	0.52
1:A:56:SER:OG	1:A:70:ALA:HB1	2.10	0.52
1:A:81:PRO:HB2	1:A:82:GLN:CA	2.39	0.52
2:L:168:SER:O	2:L:169:LYS:HB2	2.09	0.52
2:L:24:ARG:HA	2:L:69:THR:O	2.09	0.52
3:H:79:SER:HB3	5:H:302:NAG:H81	1.93	0.51
1:A:460:LYS:HB3	1:A:461:ASP:HA	1.90	0.51
3:H:51:ILE:HD12	3:H:56:SER:O	2.11	0.51
2:L:186:TYR:O	2:L:192:TYR:OH	2.29	0.51
3:H:193:THR:HG23	3:H:210:LYS:HE2	1.92	0.51
1:A:365:SER:O	4:R:15:LEU:CD1	2.59	0.50
3:H:195:ILE:HG12	3:H:210:LYS:CG	2.41	0.50
3:H:34:TRP:CH2	3:H:94:ARG:HG3	2.46	0.50
1:A:78:ASP:N	1:A:79:PRO:HA	2.26	0.50
1:A:270:ILE:HD12	1:A:344:GLN:HB3	1.93	0.50
2:L:203:SER:HB2	2:L:204:PRO:HD2	1.92	0.50
2:L:99:GLY:O	3:H:44:ARG:HD3	2.12	0.50
1:A:335:LYS:CA	1:A:414:ILE:HG13	2.41	0.50
3:H:148:GLU:CB	3:H:149:PRO:HA	2.39	0.50
1:A:272:ILE:HG23	1:A:284:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:59:TYR:CE2	3:H:68:THR:HA	2.46	0.49
1:A:83:GLU:C	1:A:84:VAL:HG22	2.31	0.49
2:L:59:PRO:HB3	6:L:301:BU3:H12	1.94	0.49
1:A:53:PHE:O	1:A:218:CYS:N	2.35	0.49
2:L:108:ARG:HG2	2:L:109:THR:N	2.26	0.49
2:L:60:SER:N	6:L:301:BU3:O6	2.39	0.49
1:A:370:GLU:HG3	1:A:384:TYR:HE2	1.78	0.49
2:L:89:GLN:HE22	3:H:100(C):PHE:HE2	1.59	0.49
3:H:38:ARG:CB	3:H:48:ILE:HD11	2.39	0.49
2:L:142:ARG:NH2	2:L:163:VAL:HB	2.28	0.49
1:A:288:LEU:HD21	1:A:345:ILE:HD11	1.95	0.49
5:A:502:NAG:H82	5:A:502:NAG:O3	2.12	0.49
1:A:66:HIS:HE1	1:A:210:PHE:CE2	2.30	0.48
2:L:134:CYS:HB2	2:L:148:TRP:CH2	2.47	0.48
2:L:158:ASN:ND2	2:L:179:LEU:HD12	2.28	0.48
1:A:84:VAL:HG23	1:A:244:THR:O	2.14	0.48
3:H:116:THR:CG2	3:H:203:SER:HB3	2.44	0.48
3:H:59:TYR:HE2	3:H:68:THR:HA	1.79	0.48
1:A:108:ILE:HD12	1:A:479:TRP:CZ2	2.48	0.48
1:A:58:ALA:HB2	1:A:213:ILE:HD12	1.96	0.48
2:L:163:VAL:HG22	2:L:175:LEU:CD1	2.44	0.48
1:A:79:PRO:HG2	3:H:31:GLY:O	2.14	0.48
3:H:51:ILE:HG13	3:H:52:LYS:N	2.28	0.48
2:L:19:VAL:CG1	2:L:78:LEU:HD21	2.44	0.48
1:A:370:GLU:HG3	1:A:384:TYR:CE2	2.48	0.47
1:A:96:TRP:HA	1:A:480:ARG:HD3	1.96	0.47
1:A:59:LYS:HD3	1:A:61:TYR:CZ	2.49	0.47
1:A:280:ASN:HB2	1:A:456:ARG:O	2.14	0.47
3:H:95:ARG:HA	3:H:100(B):PRO:O	2.15	0.47
2:L:30:OAS:HB3	2:L:30:OAS:HC23	1.77	0.47
3:H:148:GLU:HB3	3:H:149:PRO:CA	2.45	0.46
3:H:7:TRP:NE1	3:H:21:THR:HB	2.30	0.46
1:A:244:THR:OG1	1:A:245:VAL:N	2.47	0.46
1:A:373:THR:HB	1:A:385:CYS:O	2.15	0.46
5:A:503:NAG:O3	5:A:503:NAG:H82	2.14	0.46
3:H:66:ARG:HD2	3:H:82(A):THR:O	2.16	0.46
2:L:90:HIS:O	2:L:96:ARG:HA	2.15	0.46
4:R:9:ARG:O	4:R:12:SER:OG	2.27	0.46
1:A:105:HIS:HE1	1:A:475:MET:HB2	1.80	0.46
3:H:166:PHE:O	3:H:178:LEU:HD13	2.16	0.46
1:A:111:LEU:HD23	1:A:111:LEU:C	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:O	1:A:486:TYR:HA	2.15	0.46
1:A:254:VAL:HG11	1:A:261:LEU:HB2	1.98	0.46
3:H:148:GLU:HG3	3:H:176:TYR:CZ	2.51	0.45
2:L:185:ASP:O	2:L:188:LYS:HG2	2.16	0.45
1:A:272:ILE:CG2	1:A:284:ILE:HG23	2.47	0.45
1:A:86:LEU:HG	1:A:244:THR:HG22	1.97	0.45
1:A:53:PHE:HZ	3:H:100:TYR:HH	1.64	0.45
3:H:17:THR:HG22	3:H:82(A):THR:HA	1.98	0.45
1:A:201:ILE:N	1:A:201:ILE:HD12	2.32	0.45
1:A:64:GLU:HG2	1:A:209:SER:O	2.17	0.45
1:A:260:LEU:HD12	1:A:451:GLY:HA3	1.99	0.45
3:H:50:GLU:HG2	3:H:58:ASN:HB3	1.98	0.45
1:A:333:LEU:N	1:A:333:LEU:HD23	2.32	0.45
1:A:78:ASP:HB2	1:A:79:PRO:C	2.37	0.45
1:A:335:LYS:CB	1:A:414:ILE:HG13	2.46	0.44
1:A:335:LYS:HA	1:A:414:ILE:CG1	2.46	0.44
1:A:53:PHE:O	1:A:218:CYS:HB2	2.16	0.44
1:A:245:VAL:HB	1:A:246:GLN:H	1.47	0.44
3:H:22:CYS:HB2	3:H:36:TRP:CH2	2.53	0.44
1:A:345:ILE:O	1:A:349:LEU:HG	2.18	0.44
1:A:459:GLY:CA	1:A:460:LYS:CB	2.94	0.44
2:L:4:MET:HE3	2:L:23:CYS:SG	2.57	0.44
3:H:145:TYR:CE2	3:H:150:VAL:HG13	2.53	0.44
1:A:297:THR:HA	1:A:443:ILE:O	2.18	0.44
1:A:296:CYS:O	1:A:444:ARG:HA	2.18	0.44
3:H:201:LYS:N	3:H:202:PRO:CD	2.81	0.44
2:L:60:SER:H	6:L:301:BU3:HO6	1.64	0.44
2:L:89:GLN:HB2	2:L:98:PHE:CD2	2.53	0.44
1:A:254:VAL:CG1	5:A:506:NAG:H82	2.48	0.43
2:L:34:ALA:HA	2:L:49:TYR:HA	2.00	0.43
1:A:371:ILE:HD11	4:R:23:U2X:CB	2.42	0.43
2:L:156:SER:HB3	2:L:158:ASN:OD1	2.19	0.43
2:L:36:TYR:OH	3:H:100(C):PHE:HD2	2.00	0.43
1:A:84:VAL:O	1:A:244:THR:HG23	2.19	0.43
3:H:147:PRO:O	3:H:200:HIS:NE2	2.43	0.43
3:H:27:GLU:OE2	3:H:32:HIS:NE2	2.52	0.43
3:H:98:TRP:N	3:H:99:PRO:CA	2.73	0.43
1:A:252:ARG:HD2	1:A:262:ASN:HB3	2.00	0.43
1:A:230:ASP:OD1	1:A:241:ASN:N	2.52	0.43
1:A:105:HIS:CE1	1:A:475:MET:HB2	2.54	0.42
3:H:11:LEU:HD11	3:H:146:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:HB2	1:A:82:GLN:CB	2.36	0.42
1:A:272:ILE:CG2	1:A:284:ILE:CG2	2.97	0.42
1:A:333:LEU:O	1:A:414:ILE:N	2.43	0.42
3:H:34:TRP:CZ3	3:H:94:ARG:HB2	2.54	0.42
2:L:37:GLN:HG3	2:L:84:ALA:HB3	2.01	0.42
3:H:10:GLY:O	3:H:109:VAL:HA	2.20	0.42
2:L:50:ALA:O	2:L:51:ALA:HB3	2.19	0.42
1:A:66:HIS:HE1	1:A:210:PHE:CZ	2.38	0.41
3:H:59:TYR:CD1	3:H:59:TYR:N	2.88	0.41
3:H:127:SER:O	3:H:130:SER:HB2	2.20	0.41
2:L:87:TYR:CE1	2:L:101:GLY:HA3	2.55	0.41
1:A:64:GLU:OE2	1:A:66:HIS:HB2	2.21	0.41
1:A:81:PRO:CB	1:A:82:GLN:CA	2.95	0.41
2:L:9:SER:CB	2:L:102:THR:HA	2.50	0.41
2:L:149:LYS:HA	2:L:153:ALA:O	2.20	0.41
1:A:105:HIS:CD2	1:A:109:ILE:HD11	2.56	0.41
2:L:4:MET:CE	2:L:23:CYS:SG	3.09	0.41
2:L:61:ARG:NH2	2:L:81:GLU:OE2	2.53	0.41
3:H:60:HIS:HA	3:H:61:PRO:HD3	1.92	0.41
1:A:295:ASN:O	1:A:331:CYS:HA	2.22	0.41
1:A:280:ASN:ND2	1:A:458:GLY:HA3	2.31	0.41
1:A:480:ARG:O	1:A:484:TYR:HB3	2.22	0.40
3:H:159:LEU:HD21	3:H:182:VAL:HG21	2.03	0.40
3:H:188:SER:O	3:H:192:GLN:HB3	2.21	0.40
3:H:70:SER:O	3:H:78:PHE:HB2	2.21	0.40
1:A:229:ASN:HB2	1:A:241:ASN:O	2.21	0.40
2:L:160:GLN:O	2:L:177:SER:HA	2.22	0.40
3:H:100(A):LEU:HA	3:H:100(A):LEU:HD23	1.88	0.40
1:A:75:VAL:HG11	3:H:99:PRO:HG2	2.04	0.40
1:A:248:THR:HG22	1:A:486:TYR:CD1	2.57	0.40
3:H:94:ARG:HB3	3:H:102:PRO:HD2	2.04	0.40
3:H:64:LYS:HD3	3:H:64:LYS:C	2.42	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	A	334/376 (89%)	314 (94%)	17 (5%)	3 (1%)	19	62
2	L	206/209 (99%)	193 (94%)	10 (5%)	3 (2%)	11	51
3	H	217/219 (99%)	204 (94%)	9 (4%)	4 (2%)	9	47
4	R	24/28 (86%)	24 (100%)	0	0	100	100
All	All	781/832 (94%)	735 (94%)	36 (5%)	10 (1%)	13	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	245	VAL
2	L	9	SER
2	L	157	GLY
3	H	98	TRP
3	H	100(A)	LEU
3	H	100(B)	PRO
3	H	130	SER
2	L	31	SER
1	A	83	GLU

### 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	301/328 (92%)	293 (97%)	8 (3%)	48	77
2	L	181/181 (100%)	181 (100%)	0	100	100
3	H	190/190 (100%)	189 (100%)	1 (0%)	90	95
4	R	20/20 (100%)	20 (100%)	0	100	100
All	All	692/719 (96%)	683 (99%)	9 (1%)	71	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	78	ASP
1	A	83	GLU
1	A	84	VAL
1	A	211	GLU
1	A	244	THR
1	A	245	VAL
1	A	460	LYS
3	H	197	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	$\# Z  > 2$
2	OAS	L	30	2	8,8,9	0.96	0	6,9,11	0.51	0
4	DPR	R	21	4	6,7,8	0.86	0	7,8,10	1.21	1 (14%)
4	U2X	R	23	4	20,20,21	2.31	4 (20%)	24,25,27	1.70	6 (25%)

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	OAS	L	30	2	-	0/5/7/9	0/0/0/0
4	DPR	R	21	4	-	0/0/9/11	0/1/1/1
4	U2X	R	23	4	-	0/9/19/21	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	23	U2X	C4-C3	2.48	1.59	1.52
4	R	23	U2X	CE1-CZ	2.71	1.44	1.38
4	R	23	U2X	CE1-CD1	4.76	1.47	1.38
4	R	23	U2X	CE2-CD2	7.38	1.51	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	23	U2X	C1-C2-C3	-3.39	105.80	112.20
4	R	21	DPR	O-C-CA	-2.26	119.82	125.09
4	R	23	U2X	C6-C1-C2	-2.07	107.22	111.42
4	R	23	U2X	C4-C3-C7	2.65	116.90	111.41
4	R	23	U2X	OH-C7-C3	2.78	113.60	107.80
4	R	23	U2X	CG-CB-CA	2.79	119.76	114.23
4	R	23	U2X	C2-C3-C7	3.71	119.09	111.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	30	OAS	1	0
4	R	23	U2X	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

13 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	A	501	1	14,14,15	0.30	0	17,19,21	0.50	0
5	NAG	A	502	1	14,14,15	0.27	0	17,19,21	0.57	0
5	NAG	A	503	1	14,14,15	0.35	0	17,19,21	0.42	0
5	NAG	A	504	1	14,14,15	0.41	0	17,19,21	0.55	0
5	NAG	A	505	1	14,14,15	0.52	0	17,19,21	0.47	0
5	NAG	A	506	1	14,14,15	0.39	0	17,19,21	0.49	0
5	NAG	A	507	1	14,14,15	0.36	0	17,19,21	0.54	0
6	BU3	A	508	-	4,5,5	0.38	0	6,6,6	0.38	0
6	BU3	A	509	-	4,5,5	0.31	0	6,6,6	0.17	0
7	SO4	A	510	-	4,4,4	0.20	0	6,6,6	0.10	0
7	SO4	H	301	-	4,4,4	0.19	0	6,6,6	0.09	0
5	NAG	H	302	3	14,14,15	0.28	0	17,19,21	0.46	0
6	BU3	L	301	-	4,5,5	0.33	0	6,6,6	0.36	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	A	501	1	-	0/6/23/26	0/1/1/1
5	NAG	A	502	1	-	0/6/23/26	0/1/1/1
5	NAG	A	503	1	-	0/6/23/26	0/1/1/1
5	NAG	A	504	1	-	0/6/23/26	0/1/1/1
5	NAG	A	505	1	-	0/6/23/26	0/1/1/1
5	NAG	A	506	1	-	0/6/23/26	0/1/1/1
5	NAG	A	507	1	-	0/6/23/26	0/1/1/1
6	BU3	A	508	-	-	0/4/4/4	0/0/0/0
6	BU3	A	509	-	-	0/4/4/4	0/0/0/0
7	SO4	A	510	-	-	0/0/0/0	0/0/0/0
7	SO4	H	301	-	-	0/0/0/0	0/0/0/0
5	NAG	H	302	3	-	0/6/23/26	0/1/1/1
6	BU3	L	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	NAG	1	0
5	A	503	NAG	1	0
5	A	506	NAG	3	0
6	A	508	BU3	2	0
5	H	302	NAG	3	0
6	L	301	BU3	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	340/376 (90%)	0.38	30 (8%) 10 10	171, 231, 310, 417	0
2	L	208/209 (99%)	0.15	4 (1%) 66 60	171, 204, 260, 357	0
3	H	219/219 (100%)	0.14	8 (3%) 41 36	171, 203, 270, 314	0
4	R	24/28 (85%)	-0.25	0 100 100	238, 269, 298, 318	0
All	All	791/832 (95%)	0.23	42 (5%) 26 23	171, 213, 296, 417	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	GLU	5.4
1	A	353	PHE	4.8
1	A	359	ILE	4.8
1	A	360	ILE	4.6
1	A	224	ALA	4.3
1	A	358	THR	3.7
1	A	467	ILE	3.6
1	A	451	GLY	3.3
1	A	45	TRP	3.1
1	A	326	ILE	3.0
1	A	226	LEU	2.9
1	A	87	GLU	2.7
1	A	468	PHE	2.7
1	A	225	ILE	2.6
1	A	465	THR	2.6
1	A	263	GLY	2.6
2	L	2	ILE	2.6
1	A	83	GLU	2.6
3	H	194	TYR	2.5
1	A	291	SER	2.5
1	A	249	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	99	PRO	2.4
3	H	126	PRO	2.4
1	A	57	ASP	2.4
1	A	487	LYS	2.3
1	A	93	PHE	2.3
1	A	86	LEU	2.3
1	A	223	PHE	2.3
1	A	264	SER	2.2
1	A	492	GLU	2.2
3	H	29	LEU	2.2
3	H	138	LEU	2.2
1	A	78	ASP	2.1
3	H	154	TRP	2.1
1	A	271	VAL	2.1
3	H	98	TRP	2.1
1	A	85	LYS	2.1
2	L	113	PRO	2.0
2	L	15	VAL	2.0
2	L	146	VAL	2.0
3	H	36	TRP	2.0
1	A	375	SER	2.0

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

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(Å <sup>2</sup> )	Q<0.9
2	OAS	L	30	9/10	0.80	0.20	195,197,200,202	0
4	U2X	R	23	19/20	0.87	0.37	237,257,278,281	0
4	DPR	R	21	7/8	0.93	0.24	237,239,244,244	0

## 6.3 Carbohydrates ⓘ

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(Å <sup>2</sup> )	Q<0.9
5	NAG	H	302	14/15	0.65	0.24	264,268,273,274	0
7	SO4	A	510	5/5	0.69	0.25	209,209,209,210	0
5	NAG	A	505	14/15	0.71	0.31	243,254,258,260	0
5	NAG	A	503	14/15	0.71	0.35	269,280,288,293	0
7	SO4	H	301	5/5	0.77	0.42	248,248,250,253	0
5	NAG	A	504	14/15	0.77	0.31	234,246,257,257	0
6	BU3	A	508	6/6	0.79	0.13	209,209,284,287	0
5	NAG	A	507	14/15	0.88	0.23	257,262,271,272	0
6	BU3	A	509	6/6	0.90	1.59	209,209,265,266	16
5	NAG	A	502	14/15	0.91	0.15	244,254,261,262	0
6	BU3	L	301	6/6	0.91	0.17	209,209,251,253	0
5	NAG	A	501	14/15	0.91	0.20	250,254,261,262	0
5	NAG	A	506	14/15	0.94	0.21	200,205,209,210	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.