



# Full wwPDB X-ray Structure Validation Report

Oct 13, 2014 – 10:53 PM EDT

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 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/ValidationPDFNotes.html>

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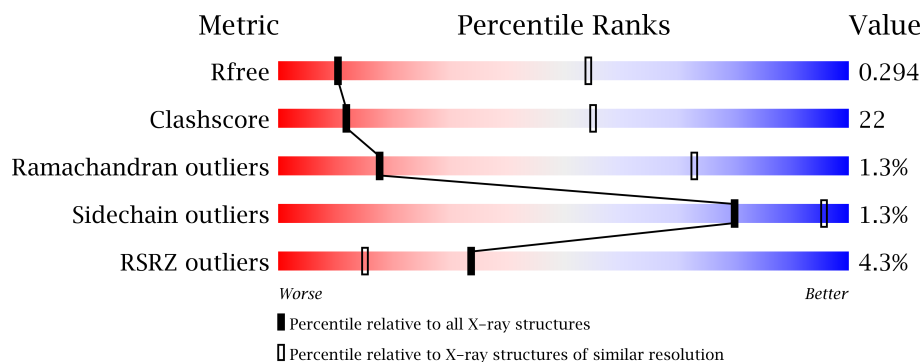
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23828

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1256 (3.74-3.30)
Clashscore	79885	1020 (3.68-3.36)
Ramachandran outliers	78287	1082 (3.70-3.34)
Sidechain outliers	78261	1082 (3.70-3.34)
RSRZ outliers	66119	1256 (3.74-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	376	
2	L	209	
3	H	219	
4	R	28	

## 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 deuterium.

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			

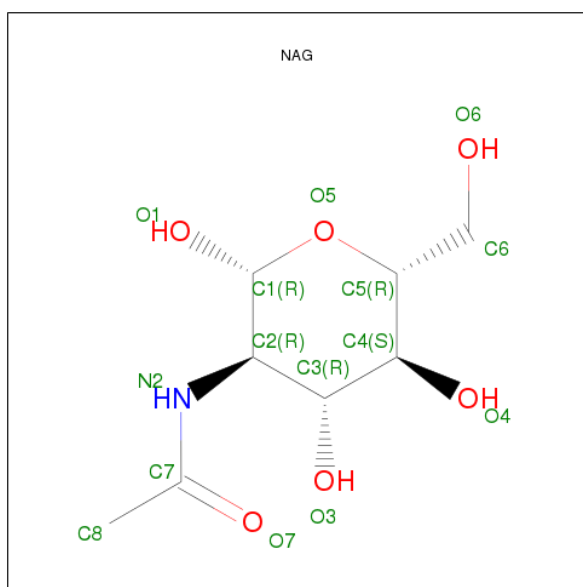
- Molecule 3 is a protein called Antibody 2.2c heavy CHAIN.

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.

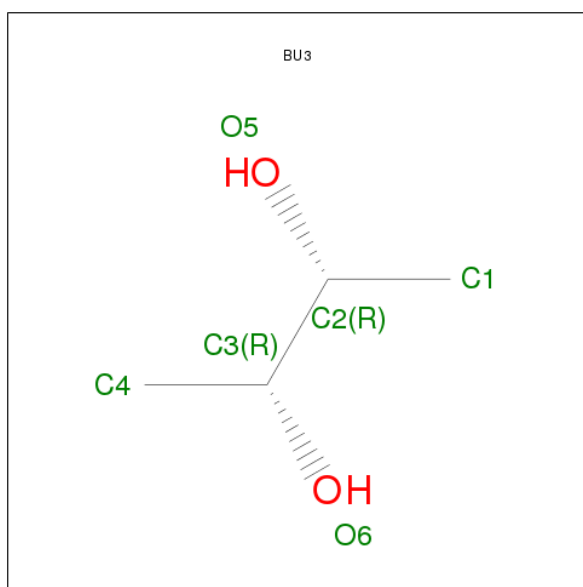
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

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



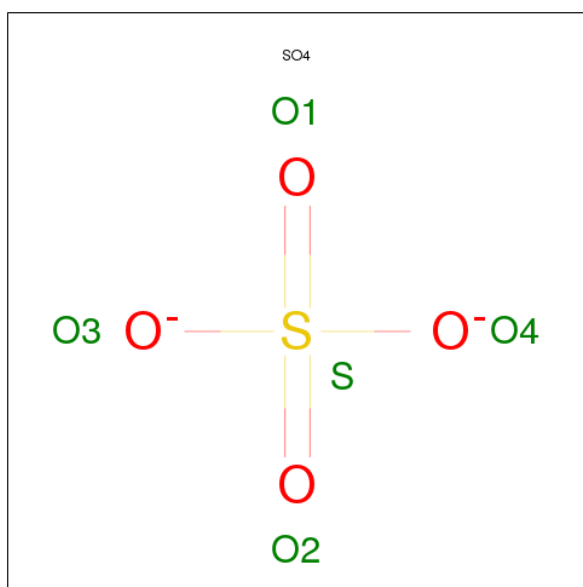
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

- 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: SO4) (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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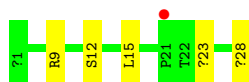
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	O	S	0	0
			5	4	1		



- Molecule 4: M48U1 peptide

Chain R: 





## 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 0.249 , 0.294	Depositor DCC
$R_{free}$ test set	1626 reflections (10.15%)	DCC
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 , 176.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 16141 reflections (0.019%)	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.

## 5 Model quality

### 5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2669	0	2590	120	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	0	1	5
6	L	6	10	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	5	0	0	0	0
7	H	5	0	0	0	0
All	All	6286	30	6119	268	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (268) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
3:H:59:TYR:CE2	3:H:67:VAL:HG12	2.25	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
3:H:195:ILE:HG12	3:H:210:LYS:HG3	1.80	0.62
1:A:79:PRO:HB3	3:H:52:LYS:HE2	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:94:ARG:HH21	3:H:102:PRO:HD3	1.73	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:99:GLY:O	3:H:44:ARG:HD3	2.12	0.50
2:L:203:SER:HB2	2:L:204:PRO:HD2	1.92	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
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:59:PRO:HB3	6:L:301:BU3:H12	1.96	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:HD12	1:A:201:ILE:N	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:296:CYS:O	1:A:444:ARG:HA	2.18	0.44
1:A:297:THR:HA	1:A:443:ILE:O	2.18	0.44
3:H:201:LYS:N	3:H:202:PRO:CD	2.81	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
2:L:60:SER:H	6:L:301:BU3:HO6	1.64	0.43
1:A:371:ILE:HD11	4:R:23:U2X:CB	2.42	0.43
2:L:36:TYR:OH	3:H:100(C):PHE:HD2	2.00	0.43
2:L:156:SER:HB3	2:L:158:ASN:OD1	2.19	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:509:BU3:H3	6:A:509:BU3:H2[3_455]	0.11	1.49
6:A:509:BU3:H41	6:A:509:BU3:H11[3_455]	0.12	1.48
6:A:509:BU3:H43	6:A:509:BU3:H13[3_455]	0.13	1.47
6:A:509:BU3:H42	6:A:509:BU3:H12[3_455]	0.15	1.45
6:A:509:BU3:HO6	6:A:509:BU3:HO5[3_455]	0.73	0.87

## 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	334/376 (89%)	314 (94%)	17 (5%)	3 (1%)	25	80
2	L	206/209 (99%)	193 (94%)	10 (5%)	3 (2%)	15	69
3	H	217/219 (99%)	204 (94%)	9 (4%)	4 (2%)	13	66
4	R	24/28 (86%)	24 (100%)	0	0	100	100
All	All	781/832 (94%)	735 (94%)	36 (5%)	10 (1%)	18	73

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%)	57	90
2	L	181/181 (100%)	181 (100%)	0	100	100
3	H	190/190 (100%)	189 (100%)	1 (0%)	94	98
4	R	20/20 (100%)	20 (100%)	0	100	100
All	All	692/719 (96%)	683 (99%)	9 (1%)	80	95

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 chains 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	6.03	1 (12%)	7,9,11	2.46	2 (28%)
4	DPR	R	21	4	7,7,8	6.71	1 (14%)	6,8,10	0.92	0
4	U2X	R	23	4	20,20,21	4.21	6 (30%)	23,25,27	1.67	5 (21%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	21	DPR	O-C	17.65	1.23	1.11
2	L	30	OAS	O-C	16.87	1.23	1.11
4	R	23	U2X	O-C	15.87	1.22	1.11
4	R	23	U2X	CE2-CD2	6.99	1.51	1.38
4	R	23	U2X	CE1-CD1	4.50	1.47	1.38
4	R	23	U2X	CE1-CZ	2.64	1.44	1.38
4	R	23	U2X	C4-C3	2.60	1.59	1.52
4	R	23	U2X	CB-CA	-2.56	1.49	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	30	OAS	C-CA-N	-6.03	107.81	113.83
4	R	23	U2X	C1-C2-C3	-3.96	105.80	112.23
4	R	23	U2X	C2-C3-C7	3.62	119.09	111.52
4	R	23	U2X	C4-C3-C7	2.57	116.90	111.52
4	R	23	U2X	OH-C7-C3	2.43	113.60	107.78
4	R	23	U2X	CG-CB-CA	2.34	119.76	114.32
2	L	30	OAS	CB-CA-N	2.13	120.22	110.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	12,14,15	0.36	0	15,19,21	0.24	0
5	NAG	A	502	1	12,14,15	0.40	0	15,19,21	0.36	0
5	NAG	A	503	1	12,14,15	0.42	0	15,19,21	0.39	0
5	NAG	A	504	1	12,14,15	0.37	0	15,19,21	0.33	0
5	NAG	A	505	1	12,14,15	0.43	0	15,19,21	0.45	0
5	NAG	A	506	1	12,14,15	0.37	0	15,19,21	0.37	0
5	NAG	A	507	1	12,14,15	0.41	0	15,19,21	0.40	0
6	BU3	A	508	-	5,5,5	0.46	0	6,6,6	0.33	0
6	BU3	A	509	-	5,5,5	0.39	0	6,6,6	0.20	0
7	SO4	A	510	-	4,4,4	0.13	0	6,6,6	0.13	0
7	SO4	H	301	-	4,4,4	0.15	0	6,6,6	0.07	0
5	NAG	H	302	3	12,14,15	0.34	0	15,19,21	0.27	0
6	BU3	L	301	-	5,5,5	0.42	0	6,6,6	0.29	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.

## 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	A	340/376 (90%)	0.48	19 (5%) 24 10	171, 231, 310, 417	0
2	L	209/209 (100%)	0.33	3 (1%) 72 39	171, 204, 260, 357	0
3	H	219/219 (100%)	0.36	11 (5%) 28 12	171, 203, 270, 314	0
4	R	27/28 (96%)	0.19	1 (3%) 39 18	238, 269, 298, 318	0
All	All	795/832 (95%)	0.40	34 (4%) 34 15	171, 213, 296, 417	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	GLU	5.0
1	A	360	ILE	4.2
1	A	359	ILE	3.7
1	A	353	PHE	3.6
4	R	21	DPR	3.3
1	A	326	ILE	3.2
1	A	358	THR	3.1
1	A	467	ILE	2.9
2	L	2	ILE	2.8
3	H	126	PRO	2.8
1	A	224	ALA	2.8
1	A	83	GLU	2.7
1	A	226	LEU	2.6
3	H	138	LEU	2.6
1	A	492	GLU	2.5
3	H	213	PRO	2.5
1	A	468	PHE	2.5
1	A	45	TRP	2.5
1	A	217	TYR	2.5
2	L	30	OAS	2.4
1	A	87	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	113	PRO	2.3
1	A	487	LYS	2.3
3	H	194	TYR	2.2
1	A	225	ILE	2.2
1	A	465	THR	2.2
3	H	63	LEU	2.2
3	H	99	PRO	2.1
3	H	98	TRP	2.1
3	H	29	LEU	2.1
3	H	100	TYR	2.1
1	A	257	THR	2.1
3	H	136	ALA	2.1
3	H	159	LEU	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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	U2X	R	23	19/20	0.38	-	237,257,278,281	0
2	OAS	L	30	9/10	0.20	-	195,197,200,202	0
4	DPR	R	21	7/8	0.27	-	237,239,244,244	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	502	14/15	0.15	-	244,254,261,262	0
5	NAG	A	506	14/15	0.30	-	200,205,209,210	0
6	BU3	A	508	6/6	0.15	-	209,209,284,287	0
5	NAG	A	501	14/15	0.20	-	250,254,261,262	0
5	NAG	H	302	14/15	0.23	-	264,268,273,274	0
7	SO4	A	510	5/5	0.21	-	209,209,209,210	0
5	NAG	A	505	14/15	0.29	-	243,254,258,260	0
5	NAG	A	504	14/15	0.27	-	234,246,257,257	0
7	SO4	H	301	5/5	0.32	-	248,248,250,253	0
5	NAG	A	503	14/15	0.33	-	269,280,288,293	0
5	NAG	A	507	14/15	0.27	-	257,262,271,272	0
6	BU3	L	301	6/6	0.12	-	209,209,251,253	0
6	BU3	A	509	6/6	1.54	-	209,209,265,266	16

## 6.5 Other polymers ⓘ

There are no such residues in this entry.