



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 01:19 AM JST

PDB ID : 7CDJ  
Title : Crystal structure of SARS-CoV-2 antibody P2C-1A3 with RBD  
Authors : Wang, X.; Zhang, L.; Ge, J.; Wang, R.  
Deposited on : 2020-06-19  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

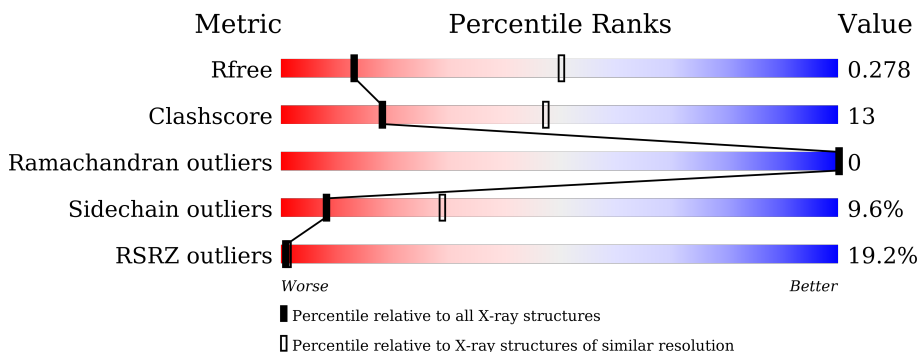
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	217	 19% 62% 25% 11%
2	H	218	 16% 59% 35% 2%
3	L	214	 20% 68% 29% 1%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4770 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	194	1536	984	256	288	8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	530	HIS	-	expression tag	UNP P0DTC2
E	531	HIS	-	expression tag	UNP P0DTC2
E	532	HIS	-	expression tag	UNP P0DTC2
E	533	HIS	-	expression tag	UNP P0DTC2
E	534	HIS	-	expression tag	UNP P0DTC2
E	535	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called antibody P2C-1A3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	212	1590	1007	265	312	6	0	0	1

- Molecule 3 is a protein called antibody P2C-1A3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	213	1630	1025	271	330	4	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

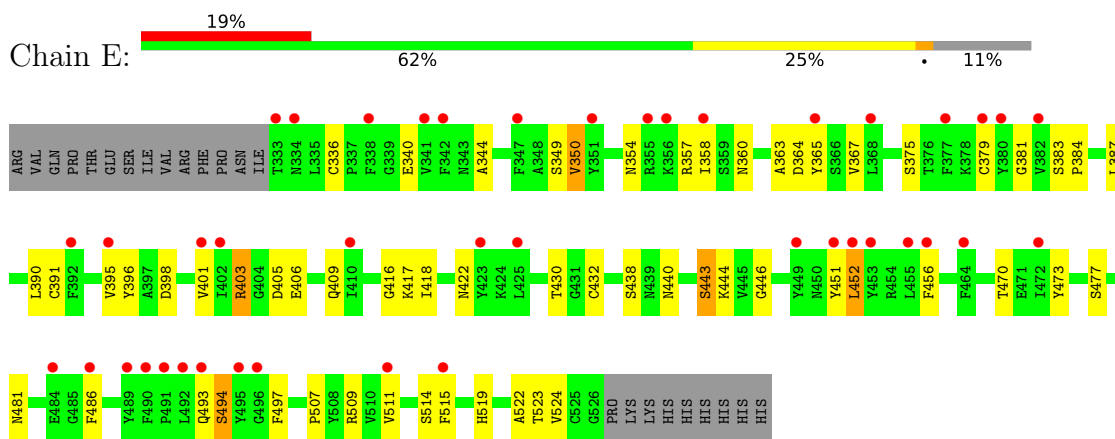


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	E	1	14	8	1	5	0	0

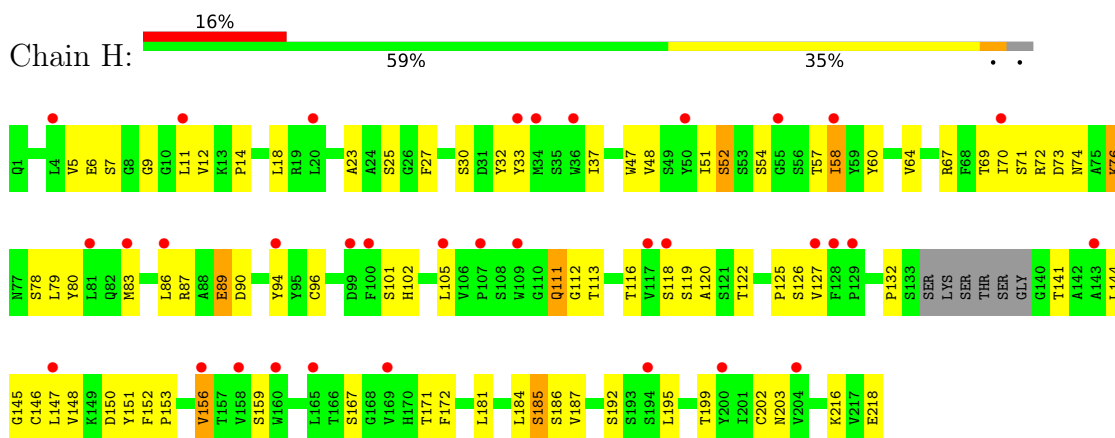
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

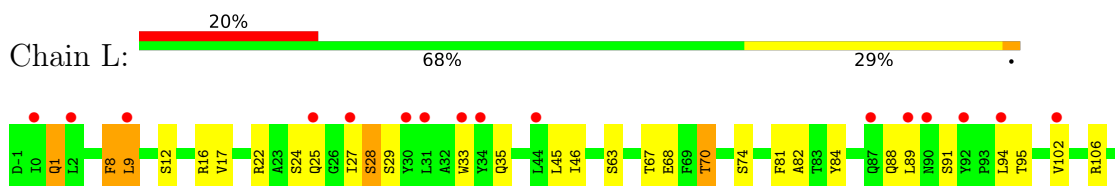
- Molecule 1: Spike protein S1

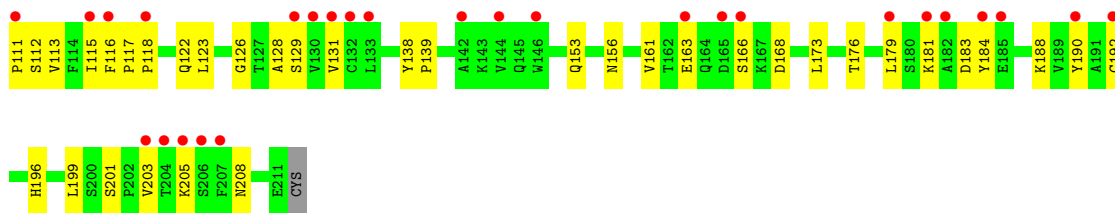


- Molecule 2: antibody P2C-1A3 heavy chain



- Molecule 3: antibody P2C-1A3 light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.41Å 89.41Å 437.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.31 – 3.40 48.66 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.31-3.40) 99.0 (48.66-3.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 3.40Å)	Xtrriage
Refinement program	PHENIX 1.15_3459	Depositor
R, $R_{free}$	0.231 , 0.271 0.239 , 0.278	Depositor DCC
$R_{free}$ test set	720 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	100.1	Xtrriage
Anisotropy	0.922	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 107.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4770	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% 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: 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	E	0.49	0/1579	0.60	0/2149
2	H	0.48	0/1628	0.65	0/2216
3	L	0.52	0/1665	0.63	0/2261
All	All	0.50	0/4872	0.63	0/6626

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	E	1536	0	1452	34	0
2	H	1590	0	1557	45	0
3	L	1630	0	1594	49	0
4	E	14	0	13	0	0
All	All	4770	0	4616	126	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 13.

All (126) 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:L:9:LEU:CD2	3:L:102:VAL:HG22	1.56	1.33
3:L:9:LEU:HD21	3:L:102:VAL:CG2	1.78	1.12
3:L:9:LEU:CD1	3:L:17:VAL:HG13	1.95	0.97
1:E:336:CYS:HB2	1:E:363:ALA:HB2	1.54	0.90
3:L:9:LEU:HD11	3:L:17:VAL:HG13	1.50	0.89
3:L:9:LEU:HD11	3:L:17:VAL:CG1	2.06	0.86
2:H:6:GLU:OE1	2:H:96:CYS:N	2.12	0.82
3:L:9:LEU:HD21	3:L:102:VAL:HG22	0.82	0.81
3:L:9:LEU:CD2	3:L:102:VAL:CG2	2.45	0.80
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.63	0.79
3:L:81:PHE:CE2	3:L:163:GLU:HG3	2.21	0.76
3:L:81:PHE:HE2	3:L:163:GLU:HG3	1.50	0.74
2:H:199:THR:HG23	2:H:216:LYS:HE3	1.76	0.67
3:L:9:LEU:O	3:L:9:LEU:HD23	1.94	0.67
2:H:145:GLY:HA3	2:H:187:VAL:HG12	1.77	0.65
1:E:360:ASN:H	1:E:523:THR:HB	1.62	0.65
3:L:9:LEU:HD23	3:L:102:VAL:HA	1.79	0.64
2:H:6:GLU:OE1	2:H:96:CYS:SG	2.55	0.64
2:H:48:VAL:HG13	2:H:64:VAL:HG21	1.81	0.63
3:L:199:LEU:HD13	3:L:203:VAL:HG23	1.80	0.63
3:L:28:SER:O	3:L:28:SER:OG	2.13	0.62
1:E:391:CYS:HB3	1:E:522:ALA:HB1	1.80	0.62
1:E:381:GLY:HA3	1:E:430:THR:HG22	1.83	0.61
2:H:120:ALA:HB3	2:H:152:PHE:CE2	2.36	0.61
1:E:384:PRO:HA	1:E:387:LEU:HD12	1.84	0.60
3:L:188:LYS:HE3	3:L:208:ASN:ND2	2.16	0.60
2:H:9:GLY:HA2	2:H:18:LEU:HD21	1.85	0.59
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.33	0.59
1:E:456:PHE:HB3	1:E:473:TYR:CD2	2.38	0.59
1:E:409:GLN:NE2	1:E:416:GLY:HA3	2.18	0.58
1:E:350:VAL:HG22	1:E:401:VAL:O	2.04	0.57
1:E:340:GLU:O	1:E:344:ALA:HB2	2.05	0.57
1:E:395:VAL:HG22	1:E:515:PHE:HD1	1.70	0.57
3:L:88:GLN:NE2	3:L:91:SER:H	2.02	0.56
1:E:493:GLN:HG3	2:H:54:SER:HB3	1.85	0.56
3:L:188:LYS:HE3	3:L:208:ASN:HD22	1.71	0.56
1:E:365:TYR:CD2	1:E:387:LEU:HB3	2.42	0.54
3:L:122:GLN:OE1	3:L:129:SER:HB2	2.08	0.54
1:E:418:ILE:HA	1:E:422:ASN:HD22	1.72	0.54
2:H:12:VAL:HG11	2:H:86:LEU:HD12	1.91	0.53
3:L:22:ARG:NH1	3:L:68:GLU:HB2	2.22	0.53
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:25:GLN:O	3:L:27:ILE:HG23	2.11	0.51
3:L:113:VAL:O	3:L:205:LYS:HG3	2.10	0.51
3:L:8:PHE:C	3:L:8:PHE:CD2	2.83	0.50
2:H:148:VAL:HB	2:H:184:LEU:HB3	1.93	0.50
2:H:9:GLY:CA	2:H:18:LEU:HD21	2.40	0.50
2:H:11:LEU:HB2	2:H:153:PRO:HG3	1.93	0.49
2:H:52:SER:O	2:H:72:ARG:NH1	2.45	0.49
2:H:132:PRO:HD3	2:H:144:LEU:HB3	1.93	0.49
3:L:33:TRP:HB2	3:L:46:ILE:HB	1.93	0.49
1:E:486:PHE:CD2	2:H:105:LEU:HD22	2.48	0.49
3:L:118:PRO:HB3	3:L:128:ALA:HB1	1.93	0.49
1:E:349:SER:OG	1:E:451:TYR:HA	2.13	0.49
2:H:171:THR:HG23	2:H:186:SER:HB2	1.94	0.48
2:H:150:ASP:HA	2:H:181:LEU:HB3	1.95	0.48
1:E:395:VAL:HG22	1:E:515:PHE:CD1	2.49	0.48
1:E:443:SER:HB2	1:E:497:PHE:HB3	1.95	0.48
2:H:148:VAL:HG11	2:H:156:VAL:HG11	1.95	0.48
1:E:452:LEU:HD23	1:E:494:SER:HA	1.96	0.48
3:L:16:ARG:HG2	3:L:74:SER:O	2.14	0.47
3:L:161:VAL:HG22	3:L:173:LEU:HD12	1.96	0.47
1:E:444:LYS:HE3	1:E:446:GLY:H	1.79	0.47
1:E:406:GLU:HG2	1:E:418:ILE:HG13	1.96	0.47
3:L:126:GLY:HA2	3:L:181:LYS:HB2	1.97	0.47
2:H:30:SER:HB2	2:H:74:ASN:ND2	2.29	0.47
1:E:391:CYS:HB3	1:E:522:ALA:CB	2.43	0.46
2:H:71:SER:OG	2:H:80:TYR:HB2	2.16	0.46
3:L:9:LEU:CD2	3:L:102:VAL:HA	2.45	0.46
3:L:35:GLN:HB2	3:L:45:LEU:HD11	1.98	0.46
3:L:179:LEU:HD22	3:L:183:ASP:HB3	1.98	0.46
2:H:184:LEU:HG	2:H:185:SER:H	1.81	0.46
1:E:379:CYS:HA	1:E:432:CYS:HA	1.97	0.46
1:E:403:ARG:HD2	1:E:406:GLU:OE2	2.16	0.45
3:L:9:LEU:HD22	3:L:102:VAL:HG22	1.80	0.45
2:H:94:TYR:O	2:H:112:GLY:HA2	2.16	0.45
1:E:497:PHE:CD1	1:E:507:PRO:HD3	2.52	0.45
2:H:60:TYR:OH	2:H:69:THR:HA	2.16	0.45
3:L:22:ARG:HA	3:L:67:THR:O	2.17	0.45
1:E:358:ILE:HG22	1:E:524:VAL:HG21	1.98	0.44
2:H:33:TYR:CD2	2:H:52:SER:HA	2.52	0.44
2:H:60:TYR:CE1	2:H:70:ILE:HG22	2.53	0.44
2:H:127:VAL:HG22	2:H:148:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:131:VAL:HG22	3:L:176:THR:HG23	1.99	0.44
1:E:395:VAL:HG21	1:E:524:VAL:HG11	2.00	0.44
2:H:111:GLN:H	2:H:111:GLN:HG3	1.50	0.44
3:L:123:LEU:CD2	3:L:128:ALA:HB2	2.46	0.44
1:E:354:ASN:O	1:E:398:ASP:HA	2.18	0.44
2:H:5:VAL:O	2:H:23:ALA:N	2.48	0.44
2:H:51:ILE:HD12	2:H:58:ILE:HD11	1.99	0.44
3:L:118:PRO:CB	3:L:128:ALA:HB1	2.48	0.44
3:L:111:PRO:HD3	3:L:196:HIS:ND1	2.33	0.44
3:L:118:PRO:HG2	3:L:184:TYR:CE1	2.54	0.43
3:L:138:TYR:CG	3:L:139:PRO:HA	2.53	0.43
3:L:82:ALA:HB3	3:L:84:TYR:CE1	2.54	0.43
1:E:357:ARG:HG3	1:E:396:TYR:CE1	2.53	0.43
2:H:172:PHE:O	2:H:184:LEU:HD11	2.18	0.43
2:H:32:TYR:CE1	2:H:101:SER:HB2	2.54	0.42
3:L:153:GLN:HB3	3:L:156:ASN:HD21	1.85	0.42
1:E:417:LYS:HD3	1:E:417:LYS:HA	1.85	0.42
1:E:440:ASN:OD1	1:E:440:ASN:N	2.53	0.42
2:H:37:ILE:HG12	2:H:47:TRP:HA	2.02	0.42
2:H:48:VAL:CG1	2:H:64:VAL:HG21	2.49	0.42
3:L:89:LEU:HD23	3:L:94:LEU:HD22	2.01	0.42
2:H:184:LEU:HA	2:H:184:LEU:HD12	1.82	0.42
1:E:364:ASP:HB3	1:E:367:VAL:HB	2.01	0.41
1:E:438:SER:CB	1:E:509:ARG:HG3	2.50	0.41
2:H:127:VAL:HA	2:H:147:LEU:O	2.20	0.41
3:L:63:SER:OG	3:L:70:THR:HG22	2.20	0.41
3:L:123:LEU:HD21	3:L:128:ALA:HB2	2.03	0.41
2:H:216:LYS:HE2	2:H:218:GLU:OE2	2.21	0.41
3:L:106:ARG:HD2	3:L:168:ASP:O	2.21	0.41
3:L:115:ILE:HD12	3:L:192:CYS:HB2	2.01	0.41
3:L:116:PHE:HA	3:L:117:PRO:HD3	1.67	0.41
3:L:184:TYR:HA	3:L:190:TYR:OH	2.20	0.41
2:H:14:PRO:HD3	2:H:118:SER:O	2.21	0.41
2:H:101:SER:OG	2:H:102:HIS:N	2.52	0.41
3:L:1:GLN:N	3:L:24:SER:OG	2.54	0.41
2:H:73:ASP:OD1	2:H:76:LYS:HG3	2.21	0.41
3:L:118:PRO:CG	3:L:128:ALA:HB1	2.51	0.41
2:H:87:ARG:HD3	2:H:89:GLU:OE2	2.20	0.40
1:E:349:SER:HB3	1:E:452:LEU:H	1.86	0.40
2:H:12:VAL:HG21	2:H:18:LEU:HB2	2.01	0.40
2:H:156:VAL:HG21	2:H:184:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:ASP:O	1:E:511:VAL:HA	2.21	0.40
3:L:35:GLN:HB3	3:L:45:LEU:HD21	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	E	192/217 (88%)	175 (91%)	17 (9%)	0	100	100
2	H	208/218 (95%)	192 (92%)	16 (8%)	0	100	100
3	L	211/214 (99%)	193 (92%)	18 (8%)	0	100	100
All	All	611/649 (94%)	560 (92%)	51 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	E	167/190 (88%)	153 (92%)	14 (8%)	11	36
2	H	179/184 (97%)	153 (86%)	26 (14%)	3	12
3	L	185/186 (100%)	174 (94%)	11 (6%)	19	49
All	All	531/560 (95%)	480 (90%)	51 (10%)	8	29

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	350	VAL
1	E	375	SER
1	E	383	SER
1	E	390	LEU
1	E	403	ARG
1	E	405	ASP
1	E	443	SER
1	E	452	LEU
1	E	470	THR
1	E	477	SER
1	E	481	ASN
1	E	494	SER
1	E	514	SER
1	E	519	HIS
2	H	7	SER
2	H	25	SER
2	H	27	PHE
2	H	52	SER
2	H	57	THR
2	H	58	ILE
2	H	76	LYS
2	H	78	SER
2	H	79	LEU
2	H	89	GLU
2	H	111	GLN
2	H	113	THR
2	H	116	THR
2	H	119	SER
2	H	122	THR
2	H	126	SER
2	H	141	THR
2	H	146	CYS
2	H	156	VAL
2	H	159	SER
2	H	167	SER
2	H	185	SER
2	H	192	SER
2	H	195	LEU
2	H	202	CYS
2	H	203	ASN
3	L	1	GLN
3	L	8	PHE

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Mol	Chain	Res	Type
3	L	9	LEU
3	L	12	SER
3	L	28	SER
3	L	29	SER
3	L	70	THR
3	L	95	THR
3	L	112	SER
3	L	166	SER
3	L	201	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	158	GLN
3	L	208	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	NAG	E	601	1	14,14,15	0.62	0	17,19,21	1.41	1 (5%)

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	NAG	E	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	601	NAG	C1-O5-C5	4.40	118.16	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	E	194/217 (89%)	1.02	42 (21%) 0 1	111, 126, 154, 170	0
2	H	212/218 (97%)	0.97	34 (16%) 1 2	81, 121, 137, 201	0
3	L	213/214 (99%)	1.14	43 (20%) 1 1	30, 120, 162, 172	0
All	All	619/649 (95%)	1.04	119 (19%) 1 1	30, 123, 156, 201	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	115	ILE	6.0
2	H	105	LEU	5.7
1	E	492	LEU	5.4
1	E	452	LEU	5.3
3	L	146	TRP	5.2
2	H	36	TRP	5.1
1	E	456	PHE	4.8
1	E	489	TYR	4.7
1	E	423	TYR	4.5
1	E	341	VAL	4.5
2	H	86	LEU	4.4
1	E	334	ASN	4.3
1	E	365	TYR	4.3
3	L	207	PHE	4.2
3	L	190	TYR	4.1
3	L	116	PHE	4.0
3	L	179	LEU	4.0
2	H	160	TRP	3.9
1	E	453	TYR	3.9
1	E	358	ILE	3.9
1	E	338	PHE	3.9
2	H	55	GLY	3.7
1	E	351	TYR	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	451	TYR	3.7
3	L	92	TYR	3.6
3	L	166	SER	3.6
2	H	33	TYR	3.5
2	H	200	TYR	3.5
1	E	464	PHE	3.4
3	L	33	TRP	3.3
3	L	132	CYS	3.3
3	L	9	LEU	3.3
3	L	118	PRO	3.3
3	L	27	ILE	3.3
3	L	205	LYS	3.2
3	L	129	SER	3.2
2	H	99	ASP	3.1
2	H	158	VAL	3.1
1	E	380	TYR	3.1
3	L	185	GLU	3.1
3	L	144	VAL	3.0
1	E	377	PHE	3.0
2	H	81	LEU	3.0
3	L	94	LEU	3.0
2	H	117	VAL	2.9
3	L	192	CYS	2.9
3	L	182	ALA	2.9
2	H	118	SER	2.9
1	E	490	PHE	2.9
1	E	382	VAL	2.9
2	H	127	VAL	2.8
2	H	100	PHE	2.8
2	H	20	LEU	2.8
1	E	495	TYR	2.8
2	H	50	TYR	2.8
3	L	142	ALA	2.8
1	E	402	ILE	2.7
1	E	410	ILE	2.7
3	L	165	ASP	2.7
3	L	2	LEU	2.7
3	L	184	TYR	2.7
2	H	83	MET	2.6
3	L	131	VAL	2.6
2	H	147	LEU	2.6
3	L	206	SER	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	379	CYS	2.6
2	H	109	TRP	2.6
3	L	89	LEU	2.6
1	E	368	LEU	2.6
1	E	484	GLU	2.6
3	L	163	GLU	2.5
1	E	486	PHE	2.5
1	E	515	PHE	2.5
3	L	31	LEU	2.5
3	L	30	TYR	2.5
3	L	87	GLN	2.5
3	L	130	VAL	2.4
2	H	156	VAL	2.4
3	L	203	VAL	2.4
2	H	143	ALA	2.4
2	H	11	LEU	2.4
2	H	58	ILE	2.4
3	L	111	PRO	2.3
2	H	94	TYR	2.3
3	L	181	LYS	2.3
1	E	333	THR	2.3
1	E	401	VAL	2.3
1	E	496	GLY	2.3
1	E	356	LYS	2.3
1	E	347	PHE	2.3
1	E	395	VAL	2.3
1	E	392	PHE	2.3
3	L	0	ILE	2.3
2	H	194	SER	2.3
2	H	204	VAL	2.3
1	E	355	ARG	2.3
3	L	25	GLN	2.3
1	E	342	PHE	2.2
1	E	491	PRO	2.2
1	E	493	GLN	2.2
3	L	102	VAL	2.2
2	H	128	PHE	2.2
1	E	455	LEU	2.2
2	H	165	LEU	2.2
3	L	44	LEU	2.1
2	H	129	PRO	2.1
3	L	204	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	70	ILE	2.1
1	E	472	ILE	2.1
3	L	90	ASN	2.1
1	E	425	LEU	2.1
2	H	169	VAL	2.1
1	E	449	TYR	2.1
2	H	107	PRO	2.1
3	L	34	TYR	2.1
3	L	133	LEU	2.1
2	H	34	MET	2.1
1	E	511	VAL	2.0
2	H	4	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
4	NAG	E	601	14/15	0.70	0.32	141,146,149,149	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.