



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2024 – 10:08 PM JST

PDB ID : 8X0X  
Title : Crystal structure of JE-5C in complex with SARS-CoV-2 RBD  
Authors : Mohapatra, A.; Chen, X.  
Deposited on : 2023-11-06  
Resolution : 3.45 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
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) : 2.36.2

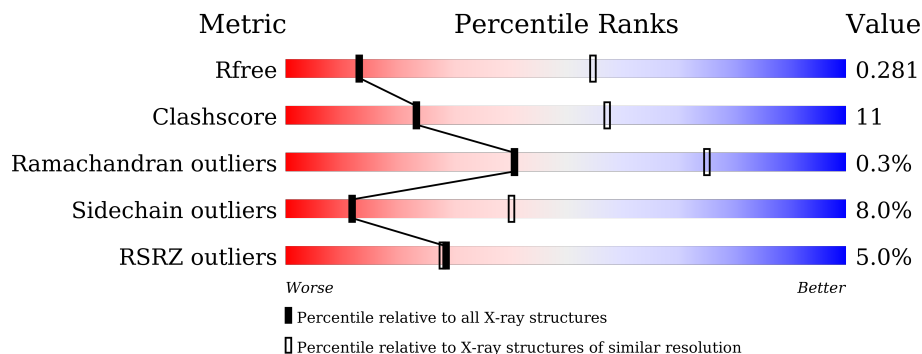
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 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	A	195	
1	E	195	
2	G	221	
2	H	221	
3	K	214	
3	L	214	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9497 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	193	1504	964	250	283	7	0	0	0
1	A	193	1515	973	249	286	7	0	0	0

- Molecule 2 is a protein called Heavy chain of JE-5C Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	218	1603	1003	273	320	7	0	0	0
2	H	218	1596	998	271	319	8	0	0	0

- Molecule 3 is a protein called Light chain of JE-5C Fab.

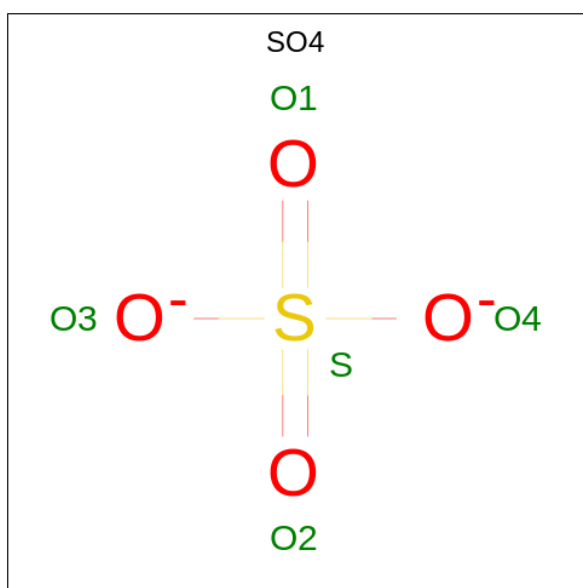
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	K	209	1611	1011	267	328	5	0	0	0
3	L	209	1620	1016	270	329	5	0	0	0

- 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
4	A	1	14	8	1	5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

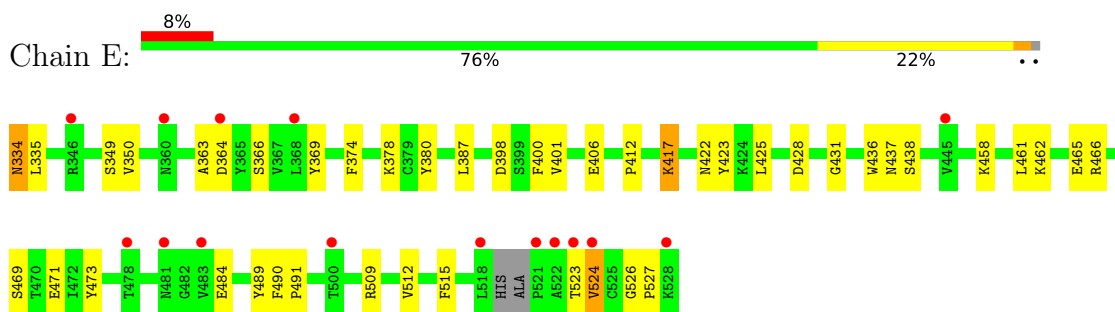
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	3	Total O 3 3	0	0
6	A	4	Total O 4 4	0	0
6	H	2	Total O 2 2	0	0
6	L	1	Total O 1 1	0	0

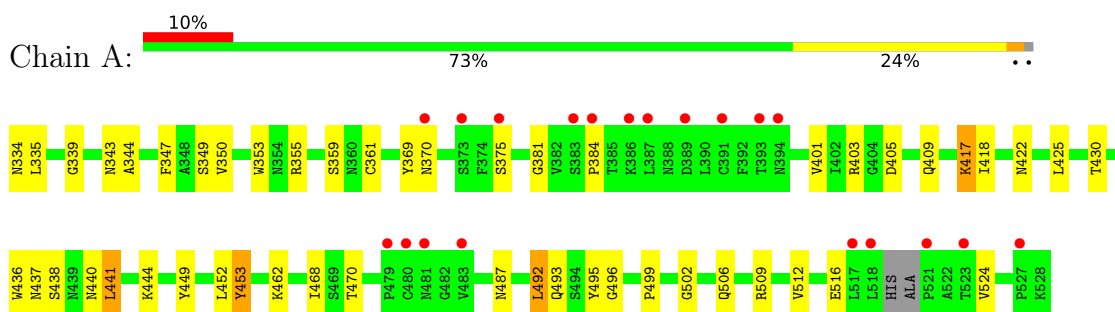
### 3 Residue-property plots [i](#)

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.

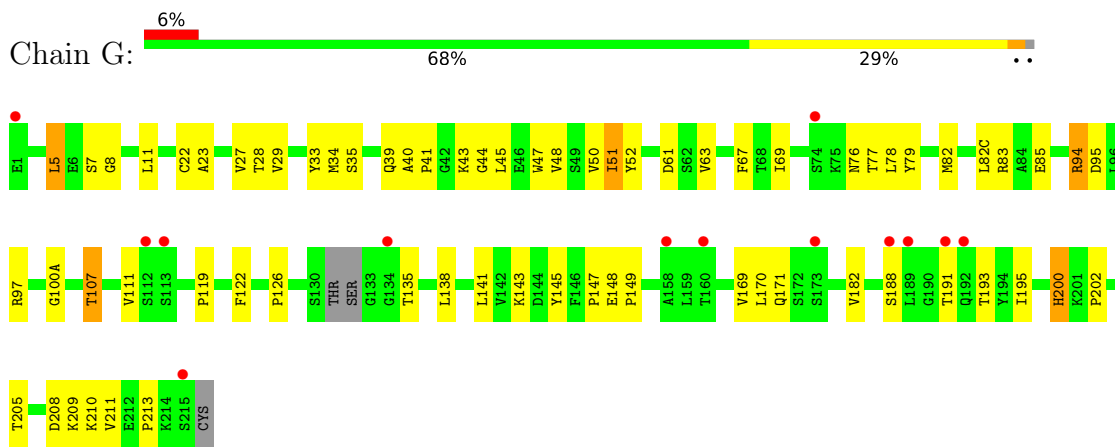
- Molecule 1: Spike protein S1



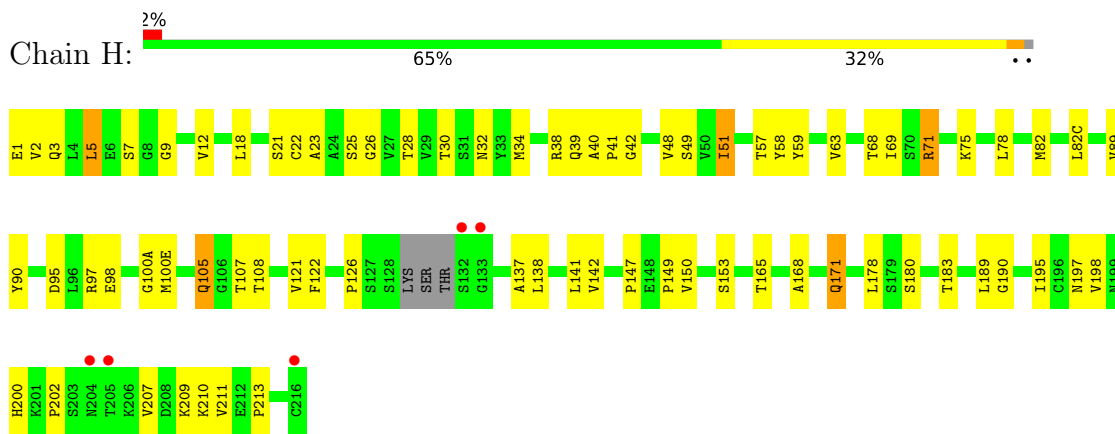
- Molecule 1: Spike protein S1



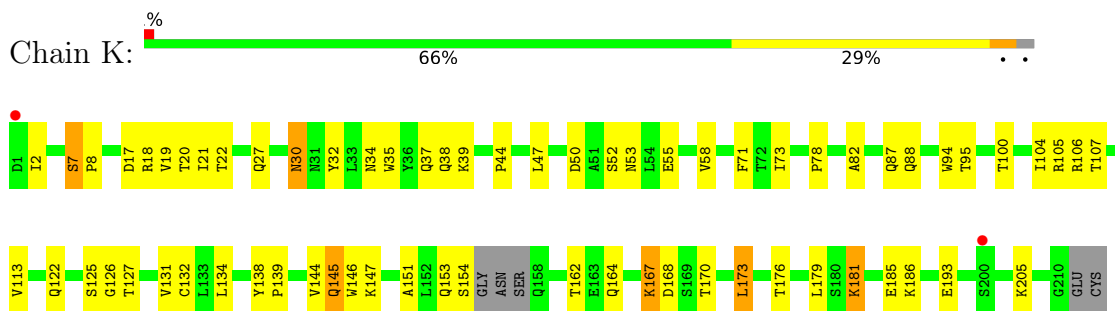
- Molecule 2: Heavy chain of JE-5C Fab



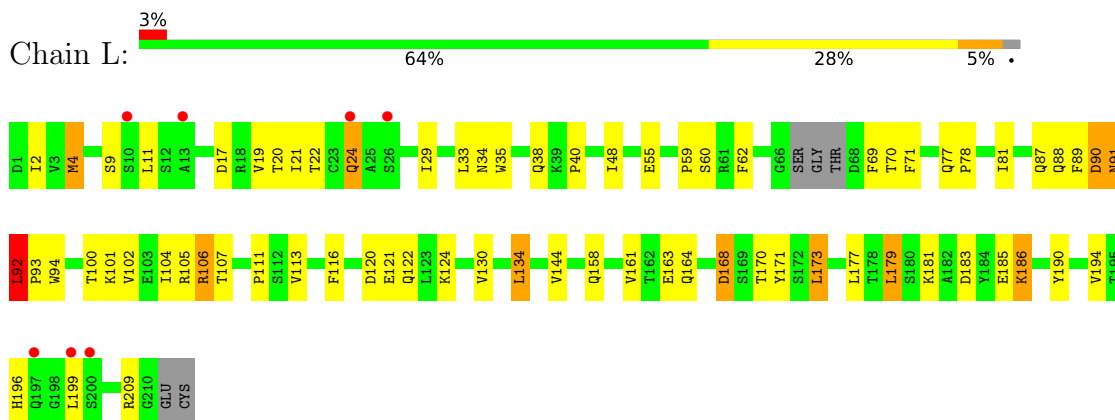
- Molecule 2: Heavy chain of JE-5C Fab



• Molecule 3: Light chain of JE-5C Fab



• Molecule 3: Light chain of JE-5C Fab



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.16Å 130.34Å 131.78Å 90.00° 105.19° 90.00°	Depositor
Resolution (Å)	36.38 – 3.45 36.38 – 3.45	Depositor EDS
% Data completeness (in resolution range)	91.3 (36.38-3.45) 91.3 (36.38-3.45)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 3.48Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.240 , 0.285 0.241 , 0.281	Depositor DCC
$R_{free}$ test set	1094 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtrriage
Anisotropy	0.958	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	9497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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, SO4

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	0.27	0/1557	0.50	0/2120
1	E	0.28	0/1546	0.49	0/2106
2	G	0.26	0/1637	0.53	0/2230
2	H	0.28	0/1630	0.56	0/2222
3	K	0.28	0/1646	0.53	0/2240
3	L	0.29	0/1655	0.56	0/2250
All	All	0.28	0/9671	0.53	0/13168

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	92	LEU	Peptide

### 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	1515	0	1419	33	0
1	E	1504	0	1393	24	1
2	G	1603	0	1567	39	0
2	H	1596	0	1553	48	0
3	K	1611	0	1543	37	0
3	L	1620	0	1559	47	1
4	A	14	0	13	2	0
4	E	14	0	13	0	0
5	E	10	0	0	0	0
6	A	4	0	0	0	0
6	E	3	0	0	0	0
6	H	2	0	0	0	0
6	L	1	0	0	0	0
All	All	9497	0	9060	210	1

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 11.

All (210) 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:113:VAL:HG11	3:L:194:VAL:HG21	1.65	0.78
2:H:34:MET:HB2	2:H:51:ILE:HD11	1.67	0.74
2:H:49:SER:HB2	2:H:69:ILE:HD11	1.70	0.72
2:G:23:ALA:HA	2:G:77:THR:HG22	1.70	0.72
1:A:453:TYR:HE1	1:A:493:GLN:HB3	1.54	0.72
1:A:381:GLY:HA3	1:A:430:THR:HA	1.72	0.71
3:L:113:VAL:HG12	3:L:134:LEU:HD22	1.71	0.71
2:G:43:LYS:HD3	2:G:44:GLY:H	1.56	0.70
3:K:113:VAL:O	3:K:205:LYS:NZ	2.24	0.69
3:K:106:ARG:HE	3:K:107:THR:HG22	1.57	0.69
1:E:380:TYR:HA	3:K:22:THR:HG21	1.74	0.68
3:L:121:GLU:HA	3:L:124:LYS:HE3	1.76	0.66
3:L:22:THR:HG22	3:L:70:THR:HG22	1.79	0.64
2:G:11:LEU:HD22	2:G:147:PRO:HD3	1.80	0.64
3:K:144:VAL:HG21	3:K:173:LEU:HD11	1.80	0.63
3:K:131:VAL:HG22	3:K:176:THR:HG22	1.79	0.63
3:L:106:ARG:HG2	3:L:107:THR:H	1.62	0.63
1:A:425:LEU:HD21	1:A:512:VAL:HG11	1.81	0.63
2:H:12:VAL:HG21	2:H:82(C):LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:138:LEU:HD23	2:G:182:VAL:HB	1.80	0.62
3:K:37:GLN:HB2	3:K:47:LEU:HD11	1.81	0.62
3:L:161:VAL:HG22	3:L:173:LEU:HB2	1.81	0.62
1:A:359:SER:HA	1:A:524:VAL:HG22	1.81	0.62
2:G:82:MET:HB3	2:G:82(C):LEU:HD21	1.82	0.61
2:G:35:SER:HB2	2:G:50:VAL:HG12	1.83	0.61
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.82	0.61
2:G:29:VAL:HG13	2:G:34:MET:HG3	1.83	0.60
2:G:34:MET:HB3	2:G:78:LEU:HD22	1.84	0.60
2:H:12:VAL:HG11	2:H:18:LEU:HB2	1.82	0.60
2:H:165:THR:HG22	2:H:180:SER:HB2	1.84	0.60
3:K:38:GLN:HG3	3:K:44:PRO:HG3	1.84	0.59
2:G:33:TYR:HB2	2:G:95:ASP:O	2.03	0.59
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.69	0.58
2:H:3:GLN:HB3	2:H:25:SER:HB2	1.85	0.58
3:L:134:LEU:HD11	3:L:144:VAL:HG22	1.85	0.58
2:G:28:THR:HA	2:G:76:ASN:HD21	1.69	0.58
2:G:195:ILE:HD11	2:G:208:ASP:HB3	1.84	0.58
3:L:106:ARG:HG2	3:L:107:THR:N	2.19	0.58
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.86	0.57
2:H:5:LEU:HA	2:H:105:GLN:HE22	1.70	0.57
2:H:100(A):GLY:HA3	3:L:34:ASN:ND2	2.20	0.56
2:H:2:VAL:HA	2:H:26:GLY:HA3	1.88	0.56
1:A:444:LYS:NZ	2:H:71:ARG:H	2.04	0.56
3:L:168:ASP:OD1	3:L:170:THR:OG1	2.20	0.55
3:L:40:PRO:HB3	3:L:163:GLU:HG3	1.88	0.55
1:A:403:ARG:HG3	1:A:495:TYR:CE1	2.42	0.54
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.90	0.54
1:E:406:GLU:OE2	1:E:417:LYS:HD2	2.08	0.54
1:E:526:GLY:H	1:E:527:PRO:HD2	1.72	0.54
2:G:8:GLY:O	2:G:107:THR:OG1	2.25	0.54
1:E:366:SER:HA	1:E:369:TYR:CZ	2.43	0.54
2:G:69:ILE:HD11	2:G:78:LEU:HD11	1.90	0.53
3:L:21:ILE:O	3:L:71:PHE:N	2.37	0.53
1:E:378:LYS:HG2	3:K:20:THR:HG21	1.90	0.53
2:G:100(A):GLY:HA3	3:K:34:ASN:ND2	2.22	0.53
3:L:81:ILE:HG13	3:L:104:ILE:HD12	1.91	0.53
2:H:5:LEU:O	2:H:23:ALA:N	2.41	0.52
2:H:95:ASP:HA	2:H:100(E):MET:H	1.74	0.52
2:H:9:GLY:HA3	2:H:18:LEU:HD11	1.91	0.52
3:L:111:PRO:HD3	3:L:196:HIS:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ASN:OD1	1:A:438:SER:N	2.42	0.52
3:L:111:PRO:HD2	3:L:199:LEU:HD23	1.91	0.52
3:K:145:GLN:HB3	3:K:193:GLU:HG2	1.91	0.52
2:G:119:PRO:HD2	2:G:205:THR:HG21	1.92	0.52
2:H:126:PRO:HD3	2:H:211:VAL:HG12	1.91	0.52
3:L:78:PRO:HA	3:L:104:ILE:HD13	1.92	0.52
3:L:130:VAL:HG23	3:L:177:LEU:HB3	1.92	0.52
3:L:91:ASN:O	3:L:92:LEU:C	2.47	0.52
1:E:350:VAL:HA	1:E:400:PHE:HB2	1.92	0.51
3:L:87:GLN:HG2	3:L:88:GLN:H	1.75	0.51
3:K:78:PRO:HB2	3:K:167:LYS:O	2.10	0.51
3:L:33:LEU:HD13	3:L:69:PHE:CG	2.46	0.51
1:A:343:ASN:HD22	4:A:601:NAG:C7	2.22	0.51
1:E:437:ASN:OD1	1:E:438:SER:N	2.44	0.51
1:A:449:TYR:HE1	1:A:496:GLY:HA2	1.76	0.51
3:L:11:LEU:HD22	3:L:102:VAL:HG13	1.92	0.51
1:A:409:GLN:HE22	1:A:417:LYS:HE3	1.76	0.51
1:A:487:ASN:OD1	2:G:94:ARG:NH2	2.39	0.51
1:A:369:TYR:CE2	1:A:384:PRO:HB3	2.46	0.51
2:H:7:SER:HB3	2:H:21:SER:HB2	1.93	0.50
2:H:49:SER:HG	2:H:59:TYR:HD2	1.59	0.50
3:K:122:GLN:O	3:K:125:SER:OG	2.27	0.50
3:L:21:ILE:HG12	3:L:100:THR:HG21	1.94	0.50
3:K:35:TRP:CE2	3:K:71:PHE:HB2	2.46	0.50
2:H:108:THR:OG1	2:H:149:PRO:HD3	2.11	0.50
3:K:146:TRP:HB2	3:K:153:GLN:HB2	1.93	0.50
2:H:147:PRO:O	2:H:200:HIS:NE2	2.37	0.50
2:H:121:VAL:HG22	2:H:142:VAL:HG22	1.93	0.50
3:L:181:LYS:O	3:L:185:GLU:HG2	2.12	0.50
2:H:28:THR:O	2:H:32:ASN:ND2	2.39	0.49
1:E:350:VAL:HG22	1:E:422:ASN:HB3	1.94	0.49
1:A:347:PHE:CE2	1:A:509:ARG:HB3	2.48	0.49
2:G:67:PHE:CZ	2:G:82:MET:HE3	2.47	0.49
3:L:40:PRO:CB	3:L:163:GLU:HG3	2.42	0.49
2:G:48:VAL:HG13	2:G:63:VAL:HG21	1.93	0.49
1:E:425:LEU:HD21	1:E:512:VAL:HG11	1.94	0.49
2:G:33:TYR:CD1	2:G:52:TYR:HA	2.47	0.49
3:K:2:ILE:O	3:K:95:THR:HG21	2.13	0.48
3:K:122:GLN:HG2	3:K:127:THR:O	2.13	0.48
1:E:374:PHE:HD1	1:E:436:TRP:HB3	1.78	0.48
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:21:ILE:HG12	3:K:100:THR:HG21	1.94	0.48
3:K:7:SER:HB3	3:K:22:THR:HB	1.95	0.48
2:H:82:MET:HB3	2:H:82(C):LEU:HD13	1.95	0.48
3:K:138:TYR:CD1	3:K:139:PRO:HA	2.49	0.48
1:A:417:LYS:HD3	2:G:97:ARG:HH22	1.78	0.48
3:L:35:TRP:CE2	3:L:71:PHE:HB2	2.49	0.48
2:G:119:PRO:HB3	2:G:145:TYR:HB3	1.95	0.47
1:E:431:GLY:HA2	1:E:515:PHE:CD2	2.49	0.47
2:H:126:PRO:HD2	2:H:213:PRO:HA	1.96	0.47
3:L:185:GLU:HA	3:L:209:ARG:NH1	2.30	0.47
1:E:473:TYR:N	1:E:489:TYR:O	2.43	0.47
3:K:39:LYS:H	3:K:82:ALA:HB1	1.79	0.47
2:H:3:GLN:N	2:H:25:SER:O	2.41	0.47
3:K:87:GLN:HG2	3:K:88:GLN:H	1.79	0.47
2:H:198:VAL:HB	2:H:207:VAL:HG23	1.97	0.46
1:A:449:TYR:CE1	1:A:496:GLY:HA2	2.50	0.46
3:K:19:VAL:HB	3:K:73:ILE:HB	1.96	0.46
3:K:47:LEU:HA	3:K:58:VAL:HG21	1.97	0.46
2:H:89:VAL:HA	2:H:108:THR:HA	1.97	0.46
2:H:195:ILE:HA	2:H:209:LYS:O	2.16	0.46
1:E:398:ASP:OD2	1:E:423:TYR:OH	2.34	0.46
2:G:27:VAL:O	2:G:76:ASN:ND2	2.49	0.46
1:A:375:SER:H	1:A:436:TRP:HA	1.81	0.46
3:K:30:ASN:C	3:K:32:TYR:N	2.70	0.46
2:H:48:VAL:HG13	2:H:63:VAL:HG21	1.98	0.46
1:A:444:LYS:O	1:A:499:PRO:HD3	2.16	0.45
2:G:169:VAL:HG13	3:K:162:THR:HG22	1.98	0.45
3:K:50:ASP:O	3:K:52:SER:N	2.44	0.45
2:H:51:ILE:HG22	2:H:57:THR:HG22	1.97	0.45
1:A:344:ALA:HB3	1:A:347:PHE:CE1	2.50	0.45
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.81	0.45
2:G:22:CYS:HB3	2:G:78:LEU:HB3	1.98	0.45
2:H:100(A):GLY:HA3	3:L:34:ASN:HD21	1.81	0.45
3:L:164:GLN:HG3	3:L:171:TYR:CE1	2.51	0.45
1:E:334:ASN:HD22	1:E:334:ASN:N	2.14	0.45
3:K:7:SER:HB3	3:K:8:PRO:HD3	1.99	0.45
1:E:462:LYS:HB2	1:E:465:GLU:OE1	2.16	0.45
1:A:470:THR:HG22	1:A:492:LEU:HD11	1.99	0.45
2:H:171:GLN:NE2	3:L:158:GLN:OE1	2.50	0.45
1:A:339:GLY:HA3	4:A:601:NAG:H82	1.98	0.45
1:E:401:VAL:HG22	1:E:509:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:105:ARG:HD3	3:K:138:TYR:OH	2.17	0.45
3:K:186:LYS:HE2	3:K:186:LYS:HB3	1.66	0.45
1:E:469:SER:OG	1:E:471:GLU:HG2	2.17	0.44
2:G:40:ALA:HB1	2:G:41:PRO:HD2	1.99	0.44
2:G:77:THR:HG1	2:G:79:TYR:HH	1.64	0.44
2:H:40:ALA:C	2:H:42:GLY:H	2.21	0.44
1:E:461:LEU:HD22	1:E:465:GLU:HG2	1.99	0.44
2:H:189:LEU:HD12	2:H:190:GLY:N	2.32	0.44
3:L:9:SER:HB3	3:L:101:LYS:HB3	2.00	0.44
2:H:3:GLN:O	2:H:25:SER:N	2.51	0.44
2:G:141:LEU:HD21	2:G:143:LYS:HD3	2.00	0.43
2:H:147:PRO:HD2	2:H:202:PRO:HB2	2.00	0.43
3:L:183:ASP:HA	3:L:186:LYS:HD2	2.00	0.43
2:G:39:GLN:HB2	2:G:45:LEU:HD23	2.00	0.43
2:G:50:VAL:HG11	3:K:94:TRP:CZ3	2.53	0.43
2:G:47:TRP:CZ2	2:G:50:VAL:HG13	2.53	0.43
2:G:191:THR:HG22	2:G:193:THR:HG23	2.00	0.43
3:K:35:TRP:CZ2	3:K:71:PHE:HB2	2.54	0.43
2:G:82(C):LEU:HD23	2:G:82(C):LEU:HA	1.82	0.43
2:G:126:PRO:HD2	2:G:213:PRO:HA	2.00	0.43
2:H:5:LEU:HA	2:H:5:LEU:HD12	1.85	0.43
3:L:163:GLU:CD	3:L:163:GLU:H	2.22	0.43
1:A:334:ASN:HB3	1:A:361:CYS:HA	2.01	0.43
3:K:126:GLY:HA2	3:K:181:LYS:HB3	2.00	0.43
3:K:138:TYR:CG	3:K:139:PRO:HA	2.54	0.43
2:H:58:TYR:CD1	3:L:92:LEU:HD13	2.54	0.43
1:A:405:ASP:OD1	1:A:405:ASP:N	2.51	0.43
3:K:132:CYS:HB2	3:K:146:TRP:CH2	2.53	0.43
2:H:39:GLN:NE2	3:L:38:GLN:OE1	2.51	0.43
1:A:444:LYS:HE2	1:A:444:LYS:HB3	1.85	0.43
2:H:150:VAL:HG12	2:H:178:LEU:HD21	2.01	0.43
2:G:148:GLU:HG2	2:G:149:PRO:HA	2.01	0.42
2:H:122:PHE:CE2	3:L:122:GLN:HG3	2.54	0.42
3:L:40:PRO:HD3	3:L:81:ILE:O	2.19	0.42
1:E:366:SER:HA	1:E:369:TYR:CE1	2.53	0.42
2:G:122:PHE:CE2	3:K:122:GLN:HG3	2.54	0.42
1:E:363:ALA:HB2	1:E:524:VAL:HG12	2.00	0.42
3:L:35:TRP:CZ2	3:L:71:PHE:HB2	2.54	0.42
3:L:179:LEU:HD11	3:L:190:TYR:HE2	1.84	0.42
1:A:353:TRP:HZ3	1:A:355:ARG:HE	1.66	0.42
2:G:51:ILE:HD13	2:G:51:ILE:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:ILE:HG13	3:L:90:ASP:HB3	2.01	0.42
1:E:335:LEU:HD22	1:E:364:ASP:HB2	2.01	0.42
1:A:349:SER:HB3	1:A:452:LEU:O	2.20	0.42
3:L:130:VAL:CG2	3:L:177:LEU:HB3	2.50	0.42
1:E:380:TYR:CZ	1:E:412:PRO:HD2	2.54	0.42
3:L:87:GLN:HG2	3:L:88:GLN:N	2.35	0.42
3:L:91:ASN:N	3:L:94:TRP:HZ3	2.17	0.42
1:A:449:TYR:HD2	2:H:68:THR:HG21	1.84	0.42
2:G:126:PRO:HD3	2:G:211:VAL:HG12	2.00	0.42
1:A:502:GLY:O	1:A:506:GLN:HG3	2.19	0.42
2:H:126:PRO:HG3	2:H:138:LEU:HB3	2.02	0.41
3:K:38:GLN:HA	3:K:44:PRO:HA	2.02	0.41
2:H:141:LEU:HD12	2:H:178:LEU:O	2.20	0.41
1:A:440:ASN:OD1	1:A:441:LEU:HG	2.20	0.41
2:G:200:HIS:ND1	2:G:202:PRO:HD2	2.35	0.41
3:L:59:PRO:HD2	3:L:62:PHE:CE1	2.56	0.41
1:E:417:LYS:H	1:E:417:LYS:HG3	1.73	0.41
1:E:490:PHE:CD1	1:E:491:PRO:HD2	2.55	0.41
1:A:350:VAL:HG22	1:A:422:ASN:HB3	2.03	0.41
2:H:137:ALA:O	3:L:116:PHE:HE1	2.04	0.41
3:L:4:MET:HA	3:L:24:GLN:O	2.21	0.41
1:A:444:LYS:HZ2	2:H:71:ARG:H	1.67	0.40
2:G:5:LEU:HG	2:G:23:ALA:HB3	2.04	0.40
2:H:153:SER:O	2:H:197:ASN:N	2.41	0.40
2:H:38:ARG:HD3	2:H:90:TYR:CE2	2.57	0.40
3:K:147:LYS:HG2	3:K:151:ALA:O	2.21	0.40
3:L:21:ILE:HB	3:L:71:PHE:HB3	2.03	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:GLU:OE2	3:L:60:SER:OG[2_656]	2.18	0.02

## 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	189/195 (97%)	175 (93%)	14 (7%)	0	100	100
1	E	189/195 (97%)	168 (89%)	20 (11%)	1 (0%)	29	66
2	G	214/221 (97%)	183 (86%)	31 (14%)	0	100	100
2	H	214/221 (97%)	186 (87%)	27 (13%)	1 (0%)	29	66
3	K	205/214 (96%)	181 (88%)	23 (11%)	1 (0%)	29	66
3	L	205/214 (96%)	182 (89%)	22 (11%)	1 (0%)	29	66
All	All	1216/1260 (96%)	1075 (88%)	137 (11%)	4 (0%)	41	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	7	SER
2	H	41	PRO
3	L	93	PRO
1	E	524	VAL

### 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	A	163/168 (97%)	154 (94%)	9 (6%)	21	53
1	E	159/168 (95%)	151 (95%)	8 (5%)	24	56
2	G	179/184 (97%)	163 (91%)	16 (9%)	9	36
2	H	178/184 (97%)	165 (93%)	13 (7%)	14	45
3	K	183/190 (96%)	165 (90%)	18 (10%)	8	31
3	L	185/190 (97%)	165 (89%)	20 (11%)	6	27
All	All	1047/1084 (97%)	963 (92%)	84 (8%)	12	40



All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	334	ASN
1	E	349	SER
1	E	387	LEU
1	E	417	LYS
1	E	428	ASP
1	E	458	LYS
1	E	466	ARG
1	E	523	THR
1	A	335	LEU
1	A	370	ASN
1	A	417	LYS
1	A	441	LEU
1	A	453	TYR
1	A	462	LYS
1	A	468	ILE
1	A	492	LEU
1	A	516	GLU
2	G	5	LEU
2	G	7	SER
2	G	51	ILE
2	G	61	ASP
2	G	83	ARG
2	G	85	GLU
2	G	94	ARG
2	G	107	THR
2	G	111	VAL
2	G	135	THR
2	G	170	LEU
2	G	171	GLN
2	G	188	SER
2	G	200	HIS
2	G	209	LYS
2	G	210	LYS
3	K	17	ASP
3	K	18	ARG
3	K	27	GLN
3	K	30	ASN
3	K	53	ASN
3	K	55	GLU
3	K	104	ILE
3	K	134	LEU
3	K	145	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	K	154	SER
3	K	164	GLN
3	K	167	LYS
3	K	168	ASP
3	K	170	THR
3	K	173	LEU
3	K	179	LEU
3	K	181	LYS
3	K	185	GLU
2	H	1	GLU
2	H	5	LEU
2	H	30	THR
2	H	51	ILE
2	H	71	ARG
2	H	75	LYS
2	H	97	ARG
2	H	98	GLU
2	H	105	GLN
2	H	107	THR
2	H	171	GLN
2	H	183	THR
2	H	210	LYS
3	L	4	MET
3	L	17	ASP
3	L	19	VAL
3	L	20	THR
3	L	24	GLN
3	L	29	ILE
3	L	55	GLU
3	L	77	GLN
3	L	89	PHE
3	L	90	ASP
3	L	91	ASN
3	L	92	LEU
3	L	105	ARG
3	L	106	ARG
3	L	120	ASP
3	L	134	LEU
3	L	168	ASP
3	L	173	LEU
3	L	179	LEU
3	L	186	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	105	GLN
2	H	171	GLN
3	L	91	ASN
3	L	158	GLN

### 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](#)

4 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	SO4	E	602	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	E	603	-	4,4,4	0.46	0	6,6,6	0.04	0
4	NAG	E	601	1	14,14,15	0.38	0	17,19,21	0.49	0
4	NAG	A	601	1	14,14,15	0.40	0	17,19,21	0.37	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	NAG	E	601	1	-	1/6/23/26	0/1/1/1
4	NAG	A	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	E	601	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAG	2	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	193/195 (98%)	0.56	20 (10%) 6 8	35, 62, 122, 133	0
1	E	193/195 (98%)	0.54	15 (7%) 13 15	39, 57, 102, 113	0
2	G	218/221 (98%)	0.36	13 (5%) 21 22	36, 55, 95, 112	0
2	H	218/221 (98%)	0.24	5 (2%) 60 58	37, 55, 80, 114	0
3	K	209/214 (97%)	0.23	2 (0%) 82 79	35, 55, 69, 82	0
3	L	209/214 (97%)	0.31	7 (3%) 46 44	41, 59, 78, 100	0
All	All	1240/1260 (98%)	0.37	62 (5%) 28 28	35, 56, 99, 133	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	LEU	7.0
1	A	521	PRO	6.0
3	K	1	ASP	5.0
2	H	132	SER	5.0
1	E	522	ALA	4.8
3	L	10	SER	4.7
1	E	521	PRO	4.4
1	E	478	THR	4.2
1	A	481	ASN	4.2
1	A	370	ASN	4.0
1	E	518	LEU	3.9
1	A	517	LEU	3.8
1	A	386	LYS	3.8
1	A	483	VAL	3.7
2	G	158	ALA	3.6
1	E	523	THR	3.4
1	A	527	PRO	3.4
1	A	391	CYS	3.4
1	A	389	ASP	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	192	GLN	3.3
1	A	383	SER	3.1
2	H	216	CYS	3.1
2	G	1	GLU	3.1
1	E	364	ASP	3.0
1	A	393	THR	3.0
2	G	215	SER	3.0
2	G	74	SER	3.0
1	A	523	THR	2.8
1	E	481	ASN	2.8
3	K	200	SER	2.8
1	A	384	PRO	2.8
2	G	188	SER	2.7
3	L	199	LEU	2.7
1	E	524	VAL	2.7
1	E	360	ASN	2.7
2	H	133	GLY	2.6
1	A	387	LEU	2.6
2	G	173	SER	2.6
1	E	368	LEU	2.6
2	G	112	SER	2.5
2	G	189	LEU	2.5
3	L	24	GLN	2.5
1	E	483	VAL	2.4
3	L	200	SER	2.4
3	L	26	SER	2.4
1	A	394	ASN	2.3
1	E	500	THR	2.3
2	G	113	SER	2.3
3	L	13	ALA	2.2
1	A	480	CYS	2.2
3	L	197	GLN	2.2
1	A	375	SER	2.2
1	E	346	ARG	2.2
2	H	204	ASN	2.2
2	G	160	THR	2.2
1	E	528	LYS	2.1
2	G	191	THR	2.1
1	A	479	PRO	2.1
2	G	134	GLY	2.1
1	A	373	SER	2.1
2	H	205	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	445	VAL	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	0.74	0.31	84,96,103,104	0
4	NAG	A	601	14/15	0.79	0.28	87,94,103,103	0
5	SO4	E	602	5/5	0.87	0.26	73,78,83,101	0
5	SO4	E	603	5/5	0.97	0.14	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.