



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2021 – 10:20 AM EDT

PDB ID : 7S0B
Title : Structure of the SARS-CoV-2 RBD in complex with neutralizing antibody N-612-056
Authors : Tanaka, S.; Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2021-08-30
Resolution : 2.90 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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	:	2.23.2
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)	:	2.23.2

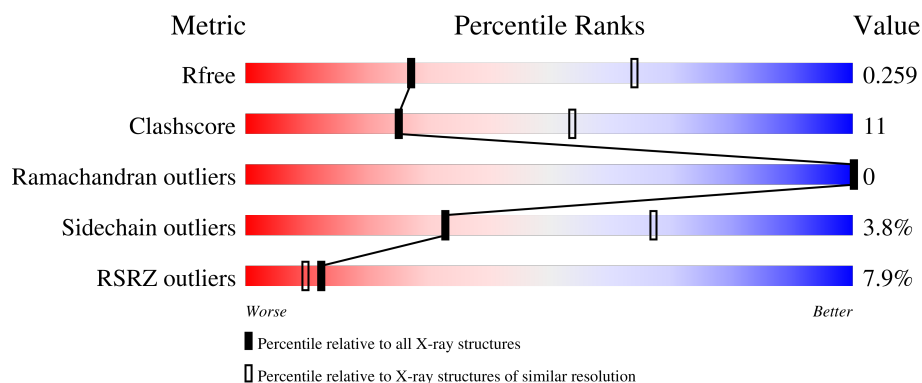
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 ≥ 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	228	<div> <div>8%</div> <div>75%</div> <div>19%</div> <div>• •</div> </div>
1	C	228	<div> <div>7%</div> <div>73%</div> <div>23%</div> <div>•</div> </div>
2	B	214	<div> <div>11%</div> <div>71%</div> <div>26%</div> <div>•</div> </div>
2	D	214	<div> <div>10%</div> <div>70%</div> <div>28%</div> <div>•</div> </div>
3	E	221	<div> <div>4%</div> <div>66%</div> <div>23%</div> <div>• 10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	221	<div><div></div><div>5%</div><div>67%</div><div>20%</div><div>10%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9828 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 N-612-056 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	5	1	0
			1621	1027	269	319	6			
1	C	219	Total	C	N	O	S	0	0	0
			1622	1027	270	319	6			

- Molecule 2 is a protein called N-612-056 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	6	2	0
			1640	1022	272	340	6			
2	D	213	Total	C	N	O	S	6	2	0
			1640	1022	272	340	6			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	199	Total	C	N	O	S	0	1	0
			1581	1013	264	296	8			
3	F	198	Total	C	N	O	S	0	1	0
			1571	1007	262	294	8			

There are 12 discrepancies between the modelled and reference sequences:

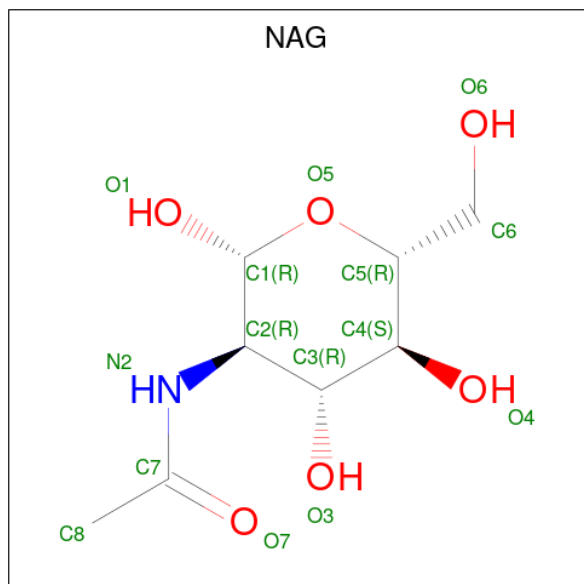
Chain	Residue	Modelled	Actual	Comment	Reference
E	534	HIS	-	expression tag	UNP P0DTC2
E	535	HIS	-	expression tag	UNP P0DTC2
E	536	HIS	-	expression tag	UNP P0DTC2
E	537	HIS	-	expression tag	UNP P0DTC2
E	538	HIS	-	expression tag	UNP P0DTC2
E	539	HIS	-	expression tag	UNP P0DTC2
F	534	HIS	-	expression tag	UNP P0DTC2
F	535	HIS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	536	HIS	-	expression tag	UNP P0DTC2
F	537	HIS	-	expression tag	UNP P0DTC2
F	538	HIS	-	expression tag	UNP P0DTC2
F	539	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	22	Total	O	0	0
			22	22		
5	C	11	Total	O	0	0
			11	11		
5	D	21	Total	O	0	0
			21	21		
5	E	24	Total	O	0	0
			24	24		

Continued on next page...

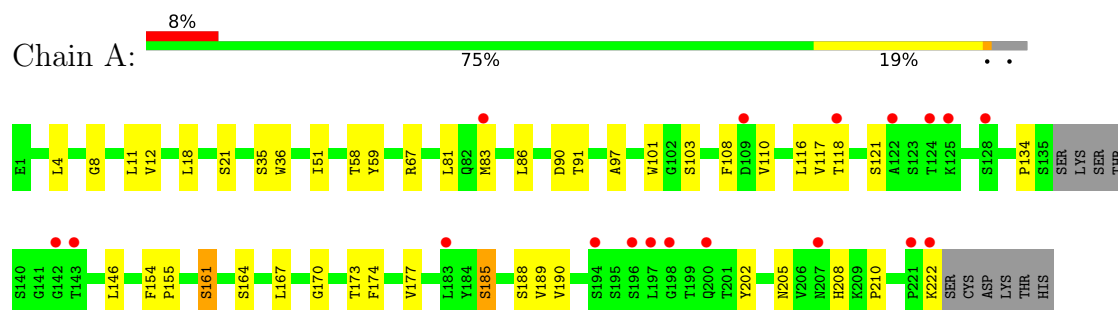
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	27	Total	O	0	0
			27	27		

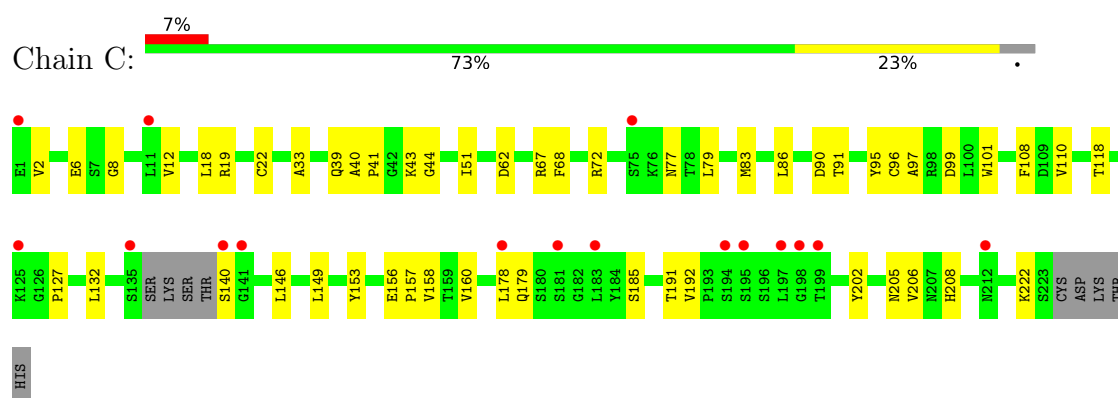
3 Residue-property plots

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.

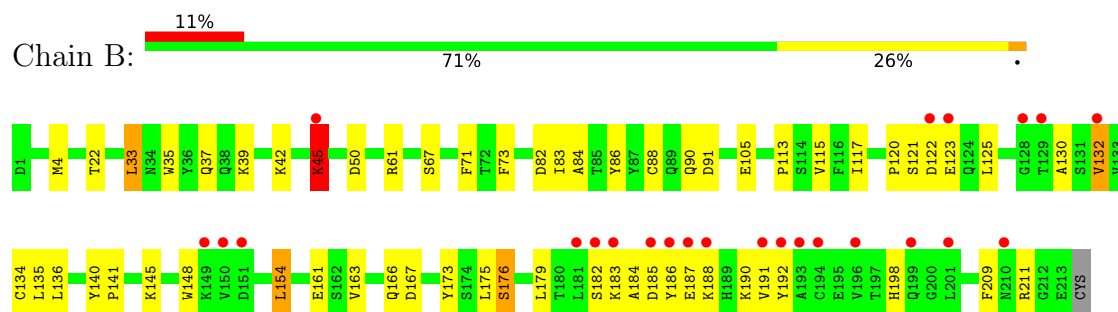
• Molecule 1: N-612-056 Fab Heavy Chain



• Molecule 1: N-612-056 Fab Heavy Chain

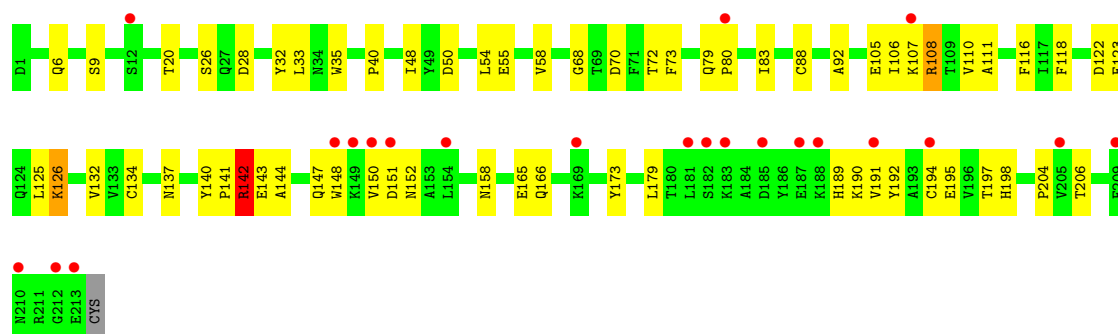


• Molecule 2: N-612-056 Light Chain

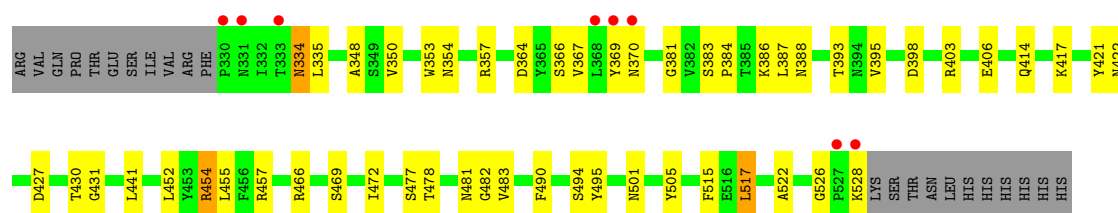


• Molecule 2: N-612-056 Light Chain

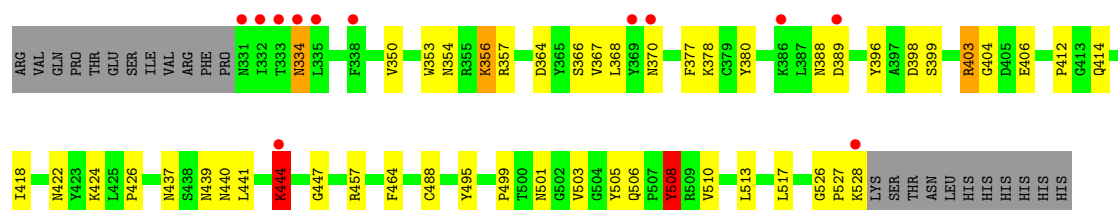




• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.30Å 153.66Å 96.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.41 – 2.90 38.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.41-2.90) 99.8 (38.96-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.215 , 0.260 0.218 , 0.259	Depositor DCC
R_{free} test set	1747 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9828	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7462e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	A	0.29	0/1663	0.57	0/2263
1	C	0.30	0/1661	0.56	0/2260
2	B	0.31	0/1679	0.66	3/2281 (0.1%)
2	D	0.33	0/1679	0.61	1/2281 (0.0%)
3	E	0.30	0/1626	0.54	1/2213 (0.0%)
3	F	0.36	1/1615 (0.1%)	0.64	4/2198 (0.2%)
All	All	0.32	1/9923 (0.0%)	0.60	9/13496 (0.1%)

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
2	D	0	1
3	F	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	508	TYR	CE2-CZ	-5.61	1.31	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	132	VAL	CG1-CB-CG2	10.39	127.53	110.90
3	F	508	TYR	CD1-CG-CD2	-6.82	110.40	117.90
3	F	444	LYS	CA-CB-CG	6.65	128.03	113.40
3	F	508	TYR	N-CA-CB	-6.20	99.44	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	45	LYS	CA-CB-CG	5.81	126.19	113.40
3	F	508	TYR	CB-CG-CD2	-5.79	117.53	121.00
2	B	154	LEU	CA-CB-CG	-5.73	102.12	115.30
2	D	143	GLU	CA-CB-CG	-5.66	100.95	113.40
3	E	517	LEU	CA-CB-CG	5.23	127.34	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	142	ARG	Sidechain
3	F	444	LYS	Peptide
3	F	508	TYR	Sidechain

5.2 Too-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 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	1621	0	1581	31	0
1	C	1622	0	1582	31	0
2	B	1640	0	1587	43	0
2	D	1640	0	1587	46	1
3	E	1581	0	1501	27	1
3	F	1571	0	1489	39	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
5	A	20	0	0	0	0
5	B	22	0	0	2	0
5	C	11	0	0	0	0
5	D	21	0	0	0	0
5	E	24	0	0	0	0
5	F	27	0	0	3	0
All	All	9828	0	9353	202	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 (202) 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:F:404:GLY:HA2	3:F:508:TYR:HD2	1.25	1.02
3:F:404:GLY:CA	3:F:508:TYR:HD2	1.77	0.97
1:A:164:SER:H	1:A:205:ASN:HD21	1.19	0.86
3:F:404:GLY:CA	3:F:508:TYR:CD2	2.58	0.86
2:D:105:GLU:OE1	2:D:173:TYR:OH	1.96	0.83
2:D:110:VAL:HG13	2:D:141:PRO:HD3	1.62	0.82
3:F:404:GLY:HA2	3:F:508:TYR:CD2	2.13	0.81
3:E:384:PRO:HA	3:E:387:LEU:HD12	1.66	0.78
2:B:122:ASP:HA	2:B:125:LEU:HD12	1.64	0.77
2:D:197:THR:HG22	2:D:204:PRO:HB3	1.67	0.76
2:B:161:GLU:HG2	2:B:175:LEU:HD11	1.68	0.74
2:B:42:LYS:NZ	5:B:302:HOH:O	2.19	0.74
3:F:444:LYS:O	3:F:499:PRO:HD3	1.87	0.74
3:F:503:VAL:HA	3:F:506:GLN:HG3	1.71	0.73
3:E:421:TYR:HB3	3:E:454:ARG:HG2	1.72	0.71
1:A:167:LEU:HD11	1:A:190:VAL:HG21	1.73	0.71
2:B:187:GLU:OE1	2:B:211:ARG:NH1	2.25	0.70
3:F:527:PRO:O	3:F:528:LYS:HB2	1.92	0.69
3:F:437:ASN:HA	3:F:508:TYR:CD1	2.28	0.69
1:A:189:VAL:HG11	2:B:135:LEU:HD22	1.74	0.68
2:B:91:ASP:OD1	5:B:301:HOH:O	2.11	0.68
3:F:388:ASN:HB3	3:F:527:PRO:HD2	1.75	0.68
2:D:144:ALA:HB2	2:D:198:HIS:HD2	1.59	0.68
1:A:222:LYS:NZ	2:B:122:ASP:OD2	2.24	0.67
3:F:404:GLY:HA3	3:F:508:TYR:CD2	2.27	0.67
2:B:163:VAL:HG22	2:B:175:LEU:HD13	1.77	0.67
3:F:403:ARG:HG2	3:F:495:TYR:CE1	2.32	0.65
2:B:182:SER:OG	2:B:185:ASP:OD2	2.15	0.65
2:D:144:ALA:HB2	2:D:198:HIS:CD2	2.32	0.65
3:F:404:GLY:HA3	3:F:508:TYR:CE2	2.34	0.63
2:D:190:LYS:HG2	2:D:191:VAL:HG23	1.80	0.63
2:B:123:GLU:OE1	2:B:123:GLU:N	2.26	0.63
3:F:437:ASN:HA	3:F:508:TYR:HD1	1.63	0.62
3:F:357:ARG:NH1	5:F:702:HOH:O	2.33	0.62
1:C:91:THR:HG23	1:C:118:THR:HA	1.81	0.62
1:C:132:LEU:HB3	2:D:118:PHE:CD1	2.35	0.61
1:C:127:PRO:HB3	1:C:153:TYR:HB3	1.83	0.61
2:D:132:VAL:HG22	2:D:179:LEU:HB3	1.83	0.60
2:D:20:THR:HG23	2:D:72:THR:HG23	1.82	0.60
1:C:97:ALA:HB1	1:C:108:PHE:HB3	1.82	0.60
3:F:366:SER:O	3:F:370:ASN:HB2	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ILE:HD13	2:B:166:GLN:HB3	1.84	0.59
2:B:154:LEU:CD1	2:D:197:THR:HG21	2.33	0.59
3:E:350:VAL:HG22	3:E:422:ASN:HB3	1.84	0.58
1:C:67:ARG:NH2	1:C:90:ASP:OD2	2.32	0.58
3:E:417:LYS:HE3	3:E:455:LEU:HD12	1.86	0.58
3:E:454:ARG:HD2	3:E:457:ARG:HD2	1.86	0.58
1:A:164:SER:H	1:A:205:ASN:ND2	1.97	0.57
2:B:187:GLU:O	2:B:211:ARG:NH2	2.38	0.56
1:C:12:VAL:HG21	1:C:86:LEU:HD13	1.87	0.56
1:C:146:LEU:HD21	1:C:202:TYR:HD1	1.70	0.56
3:F:378:LYS:HE2	3:F:380:TYR:OH	2.06	0.56
3:F:437:ASN:HB2	3:F:508:TYR:HE1	1.71	0.56
3:F:356:LYS:NZ	5:F:701:HOH:O	2.31	0.55
2:B:113:PRO:HD3	2:B:198:HIS:CD2	2.40	0.55
2:D:108:ARG:NH2	2:D:111:ALA:HB2	2.21	0.55
3:E:381:GLY:HA3	3:E:430:THR:HG22	1.88	0.55
1:C:8:GLY:O	1:C:18:LEU:HD21	2.07	0.55
3:E:366:SER:O	3:E:370:ASN:HB2	2.06	0.54
2:B:117:ILE:HG12	2:B:209:PHE:HD1	1.72	0.54
2:B:121:SER:HB2	2:B:123:GLU:OE1	2.06	0.53
2:D:80:PRO:HA	2:D:106:ILE:HD13	1.89	0.53
1:C:156:GLU:OE2	1:C:157:PRO:HA	2.08	0.53
1:A:67:ARG:NH2	1:A:90:ASP:OD2	2.42	0.53
2:B:132:VAL:HG23	2:B:179:LEU:O	2.09	0.52
1:A:4:LEU:HD12	1:A:110:VAL:HG12	1.92	0.52
2:B:140:TYR:CG	2:B:141:PRO:HA	2.45	0.52
2:B:37:GLN:HB3	2:B:45:LYS:HB3	1.92	0.51
1:A:8:GLY:O	1:A:18:LEU:HD21	2.10	0.51
2:B:4:MET:SD	2:B:90:GLN:HB3	2.50	0.51
2:B:105:GLU:OE2	2:B:173:TYR:OH	2.26	0.51
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.46	0.51
1:C:160:VAL:HG22	1:C:206:VAL:HG22	1.92	0.50
1:C:18:LEU:HD23	1:C:19:ARG:N	2.25	0.50
2:D:83:ILE:HG13	2:D:106:ILE:HD12	1.93	0.50
1:A:12:VAL:HG21	1:A:86:LEU:HD12	1.91	0.50
1:C:40:ALA:HB3	1:C:43:LYS:HG3	1.94	0.50
1:A:97:ALA:HB1	1:A:108:PHE:HB3	1.93	0.49
2:B:136:LEU:HB2	2:B:175:LEU:HB3	1.94	0.49
2:D:80:PRO:HA	2:D:106:ILE:CD1	2.42	0.49
3:F:403:ARG:HG3	3:F:406:GLU:HG3	1.93	0.49
1:A:146:LEU:HD21	1:A:202:TYR:CD2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:403:ARG:HG2	3:F:495:TYR:HE1	1.78	0.49
2:B:136:LEU:HD12	2:B:175:LEU:HD23	1.94	0.49
2:D:150:VAL:HG13	2:D:192:TYR:HE1	1.77	0.49
2:B:190:LYS:HG3	2:B:191:VAL:N	2.28	0.48
2:D:79:GLN:NE2	2:D:79:GLN:HA	2.28	0.48
2:D:134:CYS:HB2	2:D:148:TRP:CH2	2.48	0.48
1:C:146:LEU:HA	2:D:118:PHE:HE1	1.78	0.48
2:B:37:GLN:O	2:B:45:LYS:N	2.46	0.48
1:A:146:LEU:HD21	1:A:202:TYR:HD2	1.78	0.48
2:D:79:GLN:HA	2:D:79:GLN:HE21	1.78	0.48
2:D:140:TYR:CG	2:D:141:PRO:HA	2.49	0.48
2:D:83:ILE:HD13	2:D:166:GLN:HB3	1.95	0.48
1:A:51:ILE:HG13	1:A:58:THR:HG22	1.95	0.48
1:C:222:LYS:NZ	2:D:122:ASP:OD2	2.44	0.48
2:D:126:LYS:O	2:D:126:LYS:HD2	2.14	0.47
3:E:364:ASP:OD2	3:E:366:SER:OG	2.22	0.47
1:C:6:GLU:OE1	1:C:95:TYR:HA	2.15	0.47
2:D:40:PRO:HB3	2:D:165:GLU:HG3	1.95	0.47
1:C:51:ILE:HD13	1:C:72:ARG:HD2	1.97	0.47
2:D:142:ARG:HG2	2:D:173:TYR:CZ	2.49	0.47
2:B:140:TYR:CD1	2:B:141:PRO:HA	2.50	0.47
3:E:393:THR:HA	3:E:522:ALA:HA	1.96	0.47
2:B:67:SER:HA	2:B:71:PHE:CE2	2.50	0.47
3:E:334:ASN:OD1	3:E:334:ASN:N	2.48	0.47
3:E:414:GLN:OE1	3:E:414:GLN:HA	2.14	0.47
1:A:103:SER:OG	3:F:464:PHE:O	2.24	0.46
3:F:488:CYS:SG	5:F:718:HOH:O	2.61	0.46
2:D:166:GLN:HG3	2:D:173:TYR:CZ	2.50	0.46
2:D:195:GLU:HG3	2:D:206:THR:OG1	2.15	0.46
3:E:403:ARG:HG3	3:E:406:GLU:HG3	1.97	0.46
2:B:22:THR:OG1	2:D:70:ASP:HB2	2.15	0.46
1:A:134:PRO:HG3	1:A:146:LEU:HB3	1.97	0.46
3:E:403:ARG:HG2	3:E:495:TYR:CE1	2.51	0.46
2:B:33:LEU:O	2:B:50:ASP:O	2.34	0.46
1:C:191:THR:HG21	2:D:137:ASN:ND2	2.31	0.46
1:C:192:VAL:HG21	1:C:202:TYR:CE1	2.51	0.46
1:C:140:SER:HB3	2:D:116:PHE:CE2	2.51	0.45
3:E:452:LEU:HD23	3:E:494:SER:HA	1.98	0.45
2:D:151:ASP:OD2	2:D:189:HIS:ND1	2.49	0.45
3:E:388:ASN:O	3:E:526:GLY:HA3	2.16	0.45
2:D:54:LEU:HD11	2:D:58:VAL:HB	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:ASP:OD1	2:D:68:GLY:HA2	2.17	0.45
1:A:36:TRP:NE1	1:A:81:LEU:HB2	2.32	0.45
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.99	0.45
3:F:354:ASN:O	3:F:398:ASP:HA	2.17	0.45
3:F:364:ASP:O	3:F:367:VAL:HG22	2.17	0.45
1:A:11:LEU:HD12	1:A:12:VAL:N	2.32	0.45
1:C:158:VAL:HG12	1:C:208:HIS:CD2	2.51	0.45
1:A:208:HIS:CE1	1:A:210:PRO:HG2	2.52	0.44
1:C:22:CYS:HB3	1:C:79:LEU:HB3	1.98	0.44
3:E:483:VAL:CG2	3:E:490:PHE:HB2	2.47	0.44
1:A:116:LEU:HD12	1:A:117:VAL:N	2.33	0.44
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.52	0.44
1:C:12:VAL:CG1	1:C:18:LEU:HD12	2.48	0.44
2:D:123:GLU:H	2:D:123:GLU:CD	2.21	0.44
3:F:399:SER:HA	3:F:510:VAL:O	2.18	0.44
2:B:186:TYR:CE1	2:B:192:TYR:HE1	2.36	0.44
3:E:364:ASP:O	3:E:367:VAL:HG22	2.17	0.44
1:A:161:SER:HG	1:A:205:ASN:HD22	1.62	0.44
3:F:388:ASN:O	3:F:526:GLY:HA3	2.18	0.44
2:B:145:LYS:HD2	2:B:145:LYS:HA	1.79	0.44
2:B:154:LEU:HD12	2:D:197:THR:HG21	1.99	0.44
1:C:67:ARG:HH22	1:C:90:ASP:CG	2.21	0.44
3:F:444:LYS:HG3	3:F:447:GLY:O	2.17	0.44
1:C:101:TRP:CH2	3:E:357:ARG:HB2	2.53	0.43
3:E:354:ASN:O	3:E:398:ASP:HA	2.17	0.43
3:F:440:ASN:OD1	3:F:440:ASN:N	2.49	0.43
1:C:39:GLN:HG3	1:C:44:GLY:O	2.18	0.43
2:D:108:ARG:HH21	2:D:111:ALA:HB2	1.82	0.43
2:B:120:PRO:HG3	2:B:130:ALA:HB1	2.00	0.43
2:D:55:GLU:O	2:D:58:VAL:HG23	2.19	0.43
3:E:395:VAL:HG22	3:E:515:PHE:HD1	1.84	0.43
2:D:35:TRP:CE2	2:D:73:PHE:HB2	2.54	0.43
2:D:142:ARG:HG2	2:D:173:TYR:CE2	2.54	0.43
3:F:334:ASN:OD1	3:F:334:ASN:N	2.51	0.43
3:F:439:ASN:ND2	3:F:506:GLN:OE1	2.51	0.43
2:D:33:LEU:O	2:D:50:ASP:O	2.37	0.42
3:E:366:SER:HA	3:E:369:TYR:CE1	2.53	0.42
2:B:183:LYS:NZ	2:B:187:GLU:OE2	2.45	0.42
2:B:115:VAL:HG22	2:B:136:LEU:HD22	2.01	0.42
2:D:158:ASN:OD1	2:D:158:ASN:N	2.51	0.42
1:A:67:ARG:HH22	1:A:90:ASP:CG	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:TRP:HB2	2:D:48:ILE:HB	1.99	0.42
3:E:501:ASN:HB3	3:E:505:TYR:HB2	2.02	0.42
3:F:418:ILE:HA	3:F:422:ASN:HD22	1.85	0.42
2:B:37:GLN:NE2	2:B:86:TYR:OH	2.52	0.42
2:B:61:ARG:NH2	2:B:82:ASP:OD1	2.47	0.42
1:A:59:TYR:OH	3:F:457:ARG:NH2	2.52	0.42
1:A:91:THR:HG23	1:A:118:THR:HA	2.01	0.42
1:A:101:TRP:CH2	3:F:357:ARG:HB2	2.55	0.42
3:F:414:GLN:O	3:F:424:LYS:NZ	2.50	0.42
3:F:350:VAL:O	3:F:353:TRP:HD1	2.03	0.42
2:B:184:ALA:O	2:B:188:LYS:HG3	2.20	0.42
2:D:122:ASP:HA	2:D:125:LEU:HD12	2.02	0.42
3:F:367:VAL:HG23	3:F:368:LEU:HD22	2.02	0.42
1:A:154:PHE:HA	1:A:155:PRO:HA	1.88	0.41
1:A:174:PHE:CE2	2:B:176:SER:HB3	2.55	0.41
2:B:35:TRP:CE2	2:B:73:PHE:HB2	2.55	0.41
1:A:173:THR:HG23	1:A:188:SER:HB2	2.01	0.41
2:D:32:TYR:HB2	2:D:92:ALA:HB2	2.03	0.41
3:E:472:ILE:HG13	3:E:482:GLY:HA2	2.03	0.41
1:A:161:SER:OG	1:A:205:ASN:ND2	2.35	0.41
1:C:2:VAL:HG21	1:C:110:VAL:HG21	2.03	0.41
1:C:6:GLU:HG2	1:C:96:CYS:SG	2.61	0.41
3:F:501:ASN:HB3	3:F:505:TYR:HB2	2.03	0.41
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.56	0.41
1:C:33:ALA:HB3	1:C:99:ASP:HB2	2.03	0.41
1:C:68:PHE:CE1	1:C:83:MET:HB3	2.56	0.41
1:C:132:LEU:HD11	1:C:149:LEU:HB2	2.02	0.41
3:E:528:LYS:HE2	3:E:528:LYS:HB3	1.80	0.41
3:F:396:TYR:O	3:F:513:LEU:HA	2.21	0.41
1:A:170:GLY:O	1:A:190:VAL:HA	2.21	0.41
2:B:39:LYS:HG2	2:B:84:ALA:HB2	2.03	0.40
2:D:6:GLN:HE21	2:D:6:GLN:HB3	1.72	0.40
1:A:177:VAL:HG22	1:A:185:SER:O	2.21	0.40
1:C:178:LEU:HD13	1:C:179:GLN:O	2.22	0.40
3:E:353:TRP:CE2	3:E:466:ARG:HD2	2.57	0.40
3:E:431:GLY:HA2	3:E:515:PHE:CE2	2.56	0.40
3:F:412:PRO:HB3	3:F:426:PRO:O	2.22	0.40
3:E:348:ALA:HB2	3:E:354:ASN:ND2	2.36	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)
2:D:26:SER:OG	3:E:481:ASN:ND2[2_455]	2.11	0.09

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	215/228 (94%)	204 (95%)	11 (5%)	0	100	100
1	C	215/228 (94%)	208 (97%)	7 (3%)	0	100	100
2	B	213/214 (100%)	202 (95%)	11 (5%)	0	100	100
2	D	213/214 (100%)	203 (95%)	10 (5%)	0	100	100
3	E	198/221 (90%)	184 (93%)	14 (7%)	0	100	100
3	F	197/221 (89%)	184 (93%)	13 (7%)	0	100	100
All	All	1251/1326 (94%)	1185 (95%)	66 (5%)	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	A	180/189 (95%)	175 (97%)	5 (3%)	43	76
1	C	180/189 (95%)	175 (97%)	5 (3%)	43	76
2	B	189/188 (100%)	185 (98%)	4 (2%)	53	81
2	D	189/188 (100%)	180 (95%)	9 (5%)	25	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	173/194 (89%)	162 (94%)	11 (6%)	17	45
3	F	171/194 (88%)	163 (95%)	8 (5%)	26	59
All	All	1082/1142 (95%)	1040 (96%)	42 (4%)	33	66

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	35	SER
1	A	121	SER
1	A	161	SER
1	A	185	SER
2	B	33	LEU
2	B	45	LYS
2	B	167	ASP
2	B	176	SER
1	C	41	PRO
1	C	62	ASP
1	C	77	ASN
1	C	185	SER
1	C	205	ASN
2	D	9	SER
2	D	107	LYS
2	D	108	ARG
2	D	126	LYS
2	D	142	ARG
2	D	147	GLN
2	D	152	ASN
2	D	194[A]	CYS
2	D	194[B]	CYS
3	E	334	ASN
3	E	335	LEU
3	E	383	SER
3	E	386	LYS
3	E	427	ASP
3	E	441	LEU
3	E	454	ARG
3	E	469	SER
3	E	477	SER
3	E	478	THR
3	E	517	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	334	ASN
3	F	356	LYS
3	F	377	PHE
3	F	389	ASP
3	F	403	ARG
3	F	441	LEU
3	F	508	TYR
3	F	517	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
2	B	37	GLN
1	C	3	GLN
1	C	77	ASN
2	D	79	GLN
3	E	354	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](#)

2 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	$\# Z > 2$
4	NAG	E	601	3	14,14,15	0.37	0	17,19,21	0.57	0
4	NAG	F	601	3	14,14,15	0.26	0	17,19,21	0.43	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	3	-	2/6/23/26	0/1/1/1
4	NAG	F	601	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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, 95th 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 ²)	Q<0.9
1	A	218/228 (95%)	0.48	18 (8%) 11 8	45, 72, 114, 150	0
1	C	219/228 (96%)	0.47	16 (7%) 15 11	45, 71, 114, 164	0
2	B	213/214 (99%)	0.71	24 (11%) 5 4	41, 73, 137, 168	0
2	D	213/214 (99%)	0.71	22 (10%) 6 5	44, 71, 128, 175	0
3	E	199/221 (90%)	0.36	8 (4%) 38 33	43, 61, 95, 155	0
3	F	198/221 (89%)	0.34	12 (6%) 21 17	45, 63, 102, 136	0
All	All	1260/1326 (95%)	0.52	100 (7%) 12 10	41, 69, 123, 175	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	369	TYR	8.6
2	D	213	GLU	6.0
3	E	331	ASN	5.6
2	B	122	ASP	5.5
2	B	150	VAL	5.4
2	B	194[A]	CYS	5.1
2	D	194[A]	CYS	4.7
1	A	197	LEU	4.7
2	B	149	LYS	4.5
3	F	335	LEU	4.4
3	F	333	THR	4.4
2	D	151	ASP	4.2
2	B	151	ASP	3.9
1	C	135	SER	3.9
1	C	198	GLY	3.8
2	B	191	VAL	3.8
3	F	369	TYR	3.8
3	E	368	LEU	3.7
3	E	330	PRO	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	187	GLU	3.6
2	D	187	GLU	3.6
2	D	150	VAL	3.4
2	D	154	LEU	3.3
2	D	149	LYS	3.3
1	A	124	THR	3.3
1	C	141	GLY	3.3
1	C	140	SER	3.3
3	E	528	LYS	3.3
2	D	12	SER	3.3
3	F	370	ASN	3.3
3	F	332	ILE	3.2
2	B	199	GLN	3.1
2	B	210	ASN	3.1
2	D	181	LEU	3.0
3	F	528	LYS	3.0
1	C	183	LEU	2.9
2	B	45	LYS	2.9
2	B	192	TYR	2.9
1	A	128	SER	2.9
2	B	186	TYR	2.9
1	C	125	LYS	2.9
1	A	125	LYS	2.8
1	C	197	LEU	2.8
1	C	194	SER	2.8
2	B	181	LEU	2.8
1	A	222	LYS	2.8
1	C	195	SER	2.7
2	D	205	VAL	2.7
2	B	182	SER	2.6
2	B	196	VAL	2.6
2	B	201	LEU	2.6
1	A	183	LEU	2.6
2	B	188	LYS	2.6
3	F	389	ASP	2.5
1	A	122	ALA	2.5
2	B	128	GLY	2.5
3	E	370	ASN	2.5
1	C	181	SER	2.5
1	A	196	SER	2.5
2	D	148	TRP	2.5
3	F	444	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	142	GLY	2.4
3	E	333	THR	2.4
2	D	182	SER	2.4
1	A	194	SER	2.4
1	C	178	LEU	2.4
2	D	188	LYS	2.4
3	F	331	ASN	2.4
2	D	191	VAL	2.4
2	D	212	GLY	2.4
2	B	183	LYS	2.3
1	A	143	THR	2.3
2	D	209	PHE	2.3
1	C	11	LEU	2.3
1	A	198	GLY	2.3
2	D	107	LYS	2.3
1	C	199	THR	2.3
1	A	207	ASN	2.3
2	B	132	VAL	2.3
2	D	210	ASN	2.3
2	B	193	ALA	2.3
1	A	118	THR	2.2
1	A	221	PRO	2.2
2	D	169	LYS	2.2
3	F	386	LYS	2.2
2	D	185	ASP	2.2
1	C	212	ASN	2.1
3	E	527	PRO	2.1
1	A	109[A]	ASP	2.1
1	A	200	GLN	2.1
1	A	83	MET	2.1
3	F	334	ASN	2.1
2	B	123	GLU	2.1
1	C	1	GLU	2.1
2	D	183	LYS	2.1
2	B	129	THR	2.0
1	C	75	SER	2.0
3	F	338	PHE	2.0
2	B	185	ASP	2.0
2	D	80	PRO	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](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.