



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2026 – 03:36 PM JST

PDB ID : 9LF5 / pdb_00009lf5
Title : Complex structure of THC-4677 and THC-4881 Fab bound to SARS-CoV-2
WT RBD
Authors : Wang, X.; Guo, F.
Deposited on : 2025-01-08
Resolution : 2.95 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

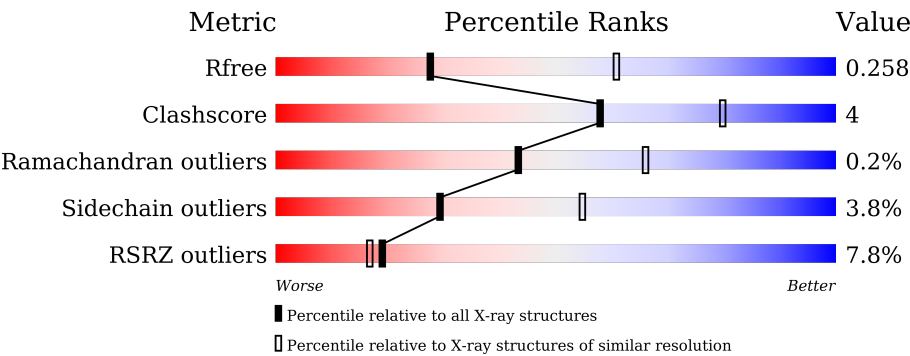
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	194	8% 88% 12%
1	B	194	11% 90% 9% .
2	C	227	12% 81% 17% .
2	E	227	10% 84% 14% ..
3	D	221	6% 91% 8% .
3	F	221	6% 89% 11%

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Mol	Chain	Length	Quality of chain
4	G	238	7% 84% 16%
4	H	238	7% 83% 16%
5	I	214	6% 91% 7%
5	J	214	6% 86% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16853 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
1	A	194	Total	C	N	O	S	0	0	0
			1536	984	256	288	8			
1	B	194	Total	C	N	O	S	0	0	0
			1536	984	256	288	8			

- Molecule 2 is a protein called THC-4677 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	225	Total	C	N	O	S	0	0	0
			1703	1082	283	331	7			
2	C	227	Total	C	N	O	S	0	0	0
			1720	1092	286	335	7			

- Molecule 3 is a protein called THC-4677 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	221	Total	C	N	O	S	0	0	0
			1699	1065	284	344	6			
3	D	221	Total	C	N	O	S	0	0	0
			1699	1065	284	344	6			

- Molecule 4 is a protein called THC-4881 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	238	Total	C	N	O	S	0	0	0
			1814	1146	305	356	7			
4	H	238	Total	C	N	O	S	0	0	0
			1814	1146	305	356	7			

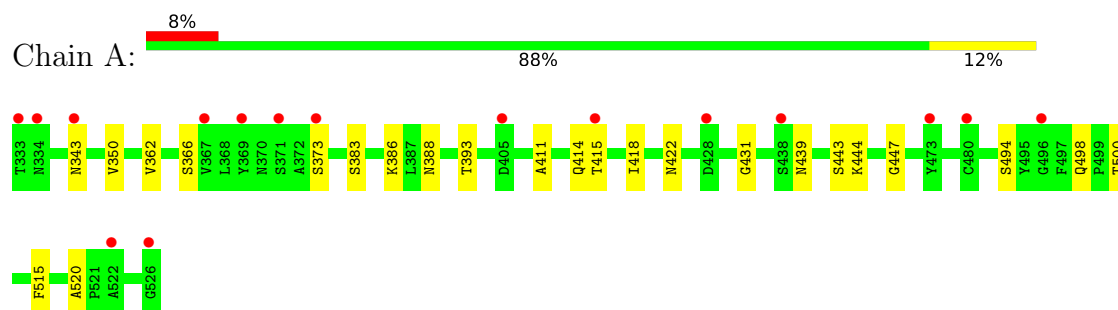
- Molecule 5 is a protein called THC-4881 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	214	Total 1666	C 1046	N 279	O 336	S 5	0	0	0
5	I	214	Total 1666	C 1046	N 279	O 336	S 5	0	0	0

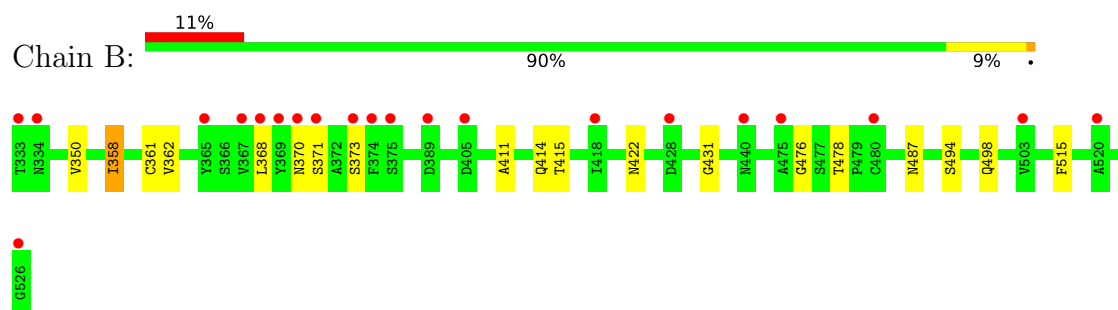
3 Residue-property plots [i](#)

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.

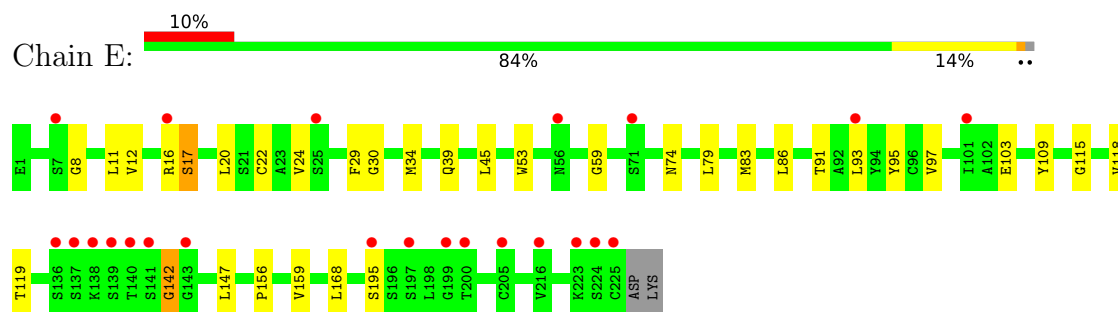
- Molecule 1: Spike protein S1



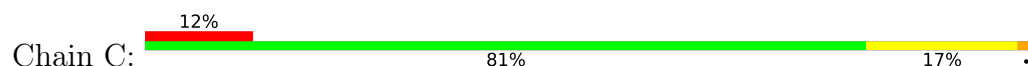
- Molecule 1: Spike protein S1

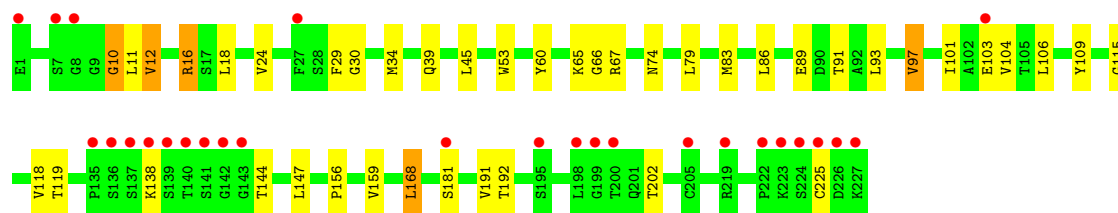


- Molecule 2: THC-4677 Heavy chain

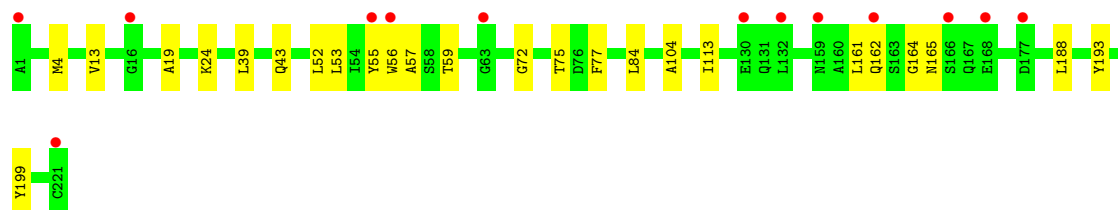
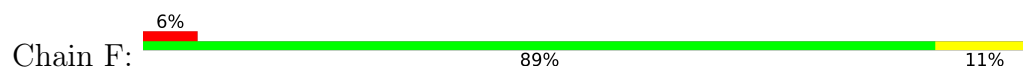


- Molecule 2: THC-4677 Heavy chain

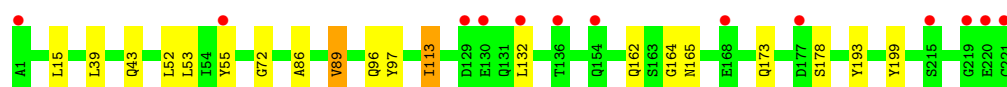




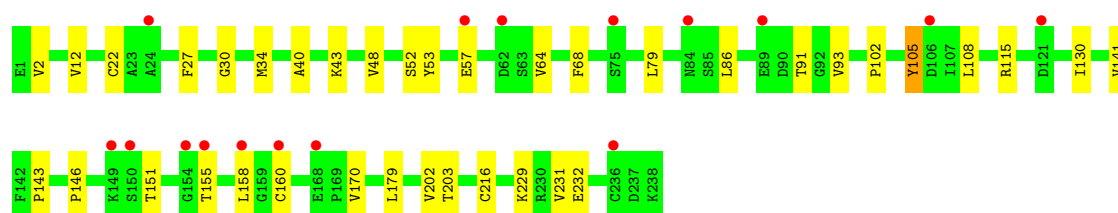
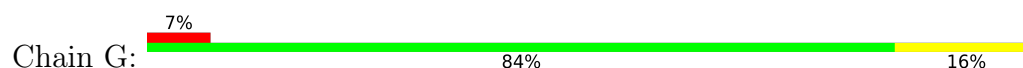
• Molecule 3: THC-4677 Light chain



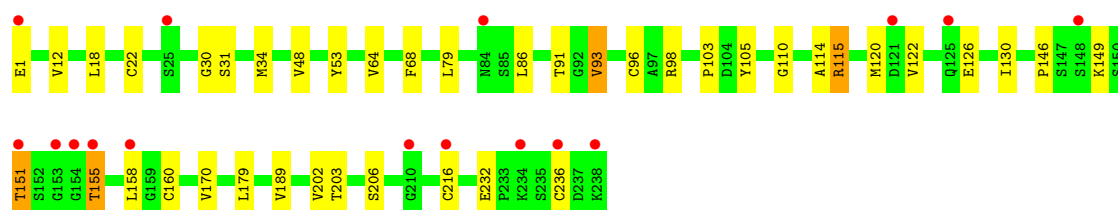
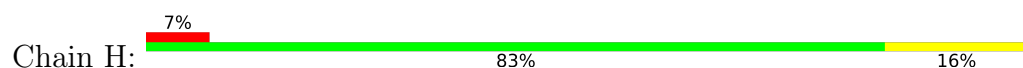
• Molecule 3: THC-4677 Light chain



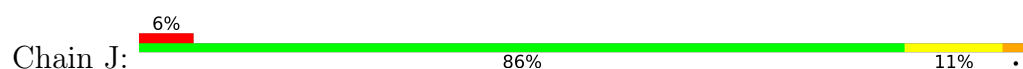
• Molecule 4: THC-4881 Heavy chain

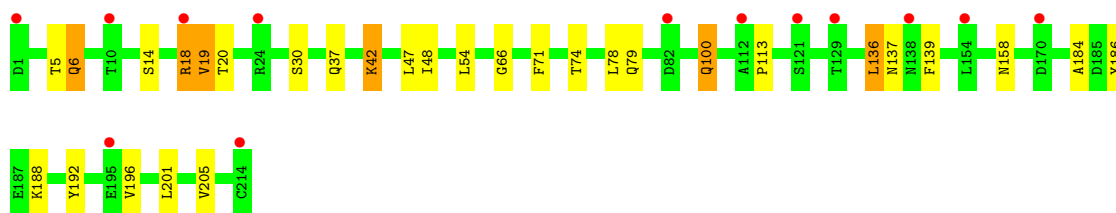


• Molecule 4: THC-4881 Heavy chain

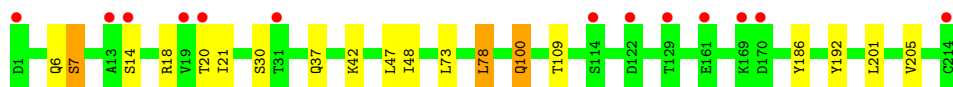
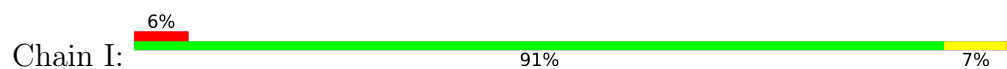


• Molecule 5: THC-4881 Light chain





● Molecule 5: THC-4881 Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.85Å 259.83Å 104.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 2.95 48.96 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.96-2.95) 99.4 (48.96-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.244 , 0.258 0.243 , 0.258	Depositor DCC
R_{free} test set	1988 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16853	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.92	0/1579	1.13	2/2149 (0.1%)
1	B	0.93	0/1579	1.13	0/2149
2	C	0.94	0/1763	1.15	1/2402 (0.0%)
2	E	0.96	0/1746	1.19	2/2380 (0.1%)
3	D	0.94	0/1736	1.16	2/2359 (0.1%)
3	F	0.94	0/1736	1.16	1/2359 (0.0%)
4	G	0.95	0/1859	1.21	1/2532 (0.0%)
4	H	0.94	0/1859	1.18	1/2532 (0.0%)
5	I	0.95	0/1703	1.17	1/2315 (0.0%)
5	J	0.94	0/1703	1.16	0/2315
All	All	0.94	0/17263	1.17	11/23492 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	7	SER	CA-C-O	-6.96	113.18	119.86
2	E	17	SER	N-CA-CB	-6.18	100.97	110.85
3	D	72	GLY	CA-C-O	-6.00	118.32	122.22
3	F	72	GLY	CA-C-O	-5.90	118.38	122.22
3	D	96	GLN	N-CA-C	-5.69	100.43	109.76
2	C	115	GLY	CA-C-O	-5.57	118.39	122.23
1	A	494	SER	N-CA-C	5.44	117.57	109.25
4	H	115	ARG	CA-C-O	-5.36	115.72	121.56
4	G	115	ARG	CA-C-O	-5.13	115.97	121.56
2	E	142	GLY	N-CA-C	-5.13	108.25	114.92
1	A	373	SER	N-CA-C	-5.06	107.11	113.28

There are no chirality outliers.

There are no planarity outliers.

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	1536	0	1453	12	0
1	B	1536	0	1453	6	0
2	C	1720	0	1690	18	9
2	E	1703	0	1673	24	0
3	D	1699	0	1639	10	0
3	F	1699	0	1639	15	1
4	G	1814	0	1769	24	0
4	H	1814	0	1769	19	8
5	I	1666	0	1620	10	0
5	J	1666	0	1620	17	0
All	All	16853	0	16325	148	9

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 4.

All (148) 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:13:VAL:HG13	3:F:84:LEU:HD22	1.34	1.04
3:F:13:VAL:CG1	3:F:84:LEU:HD22	1.90	1.00
3:F:39:LEU:HD13	3:F:77:PHE:CD2	2.11	0.86
4:G:160:CYS:CB	4:G:216:CYS:SG	2.71	0.79
2:E:93:LEU:HD22	2:E:95:TYR:CZ	2.21	0.76
2:E:93:LEU:HD21	2:E:115:GLY:HA3	1.67	0.76
2:E:97:VAL:CG1	2:E:109:TYR:HB3	2.18	0.74
3:F:13:VAL:HG13	3:F:84:LEU:CD2	2.16	0.73
4:G:160:CYS:HB2	4:G:216:CYS:SG	2.29	0.72
4:G:160:CYS:HG	4:G:216:CYS:HG	0.73	0.72
5:J:136:LEU:HD11	5:J:196:VAL:HG21	1.71	0.72
2:E:93:LEU:HD22	2:E:95:TYR:CE1	2.25	0.72
3:F:164:GLY:HA2	5:I:30:SER:HB2	1.70	0.71
4:G:160:CYS:CB	4:G:216:CYS:HG	2.04	0.70
1:A:343:ASN:O	1:A:343:ASN:OD1	2.09	0.70
4:G:12:VAL:HG21	4:G:86:LEU:HD13	1.74	0.70
2:C:11:LEU:HB2	2:C:156:PRO:HG3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:VAL:HG11	2:E:109:TYR:HB3	1.81	0.61
4:H:151:THR:HG23	4:H:155:THR:HA	1.83	0.61
2:E:93:LEU:CD2	2:E:95:TYR:CE1	2.83	0.61
2:C:101:ILE:HD12	2:C:103:GLU:HG3	1.83	0.60
4:G:179:LEU:HD21	4:G:202:VAL:HG21	1.83	0.60
4:G:12:VAL:CG2	4:G:86:LEU:HD13	2.31	0.60
4:G:141:VAL:HG13	4:G:160:CYS:SG	2.42	0.60
3:F:162:GLN:HE21	3:F:165:ASN:HD21	1.49	0.59
2:E:12:VAL:HG11	2:E:86:LEU:HD13	1.85	0.58
5:J:37:GLN:HB2	5:J:47:LEU:HD11	1.86	0.58
4:H:22:CYS:HB3	4:H:79:LEU:HB3	1.86	0.58
5:J:201:LEU:HD13	5:J:205:VAL:HG12	1.86	0.58
4:G:203:THR:HG21	5:J:137:ASN:ND2	2.18	0.58
4:G:2:VAL:HG12	4:G:27:PHE:HB3	1.86	0.56
4:H:179:LEU:HD21	4:H:202:VAL:HG21	1.87	0.55
5:J:30:SER:HB2	3:D:164:GLY:HA2	1.88	0.55
4:G:91:THR:HG23	4:G:130:ILE:HA	1.87	0.55
3:F:43:GLN:HB2	3:F:53:LEU:HD11	1.89	0.54
5:I:37:GLN:HB2	5:I:47:LEU:HD11	1.89	0.54
4:G:146:PRO:HG3	4:G:158:LEU:HD12	1.90	0.54
2:C:91:THR:HG23	2:C:119:THR:HA	1.89	0.53
2:E:11:LEU:HB2	2:E:156:PRO:HG3	1.89	0.53
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.89	0.52
4:H:18:LEU:HB2	4:H:86:LEU:HD11	1.89	0.52
4:H:91:THR:HG23	4:H:130:ILE:HA	1.90	0.52
4:H:160:CYS:SG	4:H:216:CYS:HB3	2.49	0.52
2:E:8:GLY:HA3	2:E:20:LEU:HA	1.91	0.52
4:G:22:CYS:HB3	4:G:79:LEU:HB3	1.90	0.52
4:G:203:THR:HG21	5:J:137:ASN:HD22	1.74	0.52
4:G:48:VAL:HG13	4:G:64:VAL:HG21	1.91	0.52
2:C:168:LEU:HD13	2:C:191:VAL:HG21	1.92	0.51
3:D:52:LEU:HD21	3:D:55:TYR:HB3	1.91	0.51
3:D:89:VAL:HG13	3:D:113:ILE:HD13	1.91	0.51
5:J:113:PRO:HB3	5:J:139:PHE:HB3	1.93	0.51
2:C:39:GLN:HB2	2:C:45:LEU:HD23	1.94	0.50
3:D:43:GLN:HB2	3:D:53:LEU:HD11	1.93	0.50
5:J:113:PRO:HB2	5:J:136:LEU:HD12	1.95	0.49
2:E:30:GLY:O	2:E:53:TRP:HB2	2.13	0.49
5:I:201:LEU:HD13	5:I:205:VAL:HG12	1.93	0.49
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.95	0.49
1:B:358:ILE:HG22	1:B:361:CYS:SG	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:GLN:HB3	3:D:165:ASN:HD21	1.78	0.48
3:F:52:LEU:HD21	3:F:55:TYR:HB3	1.95	0.48
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.95	0.48
2:E:142:GLY:H	2:E:195:SER:HB3	1.79	0.48
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.95	0.48
4:G:143:PRO:HD3	4:G:229:LYS:HE2	1.95	0.48
4:G:30:GLY:O	4:G:53:TYR:HB2	2.14	0.48
5:I:78:LEU:HD22	5:I:78:LEU:HA	1.74	0.47
4:G:34:MET:HB3	4:G:79:LEU:HD22	1.96	0.47
2:E:29:PHE:CE1	2:E:34:MET:HG3	2.49	0.47
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.95	0.47
3:F:193:TYR:HA	3:F:199:TYR:OH	2.14	0.47
1:B:476:GLY:HA3	1:B:487:ASN:HB3	1.97	0.47
3:F:13:VAL:HG11	3:F:19:ALA:HB2	1.96	0.46
2:E:39:GLN:HB2	2:E:45:LEU:HD23	1.96	0.46
3:F:162:GLN:HB3	3:F:165:ASN:HD21	1.80	0.46
4:G:158:LEU:HD21	4:G:231:VAL:HB	1.96	0.46
2:C:106:LEU:CD2	3:D:97:TYR:HA	2.46	0.46
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.51	0.46
5:I:186:TYR:HA	5:I:192:TYR:OH	2.15	0.46
3:F:4:MET:HG3	3:F:104:ALA:O	2.16	0.45
5:J:42:LYS:HA	5:J:42:LYS:HD2	1.66	0.45
2:E:91:THR:HG23	2:E:119:THR:HA	1.97	0.45
2:E:97:VAL:HG11	2:E:109:TYR:CG	2.51	0.45
5:J:186:TYR:HA	5:J:192:TYR:OH	2.17	0.45
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.52	0.45
1:A:350:VAL:HG21	1:A:418:ILE:HG23	1.99	0.45
2:C:106:LEU:HD23	3:D:97:TYR:HA	1.99	0.45
4:G:64:VAL:HB	4:G:68:PHE:CD2	2.52	0.45
4:G:141:VAL:CG1	4:G:160:CYS:SG	3.05	0.45
2:C:30:GLY:O	2:C:53:TRP:HB2	2.16	0.45
4:H:30:GLY:O	4:H:53:TYR:HB2	2.17	0.44
2:C:60:TYR:HB2	2:C:65:LYS:HD3	1.99	0.44
2:E:97:VAL:HG11	2:E:109:TYR:CB	2.47	0.44
5:J:184:ALA:O	5:J:188:LYS:HG2	2.18	0.44
2:C:12:VAL:HG11	2:C:86:LEU:HD13	1.98	0.43
1:A:366:SER:H	1:A:388:ASN:HD21	1.67	0.43
1:A:500:THR:HG21	2:E:59:GLY:HA3	2.00	0.43
3:F:24:LYS:HA	3:F:75:THR:O	2.18	0.43
5:J:18:ARG:O	5:J:19:VAL:HB	2.18	0.43
5:J:20:THR:HG22	5:J:74:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLY:HA2	1:A:498:GLN:HG2	2.01	0.42
2:E:83:MET:HE3	2:E:86:LEU:HD11	2.00	0.42
4:G:52:SER:HB3	4:G:57:GLU:HG3	2.01	0.42
4:H:93:VAL:HG13	4:H:126:GLU:HB2	2.01	0.42
5:I:42:LYS:HD2	5:I:42:LYS:HA	1.69	0.42
1:A:393:THR:HG21	1:A:520:ALA:HB3	2.01	0.42
3:F:161:LEU:HD23	3:F:161:LEU:HA	1.91	0.42
2:E:97:VAL:HG11	2:E:109:TYR:CD1	2.55	0.42
5:J:6:GLN:HE21	5:J:6:GLN:HB3	1.55	0.42
2:C:97:VAL:CG1	2:C:109:TYR:HB3	2.50	0.42
5:I:21:ILE:HD11	5:I:73:LEU:HD23	2.00	0.42
4:H:64:VAL:HB	4:H:68:PHE:CD2	2.54	0.42
2:C:10:GLY:HA2	2:C:118:VAL:HA	2.02	0.42
2:C:16:ARG:HA	2:C:16:ARG:HD2	1.85	0.42
2:C:29:PHE:HD2	2:C:74:ASN:HA	1.85	0.42
2:E:16:ARG:HG3	2:E:17:SER:N	2.35	0.42
2:E:83:MET:HE1	2:E:118:VAL:HG11	2.01	0.42
1:B:411:ALA:HB3	1:B:414:GLN:HG3	2.02	0.41
4:H:98:ARG:O	4:H:120:MET:HA	2.20	0.41
4:H:31:SER:HB3	4:H:103:PRO:HB3	2.01	0.41
4:H:110:GLY:HA2	4:H:114:ALA:HB2	2.01	0.41
4:H:146:PRO:HG3	4:H:158:LEU:HD12	2.02	0.41
4:G:102:PRO:HB2	4:G:105:TYR:CD1	2.55	0.41
1:A:383:SER:HB3	1:A:386:LYS:HD2	2.02	0.41
2:E:22:CYS:HB3	2:E:79:LEU:HB3	2.02	0.41
5:J:5:THR:HG23	5:J:100:GLN:HE21	1.86	0.41
1:B:371:SER:C	1:B:373:SER:H	2.28	0.41
2:C:83:MET:HE3	2:C:86:LEU:HD11	2.03	0.41
4:H:34:MET:HB3	4:H:79:LEU:HD22	2.03	0.41
2:C:83:MET:HE1	2:C:118:VAL:HG11	2.03	0.41
4:H:64:VAL:HB	4:H:68:PHE:CG	2.55	0.41
5:J:188:LYS:HD3	5:J:188:LYS:HA	1.88	0.41
5:I:6:GLN:HE21	5:I:6:GLN:HB3	1.52	0.41
4:G:40:ALA:HB3	4:G:43:LYS:HB3	2.01	0.41
2:C:18:LEU:HD12	2:C:18:LEU:HA	1.95	0.41
3:D:86:ALA:O	3:D:89:VAL:HG22	2.21	0.41
4:H:98:ARG:HH11	4:H:122:VAL:HG23	1.86	0.41
5:I:100:GLN:HE21	5:I:100:GLN:HB2	1.71	0.41
3:D:193:TYR:HA	3:D:199:TYR:OH	2.21	0.41
4:H:155:THR:HG22	4:H:206:SER:HB2	2.03	0.41
1:A:439:ASN:O	1:A:443:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:PHE:HD2	2:E:74:ASN:HA	1.86	0.40
5:J:66:GLY:HA3	5:J:71:PHE:HA	2.02	0.40
3:D:173:GLN:HG2	3:D:178:SER:HA	2.02	0.40
4:H:98:ARG:HD3	4:H:122:VAL:CG2	2.51	0.40
5:I:18:ARG:HG3	5:I:20:THR:HG23	2.02	0.40
3:F:56:TRP:O	3:F:57:ALA:HB3	2.22	0.40
4:H:48:VAL:HG13	4:H:64:VAL:HG21	2.03	0.40
1:A:444:LYS:HD2	1:A:444:LYS:HA	1.78	0.40

All (9) 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:C:66:GLY:O	4:H:149:LYS:CE[2_455]	0.78	1.42
2:C:67:ARG:N	4:H:149:LYS:NZ[2_455]	0.80	1.40
2:C:67:ARG:CA	4:H:149:LYS:NZ[2_455]	1.01	1.19
2:C:66:GLY:C	4:H:149:LYS:NZ[2_455]	1.45	0.75
2:C:66:GLY:C	4:H:149:LYS:CE[2_455]	1.50	0.70
3:F:59:THR:OG1	2:C:138:LYS:O[4_555]	1.84	0.36
2:C:66:GLY:O	4:H:149:LYS:NZ[2_455]	1.93	0.27
2:C:67:ARG:N	4:H:149:LYS:CE[2_455]	2.07	0.13
2:C:66:GLY:O	4:H:149:LYS:CD[2_455]	2.13	0.07

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	192/194 (99%)	188 (98%)	4 (2%)	0	100	100
1	B	192/194 (99%)	186 (97%)	6 (3%)	0	100	100
2	C	225/227 (99%)	218 (97%)	6 (3%)	1 (0%)	30	53
2	E	223/227 (98%)	214 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
3	F	219/221 (99%)	216 (99%)	3 (1%)	0	100	100
4	G	236/238 (99%)	233 (99%)	3 (1%)	0	100	100
4	H	236/238 (99%)	231 (98%)	5 (2%)	0	100	100
5	I	212/214 (99%)	206 (97%)	5 (2%)	1 (0%)	24	49
5	J	212/214 (99%)	204 (96%)	5 (2%)	3 (1%)	9	24
All	All	2166/2188 (99%)	2111 (98%)	50 (2%)	5 (0%)	43	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	J	19	VAL
5	J	18	ARG
5	J	14	SER
5	I	14	SER
2	C	10	GLY

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	167/167 (100%)	165 (99%)	2 (1%)	63	79
1	B	167/167 (100%)	159 (95%)	8 (5%)	23	48
2	C	194/194 (100%)	179 (92%)	15 (8%)	12	30
2	E	192/194 (99%)	187 (97%)	5 (3%)	40	65
3	D	190/190 (100%)	185 (97%)	5 (3%)	40	65
3	F	190/190 (100%)	188 (99%)	2 (1%)	65	80
4	G	202/202 (100%)	195 (96%)	7 (4%)	32	57
4	H	202/202 (100%)	189 (94%)	13 (6%)	16	38
5	I	189/189 (100%)	184 (97%)	5 (3%)	40	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	189/189 (100%)	180 (95%)	9 (5%)	23	48
All	All	1882/1884 (100%)	1811 (96%)	71 (4%)	29	55

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	VAL
1	A	415	THR
2	E	24	VAL
2	E	103	GLU
2	E	147	LEU
2	E	159	VAL
2	E	168	LEU
3	F	113	ILE
3	F	188	LEU
4	G	93	VAL
4	G	105	TYR
4	G	108	LEU
4	G	151	THR
4	G	155	THR
4	G	170	VAL
4	G	232	GLU
5	J	6	GLN
5	J	42	LYS
5	J	48	ILE
5	J	54	LEU
5	J	78	LEU
5	J	79	GLN
5	J	100	GLN
5	J	136	LEU
5	J	158	ASN
1	B	358	ILE
1	B	362	VAL
1	B	368	LEU
1	B	370	ASN
1	B	415	THR
1	B	478	THR
1	B	494	SER
1	B	498	GLN
2	C	12	VAL
2	C	16	ARG
2	C	24	VAL

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Mol	Chain	Res	Type
2	C	89	GLU
2	C	93	LEU
2	C	97	VAL
2	C	104	VAL
2	C	144	THR
2	C	147	LEU
2	C	159	VAL
2	C	168	LEU
2	C	181	SER
2	C	192	THR
2	C	202	THR
2	C	225	CYS
3	D	15	LEU
3	D	39	LEU
3	D	89	VAL
3	D	113	ILE
3	D	132	LEU
4	H	1	GLU
4	H	12	VAL
4	H	93	VAL
4	H	96	CYS
4	H	105	TYR
4	H	115	ARG
4	H	151	THR
4	H	155	THR
4	H	170	VAL
4	H	189	VAL
4	H	203	THR
4	H	232	GLU
4	H	236	CYS
5	I	7	SER
5	I	48	ILE
5	I	78	LEU
5	I	100	GLN
5	I	109	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	ASN
1	A	481	ASN
1	A	493	GLN

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Mol	Chain	Res	Type
2	E	56	ASN
2	E	180	GLN
2	E	201	GLN
3	F	22	ASN
3	F	102	GLN
3	F	162	GLN
3	F	196	HIS
3	F	206	GLN
4	G	39	GLN
4	G	84	ASN
4	G	125	GLN
4	G	191	GLN
4	G	212	GLN
4	G	224	ASN
5	J	3	GLN
5	J	38	GLN
5	J	56	ASN
5	J	100	GLN
5	J	137	ASN
5	J	138	ASN
5	J	147	GLN
5	J	210	ASN
1	B	334	ASN
1	B	354	ASN
1	B	437	ASN
1	B	439	ASN
1	B	481	ASN
2	C	56	ASN
2	C	114	GLN
2	C	173	HIS
3	D	22	ASN
3	D	35	ASN
3	D	36	GLN
3	D	85	GLN
3	D	144	ASN
4	H	84	ASN
4	H	184	HIS
4	H	212	GLN
5	I	100	GLN
5	I	160	GLN
5	I	189	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	194/194 (100%)	0.76	16 (8%) 17 15	24, 38, 60, 69	0
1	B	194/194 (100%)	0.91	21 (10%) 11 10	25, 39, 72, 103	0
2	C	227/227 (100%)	0.99	27 (11%) 9 8	28, 44, 92, 222	0
2	E	225/227 (99%)	0.86	23 (10%) 12 11	29, 45, 81, 128	0
3	D	221/221 (100%)	0.70	13 (5%) 28 23	25, 39, 68, 108	0
3	F	221/221 (100%)	0.66	13 (5%) 28 23	26, 40, 58, 98	0
4	G	238/238 (100%)	0.64	16 (6%) 24 20	28, 38, 58, 81	0
4	H	238/238 (100%)	0.70	16 (6%) 24 20	25, 38, 61, 81	0
5	I	214/214 (100%)	0.79	13 (6%) 27 22	28, 44, 61, 80	0
5	J	214/214 (100%)	0.80	13 (6%) 27 22	28, 47, 63, 81	0
All	All	2186/2188 (99%)	0.78	171 (7%) 19 17	24, 41, 66, 222	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	140	THR	7.2
2	C	142	GLY	6.9
5	I	214	CYS	6.3
2	C	141	SER	5.8
2	E	140	THR	5.6
2	C	139	SER	4.9
3	D	221	CYS	4.8
1	B	369	TYR	4.6
2	C	226	ASP	4.5
4	G	154	GLY	4.4
2	C	138	LYS	4.2
3	F	1	ALA	4.2
4	H	1	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
4	G	121	ASP	4.0
2	C	227	LYS	4.0
5	I	14	SER	4.0
3	D	154	GLN	4.0
2	E	224	SER	3.9
4	G	158	LEU	3.9
3	F	55	TYR	3.9
2	C	137	SER	3.8
1	B	367	VAL	3.7
2	C	195	SER	3.7
5	I	170	ASP	3.7
4	H	121	ASP	3.7
4	H	153	GLY	3.7
2	E	139	SER	3.6
2	C	143	GLY	3.6
1	B	428	ASP	3.5
4	H	154	GLY	3.4
2	C	136	SER	3.3
2	E	138	LYS	3.3
2	C	200	THR	3.3
1	B	526	GLY	3.3
1	A	371	SER	3.2
5	I	13	ALA	3.2
3	F	56	TRP	3.2
1	B	368	LEU	3.1
1	A	428	ASP	3.1
1	B	371	SER	3.1
3	F	221	CYS	3.1
5	J	214	CYS	3.1
3	D	168	GLU	3.1
1	B	374	PHE	3.0
5	J	121	SER	3.0
2	C	199	GLY	3.0
2	E	136	SER	3.0
2	E	195	SER	3.0
5	J	170	ASP	3.0
2	E	199	GLY	3.0
4	H	210	GLY	3.0
1	A	367	VAL	3.0
3	D	219	GLY	3.0
4	H	155	THR	3.0
1	A	526	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	137	SER	2.9
3	D	136	THR	2.9
2	C	223	LYS	2.9
2	E	223	LYS	2.9
5	I	122	ASP	2.9
1	B	333	THR	2.9
4	G	155	THR	2.9
1	B	480	CYS	2.9
2	C	198	LEU	2.8
2	E	101	ILE	2.8
1	B	334	ASN	2.8
5	J	1	ASP	2.8
4	H	25	SER	2.8
2	C	224	SER	2.7
5	I	20	THR	2.7
2	E	143	GLY	2.7
2	C	7	SER	2.7
4	G	150	SER	2.7
1	B	370	ASN	2.7
3	F	162	GLN	2.7
1	A	522	ALA	2.7
3	D	55	TYR	2.7
2	C	8	GLY	2.7
5	I	19	VAL	2.7
1	B	365	TYR	2.6
4	H	125	GLN	2.6
1	A	480	CYS	2.6
2	E	200	THR	2.6
5	I	169	LYS	2.6
4	H	158	LEU	2.6
4	G	75	SER	2.6
4	H	216	CYS	2.6
4	H	238	LYS	2.6
5	J	129	THR	2.6
5	I	129	THR	2.6
5	J	112	ALA	2.6
5	I	1	ASP	2.6
2	C	219	ARG	2.5
2	E	197	SER	2.5
4	H	148	SER	2.5
2	C	103	GLU	2.5
3	D	130	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
4	G	236	CYS	2.5
3	D	132	LEU	2.5
2	E	216	VAL	2.5
1	A	438	SER	2.5
2	E	7	SER	2.4
4	G	89	GLU	2.4
2	C	222	PRO	2.4
1	A	415	THR	2.4
4	H	151	THR	2.4
2	E	93	LEU	2.4
1	B	373	SER	2.4
2	E	25	SER	2.4
1	A	369	TYR	2.4
1	A	334	ASN	2.3
1	A	496	GLY	2.3
5	J	18	ARG	2.3
5	J	138	ASN	2.3
1	B	389	ASP	2.3
5	J	82	ASP	2.3
5	I	31	THR	2.3
2	C	27	PHE	2.3
3	F	168	GLU	2.3
4	G	149	LYS	2.3
1	B	418	ILE	2.3
3	F	130	GLU	2.2
3	D	129	ASP	2.2
2	E	225	CYS	2.2
1	B	475	ALA	2.2
4	G	57	GLU	2.2
5	J	10	THR	2.2
3	D	215	SER	2.2
1	B	520	ALA	2.2
4	G	24	ALA	2.2
1	B	440	ASN	2.2
2	E	16	ARG	2.2
2	C	135	PRO	2.2
4	G	160	CYS	2.2
2	E	141	SER	2.2
1	A	405	ASP	2.2
4	G	62	ASP	2.2
4	G	106	ASP	2.2
1	A	333	THR	2.2

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Mol	Chain	Res	Type	RSRZ
4	H	236	CYS	2.2
5	J	195	GLU	2.2
5	J	24	ARG	2.1
2	E	56	ASN	2.1
4	H	84	ASN	2.1
3	F	63	GLY	2.1
3	F	132	LEU	2.1
1	B	375	SER	2.1
2	C	181	SER	2.1
4	H	234	LYS	2.1
2	E	205	CYS	2.1
2	C	1	GLU	2.1
3	D	220	GLU	2.1
1	B	405	ASP	2.1
3	F	16	GLY	2.1
3	F	177	ASP	2.1
5	J	154	LEU	2.1
2	C	225	CYS	2.1
3	F	166	SER	2.1
1	B	503	VAL	2.1
3	D	1	ALA	2.1
1	A	473	TYR	2.1
1	A	373	SER	2.0
3	F	159	ASN	2.0
4	G	84	ASN	2.0
5	I	161	GLU	2.0
2	E	71	SER	2.0
5	I	114	SER	2.0
2	C	205	CYS	2.0
1	A	343	ASN	2.0
3	D	177	ASP	2.0
4	G	168	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.