



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:27 AM UTC

PDB ID : 7XEI / pdb_00007xei
Title : SARS-CoV-2-prototyped-RBD and CB6-092-Fab complex
Authors : Wang, Y.; Feng, Y.
Deposited on : 2022-03-31
Resolution : 2.76 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

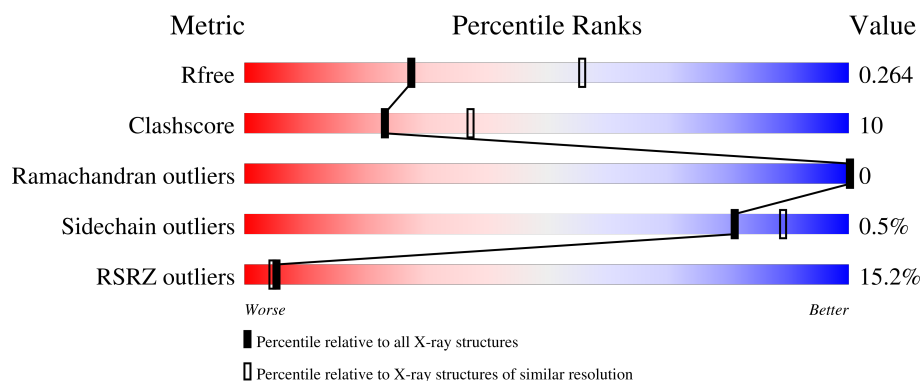
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	227	17% 66% 20% 14%
1	B	227	20% 68% 17% 14%
2	C	233	12% 65% 26% 7%
2	E	233	9% 76% 18% 6%
3	D	216	9% 88% 11%

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Mol	Chain	Length	Quality of chain
3	F	216	17% 73% 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9648 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	196	Total	C	N	O	S	0	0	0
			1552	995	259	290	8			
1	B	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	538	HIS	-	expression tag	UNP P0DTC2
A	539	HIS	-	expression tag	UNP P0DTC2
A	540	HIS	-	expression tag	UNP P0DTC2
A	541	HIS	-	expression tag	UNP P0DTC2
A	542	HIS	-	expression tag	UNP P0DTC2
A	543	HIS	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
B	538	HIS	-	expression tag	UNP P0DTC2
B	539	HIS	-	expression tag	UNP P0DTC2
B	540	HIS	-	expression tag	UNP P0DTC2
B	541	HIS	-	expression tag	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CB6-092-Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	216	Total	C	N	O	S	0	0	0
			1619	1028	269	314	8			
2	E	218	Total	C	N	O	S	0	0	0
			1632	1035	271	318	8			

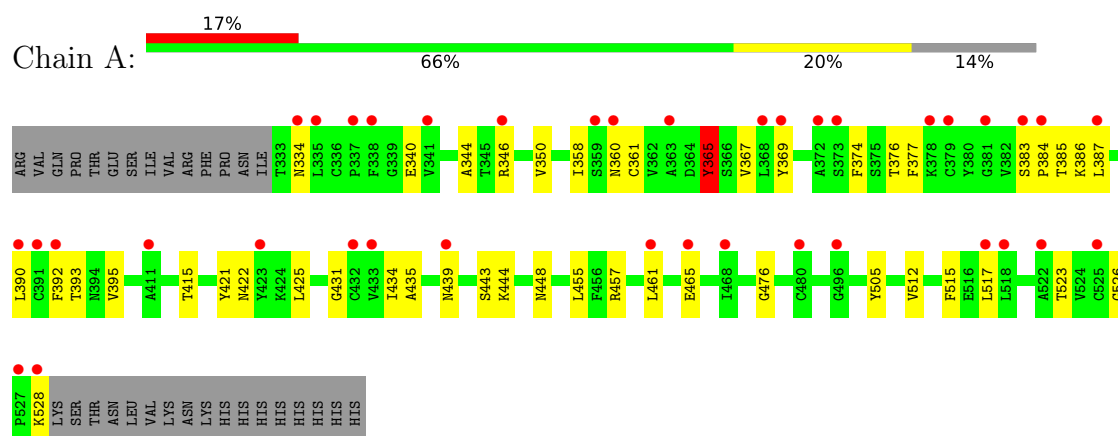
- Molecule 3 is a protein called CB6-092-Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	215	Total	C	N	O	S	0	0	0
			1651	1030	277	339	5			
3	F	215	Total	C	N	O	S	0	0	0
			1651	1030	277	339	5			

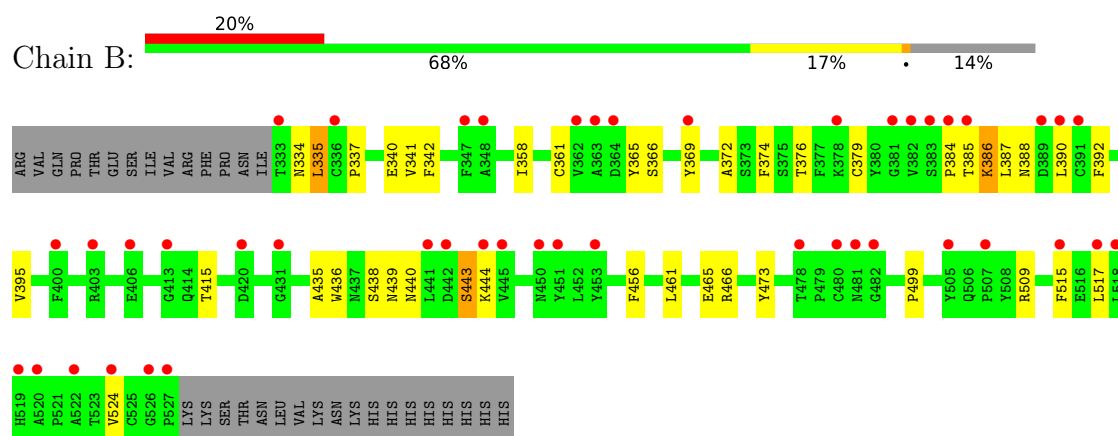
3 Residue-property plots [i](#)

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.

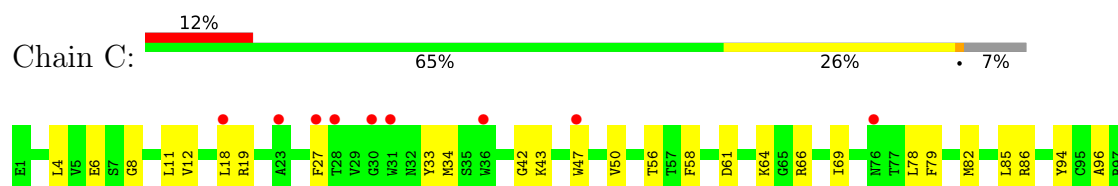
• Molecule 1: Spike protein S1

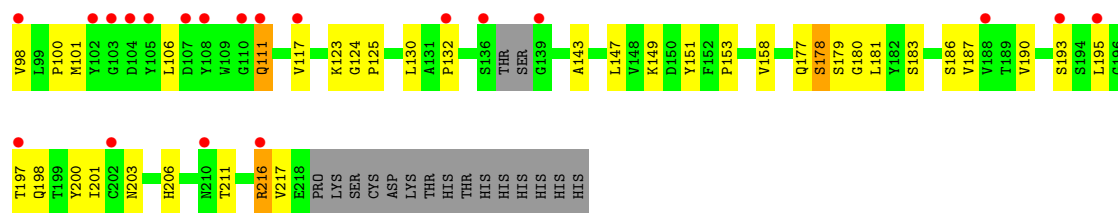


• Molecule 1: Spike protein S1

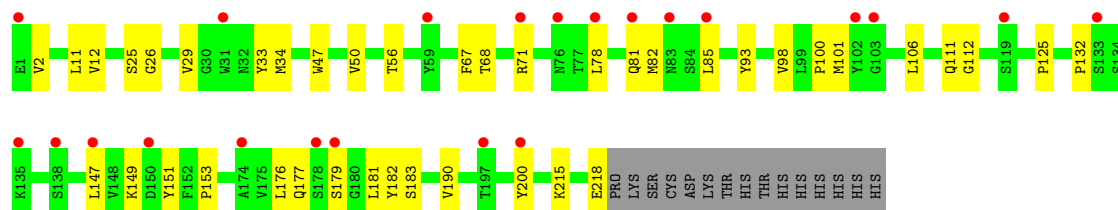
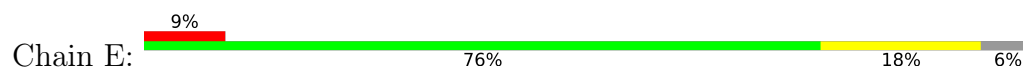


• Molecule 2: CB6-092-Fab heavy chain

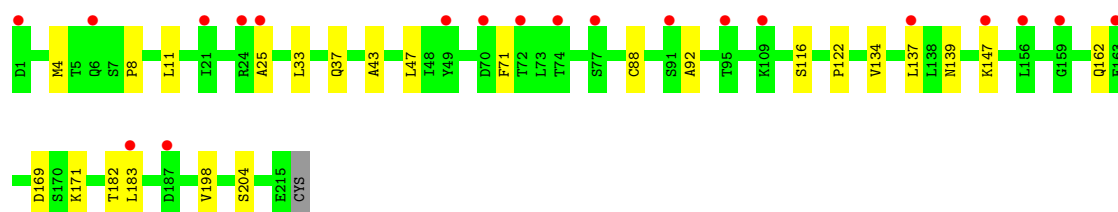
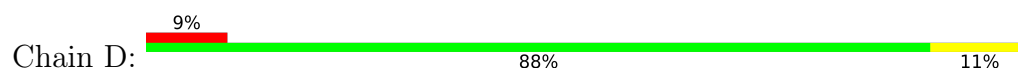




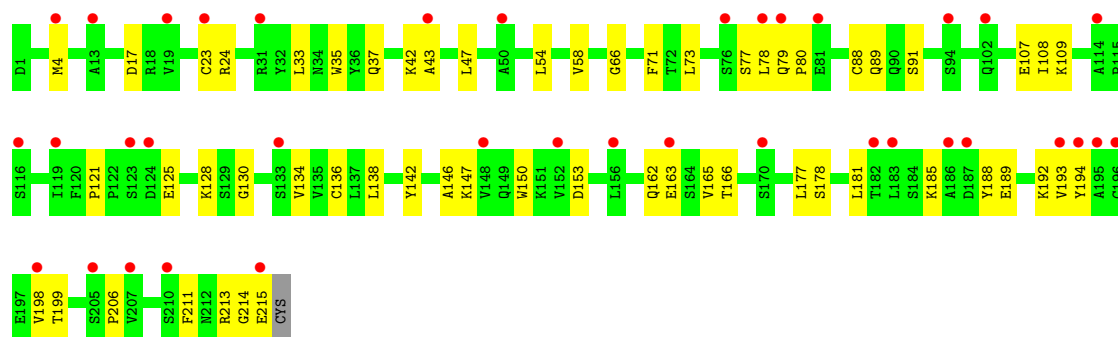
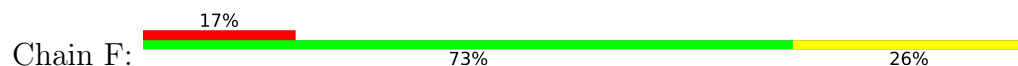
• Molecule 2: CB6-092-Fab heavy chain



• Molecule 3: CB6-092-Fab light chain



• Molecule 3: CB6-092-Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.05Å 112.20Å 101.74Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	49.95 – 2.76 49.95 – 2.76	Depositor EDS
% Data completeness (in resolution range)	91.4 (49.95-2.76) 91.5 (49.95-2.76)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.215 , 0.263 0.221 , 0.264	Depositor DCC
R_{free} test set	2015 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9648	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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

5.1 Standard geometry

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	0.32	1/1596 (0.1%)	0.66	4/2172 (0.2%)
1	B	0.37	0/1587	0.69	1/2161 (0.0%)
2	C	0.32	0/1659	0.64	5/2262 (0.2%)
2	E	0.18	0/1673	0.49	0/2283
3	D	0.17	0/1685	0.46	0/2287
3	F	0.29	0/1685	0.60	2/2287 (0.1%)
All	All	0.28	1/9885 (0.0%)	0.59	12/13452 (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
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	ARG	CD-NE	-5.30	1.38	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	24	ARG	CA-CB-CG	8.37	130.84	114.10
1	A	346	ARG	NE-CZ-NH2	8.26	126.63	119.20
2	C	111	GLN	CA-CB-CG	-8.07	97.97	114.10
1	B	386	LYS	CA-CB-CG	8.02	130.14	114.10
2	C	180	GLY	N-CA-C	-7.50	104.70	115.27
3	F	24	ARG	CB-CA-C	7.11	123.82	109.38
1	A	346	ARG	NE-CZ-NH1	-5.89	115.61	121.50
2	C	216	ARG	CB-CG-CD	5.81	124.66	111.30
1	A	365	TYR	CA-C-N	5.79	127.96	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	TYR	C-N-CA	5.79	127.96	120.44
2	C	178	SER	CA-C-N	5.03	127.03	120.28
2	C	178	SER	C-N-CA	5.03	127.03	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	443	SER	Peptide

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	1552	0	1473	37	0
1	B	1543	0	1460	42	1
2	C	1619	0	1580	48	1
2	E	1632	0	1595	29	0
3	D	1651	0	1605	16	0
3	F	1651	0	1605	39	0
All	All	9648	0	9318	195	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 10.

All (195) 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)
1:A:374:PHE:O	1:B:386:LYS:NZ	1.95	0.98
1:B:365:TYR:N	1:B:388:ASN:HD21	1.66	0.93
1:B:365:TYR:H	1:B:388:ASN:HD21	1.17	0.88
1:B:365:TYR:H	1:B:388:ASN:ND2	1.76	0.84
1:B:387:LEU:HA	1:B:390:LEU:CD1	2.08	0.82
1:B:386:LYS:O	1:B:390:LEU:HD12	1.80	0.82
2:E:47:TRP:HE1	2:E:50:VAL:HG23	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:TYR:CE2	1:B:385:THR:HB	2.20	0.77
2:C:111:GLN:HG3	3:D:43:ALA:HB2	1.68	0.76
1:A:358:ILE:HB	1:A:395:VAL:HG23	1.68	0.75
3:F:189:GLU:HA	3:F:213:ARG:HD2	1.69	0.73
2:E:2:VAL:HA	2:E:25:SER:O	1.89	0.71
1:B:386:LYS:O	1:B:390:LEU:CD1	2.39	0.71
1:B:387:LEU:HA	1:B:390:LEU:HD13	1.72	0.70
2:E:2:VAL:HG12	2:E:26:GLY:HA3	1.73	0.69
2:C:187:VAL:HG21	3:D:137:LEU:HD11	1.76	0.66
2:C:100:PRO:HD2	2:C:101:MET:HE2	1.78	0.65
2:E:177:GLN:HA	3:F:162:GLN:HE22	1.60	0.65
3:F:134:VAL:HG23	3:F:181:LEU:HB3	1.77	0.65
2:E:11:LEU:HB2	2:E:153:PRO:HG3	1.79	0.64
3:F:138:LEU:HD21	3:F:198:VAL:HG21	1.80	0.64
2:C:177:GLN:HA	3:D:162:GLN:HE22	1.64	0.63
1:B:439:ASN:O	1:B:443:SER:HB2	1.99	0.62
2:E:125:PRO:HB3	2:E:151:TYR:HB3	1.81	0.62
2:C:201:ILE:HG12	2:C:216:ARG:HB2	1.81	0.62
1:B:369:TYR:HE2	1:B:385:THR:HB	1.64	0.62
3:D:169:ASP:OD1	3:D:171:LYS:HG2	2.00	0.62
2:C:149:LYS:HA	2:C:183:SER:HB2	1.82	0.61
2:C:190:VAL:HG21	2:C:195:LEU:HD21	1.83	0.61
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.34	0.61
2:E:215:LYS:NZ	3:F:125:GLU:OE1	2.33	0.61
1:A:386:LYS:HE2	1:B:374:PHE:O	2.01	0.61
1:B:387:LEU:CA	1:B:390:LEU:HD12	2.31	0.60
1:A:369:TYR:CE1	1:A:384:PRO:HB2	2.36	0.60
2:E:98:VAL:HG22	2:E:106:LEU:HG	1.82	0.60
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.83	0.59
1:B:444:LYS:H	1:B:499:PRO:HD3	1.68	0.59
1:B:387:LEU:CA	1:B:390:LEU:CD1	2.81	0.58
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.86	0.58
1:A:383:SER:HB3	1:A:386:LYS:HD2	1.85	0.57
3:F:189:GLU:HA	3:F:213:ARG:CD	2.34	0.57
1:A:365:TYR:N	1:A:365:TYR:CD2	2.72	0.57
2:C:125:PRO:HB3	2:C:151:TYR:HB3	1.87	0.57
2:E:132:PRO:HD2	2:E:218:GLU:HB2	1.87	0.57
1:A:476:GLY:HA2	2:C:27:PHE:HA	1.86	0.56
2:E:68:THR:HG23	2:E:81:GLN:HB3	1.88	0.55
1:B:461:LEU:HD22	1:B:465:GLU:HB3	1.89	0.55
1:A:461:LEU:HD22	1:A:465:GLU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:TYR:CE1	1:B:384:PRO:HB2	2.42	0.54
2:C:12:VAL:HG11	2:C:85:LEU:HD13	1.89	0.54
3:F:109:LYS:HA	3:F:142:TYR:OH	2.08	0.54
1:B:365:TYR:H	1:B:388:ASN:CG	2.16	0.53
2:E:176:LEU:HD13	2:E:182:TYR:CE2	2.43	0.53
1:A:395:VAL:HG12	1:A:515:PHE:HA	1.90	0.53
3:D:8:PRO:HG3	3:D:11:LEU:HD13	1.91	0.53
1:A:365:TYR:CD1	1:A:387:LEU:HG	2.44	0.52
3:F:188:TYR:O	3:F:194:TYR:OH	2.25	0.52
3:D:122:PRO:HD3	3:D:134:VAL:HG22	1.92	0.52
1:A:387:LEU:HD11	1:A:515:PHE:CZ	2.45	0.52
2:C:4:LEU:HD21	2:C:27:PHE:HE2	1.75	0.52
3:D:33:LEU:HD11	3:D:88:CYS:HB2	1.90	0.52
3:D:147:LYS:O	3:D:198:VAL:HA	2.10	0.51
1:B:365:TYR:N	1:B:388:ASN:ND2	2.41	0.51
2:C:12:VAL:HG21	2:C:85:LEU:HD12	1.92	0.51
1:B:385:THR:C	1:B:387:LEU:H	2.19	0.51
1:A:386:LYS:NZ	1:B:372:ALA:O	2.40	0.51
2:E:12:VAL:HG11	2:E:85:LEU:HD12	1.93	0.51
2:E:47:TRP:NE1	2:E:50:VAL:HG23	2.21	0.51
2:C:33:TYR:CE2	2:C:100:PRO:HG3	2.46	0.51
2:C:123:LYS:HD2	2:C:124:GLY:N	2.25	0.50
3:F:153:ASP:OD1	3:F:192:LYS:HB2	2.12	0.50
2:C:42:GLY:C	2:C:43:LYS:HD3	2.37	0.50
2:E:93:TYR:O	2:E:112:GLY:HA2	2.11	0.50
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.94	0.50
2:C:8:GLY:O	2:C:18:LEU:HD11	2.12	0.49
2:C:12:VAL:HG13	2:C:117:VAL:HB	1.94	0.49
2:E:179:SER:HB2	2:E:181:LEU:H	1.77	0.49
1:A:393:THR:OG1	1:A:517:LEU:HA	2.12	0.49
1:B:415:THR:HB	2:E:56:THR:HG21	1.94	0.49
2:C:18:LEU:HD22	2:C:19:ARG:H	1.77	0.49
2:E:111:GLN:HA	3:F:43:ALA:HB2	1.94	0.49
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.67	0.49
2:C:216:ARG:HG2	2:C:217:VAL:N	2.28	0.49
3:F:33:LEU:HD21	3:F:88:CYS:HB2	1.95	0.48
2:C:47:TRP:HZ2	2:C:50:VAL:HG12	1.78	0.48
2:C:78:LEU:HD12	2:C:79:PHE:H	1.79	0.48
3:F:89:GLN:NE2	3:F:91:SER:OG	2.45	0.48
3:D:4:MET:HE1	3:D:25:ALA:HB2	1.94	0.48
1:A:415:THR:HB	2:C:56:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:ARG:HD3	2:C:86:ARG:NH2	2.29	0.48
2:E:190:VAL:HG21	2:E:200:TYR:CZ	2.48	0.48
2:E:147:LEU:HG	2:E:149:LYS:HG3	1.96	0.48
3:F:198:VAL:O	3:F:206:PRO:HA	2.14	0.48
3:F:42:LYS:HA	3:F:42:LYS:HD2	1.69	0.47
3:F:121:PRO:HB3	3:F:211:PHE:CE1	2.50	0.47
1:B:395:VAL:HG23	1:B:524:VAL:HG21	1.96	0.47
3:F:146:ALA:O	3:F:147:LYS:HD2	2.15	0.47
1:B:358:ILE:HB	1:B:395:VAL:HB	1.96	0.47
3:D:116:SER:OG	3:D:139:ASN:HB3	2.14	0.47
1:B:466:ARG:HH21	1:B:466:ARG:HB3	1.79	0.47
3:D:33:LEU:HD22	3:D:71:PHE:CG	2.50	0.47
1:B:376:THR:HB	1:B:435:ALA:HB3	1.97	0.47
2:C:200:TYR:O	2:C:216:ARG:HA	2.15	0.47
3:F:66:GLY:HA3	3:F:71:PHE:HA	1.97	0.47
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.97	0.47
1:B:335:LEU:H	1:B:335:LEU:HG	1.54	0.46
1:B:456:PHE:HB3	1:B:473:TYR:CD2	2.50	0.46
2:E:149:LYS:HA	2:E:183:SER:HB2	1.96	0.46
3:F:54:LEU:HD11	3:F:58:VAL:HB	1.96	0.46
3:D:182:THR:O	3:D:183:LEU:HD23	2.15	0.46
3:F:4:MET:HE3	3:F:23:CYS:SG	2.55	0.46
1:B:392:PHE:CD2	1:B:515:PHE:HB3	2.51	0.46
1:B:379:CYS:SG	1:B:384:PRO:HB3	2.54	0.46
2:E:67:PHE:CE1	2:E:82:MET:HB3	2.51	0.46
3:F:77:SER:HB2	3:F:79:GLN:NE2	2.30	0.46
3:F:80:PRO:HA	3:F:108:ILE:HG13	1.96	0.46
1:A:392:PHE:CG	1:A:515:PHE:HB3	2.51	0.46
2:C:130:LEU:HD21	2:C:147:LEU:HB2	1.97	0.46
1:A:360:ASN:ND2	1:A:523:THR:HB	2.31	0.46
1:A:455:LEU:HD11	2:C:101:MET:HG3	1.97	0.45
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.98	0.45
1:A:369:TYR:HE1	1:A:384:PRO:HB2	1.80	0.45
1:A:385:THR:OG1	1:A:386:LYS:N	2.50	0.45
2:C:11:LEU:HB2	2:C:153:PRO:HG3	1.99	0.45
3:F:17:ASP:O	3:F:78:LEU:N	2.42	0.45
1:B:366:SER:H	1:B:388:ASN:HD21	1.65	0.45
2:C:61:ASP:HA	2:C:64:LYS:HG3	1.99	0.45
2:C:158:VAL:HA	2:C:203:ASN:O	2.17	0.45
2:E:29:VAL:HG13	2:E:34:MET:HG3	1.97	0.45
3:F:79:GLN:HB3	3:F:80:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLY:HA2	1:A:515:PHE:HD2	1.78	0.45
1:B:386:LYS:HB3	1:B:386:LYS:HE3	1.68	0.45
2:E:82:MET:CB	2:E:85:LEU:HD21	2.46	0.45
2:E:100:PRO:HD2	2:E:101:MET:HE3	1.97	0.45
1:A:376:THR:HB	1:A:435:ALA:HB3	1.99	0.44
2:C:187:VAL:HG11	3:D:137:LEU:HD11	2.00	0.44
1:A:334:ASN:ND2	1:A:360:ASN:O	2.50	0.44
1:B:337:PRO:HB2	1:B:340:GLU:HG3	1.99	0.44
2:C:197:THR:OG1	2:C:198:GLN:N	2.51	0.44
3:F:134:VAL:CG2	3:F:181:LEU:HB3	2.45	0.44
3:F:165:VAL:HG22	3:F:177:LEU:HD12	2.00	0.44
3:F:153:ASP:CG	3:F:192:LYS:HB2	2.43	0.44
3:F:214:GLY:O	3:F:215:GLU:HB3	2.17	0.44
2:C:34:MET:HB3	2:C:78:LEU:HD22	1.99	0.43
2:C:96:ALA:HB3	2:C:106:LEU:HD23	1.99	0.43
3:F:163:GLU:HA	3:F:178:SER:O	2.18	0.43
1:A:526:GLY:O	1:A:528:LYS:N	2.50	0.43
3:F:128:LYS:HB2	3:F:128:LYS:HE2	1.83	0.43
3:F:107:GLU:HG2	3:F:108:ILE:N	2.33	0.43
3:F:199:THR:HG23	3:F:206:PRO:HG3	2.00	0.43
1:A:431:GLY:HA2	1:A:515:PHE:CE2	2.53	0.43
1:B:334:ASN:O	1:B:361:CYS:HB2	2.18	0.43
2:C:50:VAL:CG1	2:C:58:PHE:HB2	2.47	0.43
3:F:130:GLY:HA2	3:F:185:LYS:HE3	2.01	0.43
2:C:82:MET:HE2	2:C:85:LEU:HD21	2.01	0.43
2:C:98:VAL:HG22	2:C:106:LEU:HG	2.00	0.42
2:C:201:ILE:HA	2:C:216:ARG:HA	2.01	0.42
2:C:132:PRO:HB3	2:C:143:ALA:O	2.19	0.42
2:E:82:MET:HB2	2:E:85:LEU:HD21	2.02	0.42
3:F:193:VAL:HG23	3:F:211:PHE:O	2.20	0.42
1:B:387:LEU:C	1:B:390:LEU:HD12	2.44	0.42
2:C:187:VAL:HG11	3:D:137:LEU:CD1	2.49	0.42
2:E:71:ARG:HG2	2:E:78:LEU:HD12	2.01	0.42
2:C:4:LEU:HD21	2:C:27:PHE:CE2	2.54	0.42
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.55	0.42
2:C:158:VAL:HG21	2:C:186:SER:HB2	2.01	0.42
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.54	0.42
1:A:444:LYS:HG2	1:A:448:ASN:HB2	2.02	0.42
1:B:366:SER:H	1:B:388:ASN:ND2	2.17	0.42
1:A:365:TYR:N	1:A:365:TYR:HD2	2.15	0.41
1:B:341:VAL:HG13	1:B:342:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:ARG:O	2:C:117:VAL:HG11	2.19	0.41
2:E:190:VAL:HG21	2:E:200:TYR:OH	2.20	0.41
1:A:340:GLU:O	1:A:344:ALA:HB2	2.20	0.41
3:F:193:VAL:HG23	3:F:211:PHE:C	2.45	0.41
1:A:425:LEU:HD21	1:A:512:VAL:HG11	2.02	0.41
1:A:439:ASN:O	1:A:443:SER:OG	2.37	0.41
1:A:505:TYR:OH	3:D:92:ALA:HB1	2.20	0.41
2:C:123:LYS:HD2	2:C:124:GLY:H	1.84	0.41
1:B:517:LEU:C	1:B:517:LEU:HD23	2.46	0.41
2:C:6:GLU:OE1	2:C:94:TYR:HA	2.21	0.41
3:F:153:ASP:OD2	3:F:192:LYS:HB2	2.20	0.41
1:A:392:PHE:CD2	1:A:515:PHE:HB3	2.55	0.41
1:B:395:VAL:HG22	1:B:515:PHE:HD2	1.85	0.41
2:E:176:LEU:HD13	2:E:182:TYR:CD2	2.55	0.41
3:F:136:CYS:HB2	3:F:150:TRP:CZ2	2.55	0.41
1:A:334:ASN:ND2	1:A:361:CYS:HA	2.36	0.40
1:B:387:LEU:HA	1:B:390:LEU:HD12	1.86	0.40
2:C:50:VAL:HG13	2:C:58:PHE:HB2	2.02	0.40
2:C:69:ILE:CG1	2:C:78:LEU:HD11	2.51	0.40
2:C:206:HIS:HB3	2:C:211:THR:OG1	2.21	0.40
3:F:35:TRP:CG	3:F:73:LEU:HD23	2.56	0.40
2:C:179:SER:HB3	2:C:181:LEU:H	1.87	0.40
2:E:33:TYR:CE2	2:E:100:PRO:HG3	2.57	0.40
3:F:165:VAL:HG12	3:F:166:THR:O	2.22	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:B:440:ASN:OD1	2:C:193:SER:OG[1_556]	2.18	0.02

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	194/227 (86%)	187 (96%)	7 (4%)	0	100	100
1	B	193/227 (85%)	182 (94%)	11 (6%)	0	100	100
2	C	212/233 (91%)	202 (95%)	10 (5%)	0	100	100
2	E	216/233 (93%)	208 (96%)	8 (4%)	0	100	100
3	D	213/216 (99%)	205 (96%)	8 (4%)	0	100	100
3	F	213/216 (99%)	202 (95%)	11 (5%)	0	100	100
All	All	1241/1352 (92%)	1186 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	169/200 (84%)	167 (99%)	2 (1%)	63	78
1	B	168/200 (84%)	167 (99%)	1 (1%)	78	88
2	C	180/197 (91%)	179 (99%)	1 (1%)	78	88
2	E	182/197 (92%)	182 (100%)	0	100	100
3	D	189/190 (100%)	188 (100%)	1 (0%)	81	89
3	F	189/190 (100%)	189 (100%)	0	100	100
All	All	1077/1174 (92%)	1072 (100%)	5 (0%)	81	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	TYR
1	A	367	VAL
1	B	335	LEU
2	C	178	SER
3	D	204	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	ASN
1	A	414	GLN
1	B	388	ASN
1	B	450	ASN
3	D	162	GLN
2	E	39	GLN
3	F	126	GLN
3	F	162	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 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	196/227 (86%)	1.34	38 (19%) 3 2	36, 54, 112, 156	0
1	B	195/227 (85%)	1.45	45 (23%) 2 1	39, 66, 140, 165	0
2	C	216/233 (92%)	1.25	29 (13%) 7 5	31, 53, 86, 153	0
2	E	218/233 (93%)	1.08	22 (10%) 12 11	37, 54, 81, 113	0
3	D	215/216 (99%)	1.01	20 (9%) 14 14	37, 51, 79, 104	0
3	F	215/216 (99%)	1.20	37 (17%) 4 3	40, 59, 100, 134	0
All	All	1255/1352 (92%)	1.22	191 (15%) 5 4	31, 56, 107, 165	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	520	ALA	6.0
2	C	136	SER	5.3
2	C	139	GLY	5.2
1	A	518	LEU	4.8
1	B	518	LEU	4.5
2	C	110	GLY	4.4
2	E	31	TRP	4.3
1	A	346	ARG	4.1
1	A	369	TYR	4.1
1	B	364	ASP	4.1
3	F	210	SER	3.9
3	D	187	ASP	3.9
1	A	363	ALA	3.8
1	A	391	CYS	3.8
3	F	196	CYS	3.7
2	C	102	TYR	3.7
3	F	79	GLN	3.7
3	F	183	LEU	3.6
2	C	202	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
3	F	116	SER	3.6
1	A	359	SER	3.6
3	F	207	VAL	3.6
2	E	102	TYR	3.6
1	B	384	PRO	3.5
3	F	78	LEU	3.5
1	B	515	PHE	3.4
2	E	179	SER	3.4
1	A	392	PHE	3.4
1	A	390	LEU	3.3
1	B	480	CYS	3.3
1	B	391	CYS	3.3
2	C	31	TRP	3.3
1	B	505	TYR	3.3
3	D	159	GLY	3.3
2	C	216	ARG	3.2
1	A	360	ASN	3.2
2	C	103	GLY	3.2
1	B	527	PRO	3.1
1	A	379	CYS	3.1
1	A	373	SER	3.1
2	C	104	ASP	3.1
1	A	527	PRO	3.1
1	A	387	LEU	3.1
3	F	152	VAL	3.0
1	A	480	CYS	3.0
2	E	150	ASP	3.0
1	B	363	ALA	3.0
1	B	445	VAL	3.0
2	C	108	TYR	2.9
3	D	72	THR	2.9
2	C	107	ASP	2.9
1	B	524	VAL	2.9
3	F	148	VAL	2.9
2	C	30	GLY	2.9
1	A	461	LEU	2.9
3	D	1	ASP	2.9
2	C	132	PRO	2.8
2	E	71	ARG	2.8
2	E	135	LYS	2.8
3	F	119	ILE	2.8
1	B	444	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	378	LYS	2.8
3	D	21	ILE	2.8
3	F	94	SER	2.8
1	B	413	GLY	2.8
1	B	517	LEU	2.8
3	F	198	VAL	2.8
1	B	382	VAL	2.7
1	A	423	TYR	2.7
1	B	381	GLY	2.7
1	B	383	SER	2.7
3	F	50	ALA	2.7
1	A	432	CYS	2.7
1	A	381	GLY	2.7
3	D	74	THR	2.7
3	D	91	SER	2.7
1	A	528	LYS	2.7
3	D	147	LYS	2.7
1	A	335	LEU	2.6
2	E	85	LEU	2.6
2	E	119	SER	2.6
3	D	70	ASP	2.6
1	B	420	ASP	2.6
3	F	4	MET	2.6
2	E	200	TYR	2.6
2	E	1	GLU	2.6
3	F	81	GLU	2.6
1	B	390	LEU	2.6
1	A	411	ALA	2.6
2	E	138	SER	2.5
3	F	205	SER	2.5
1	B	389	ASP	2.5
1	A	468	ILE	2.5
1	B	431	GLY	2.5
3	F	195	ALA	2.5
1	A	383	SER	2.5
1	B	482	GLY	2.5
1	B	478	THR	2.5
1	B	519	HIS	2.5
3	F	123	SER	2.5
1	B	450	ASN	2.4
2	C	36	TRP	2.4
2	E	103	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	188	VAL	2.4
2	E	174	ALA	2.4
2	E	83	ASN	2.4
3	F	19	VAL	2.4
2	C	28	THR	2.4
3	F	102	GLN	2.4
1	B	369	TYR	2.4
2	C	18	LEU	2.4
2	C	197	THR	2.4
1	B	406	GLU	2.4
2	C	195	LEU	2.3
3	D	24	ARG	2.3
1	A	368	LEU	2.3
1	B	385	THR	2.3
1	B	442	ASP	2.3
2	C	47	TRP	2.3
1	B	348	ALA	2.3
1	A	496	GLY	2.3
3	F	156	LEU	2.3
2	C	23	ALA	2.3
3	F	114	ALA	2.3
2	E	178	SER	2.3
1	A	517	LEU	2.3
1	B	336	CYS	2.2
3	D	25	ALA	2.2
3	F	23	CYS	2.2
3	F	163	GLU	2.2
3	F	31	ARG	2.2
2	E	133	SER	2.2
2	C	117	VAL	2.2
1	A	522	ALA	2.2
3	F	215	GLU	2.2
2	C	105	TYR	2.2
1	A	334	ASN	2.2
1	B	481	ASN	2.2
3	F	187	ASP	2.2
3	D	137	LEU	2.2
3	D	183	LEU	2.2
3	F	193	VAL	2.2
1	B	347	PHE	2.2
1	B	522	ALA	2.2
2	E	76	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	384	PRO	2.2
3	F	76	SER	2.2
2	C	98	VAL	2.2
2	C	27	PHE	2.2
3	D	95	THR	2.2
2	E	81	GLN	2.2
1	B	526	GLY	2.2
2	E	147	LEU	2.2
1	A	341	VAL	2.2
1	B	333	THR	2.1
2	C	111	GLN	2.1
3	F	194	TYR	2.1
1	B	400	PHE	2.1
3	F	43	ALA	2.1
3	F	186	ALA	2.1
1	A	465	GLU	2.1
1	B	403	ARG	2.1
1	A	378	LYS	2.1
3	D	49	TYR	2.1
1	A	372	ALA	2.1
3	D	109	LYS	2.1
3	D	6	GLN	2.1
2	E	78	LEU	2.1
2	E	59	TYR	2.1
1	A	338	PHE	2.1
3	F	13	ALA	2.1
3	F	182	THR	2.1
2	C	76	ASN	2.1
2	C	210	ASN	2.1
1	A	525	CYS	2.1
1	A	433	VAL	2.1
3	F	124	ASP	2.0
2	C	193	SER	2.0
3	D	77	SER	2.0
3	F	133	SER	2.0
3	F	170	SER	2.0
1	A	337	PRO	2.0
1	B	507	PRO	2.0
3	D	156	LEU	2.0
1	B	451	TYR	2.0
3	D	163	GLU	2.0
2	E	197	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	441	LEU	2.0
1	A	439	ASN	2.0
1	B	362	VAL	2.0
1	B	453	TYR	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.