



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2026 – 03:27 PM JST

PDB ID : 9LFO / pdb_00009lfo
Title : Complex structure of THC-2199 Fab bound to SARS-CoV-2 XBB.1.5 RBD
Authors : Wang, X.; Guo, F.
Deposited on : 2025-01-08
Resolution : 2.91 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

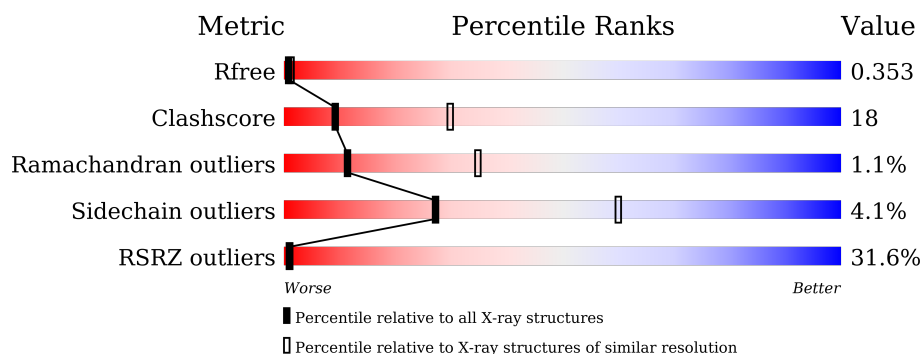
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	C	219	26% 71% 15% • 12%
1	F	219	22% 58% 30% • 12%
2	A	232	27% 63% 34% •
2	D	232	35% 71% 25% • •
3	B	219	27% 71% 26% •
3	E	219	45% 63% 32% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9932 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	C	192	Total	C	N	O	S	0	0	0
			1527	987	255	277	8			
1	F	193	Total	C	N	O	S	0	0	0
			1535	991	257	279	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
F	339	HIS	GLY	variant	UNP P0DTC2
F	346	THR	ARG	variant	UNP P0DTC2
F	368	ILE	LEU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	376	ALA	THR	variant	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	445	PRO	VAL	variant	UNP P0DTC2
F	446	SER	GLY	variant	UNP P0DTC2
F	460	LYS	ASN	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2
F	478	LYS	THR	variant	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	486	PRO	PHE	variant	UNP P0DTC2
F	490	SER	PHE	variant	UNP P0DTC2
F	498	ARG	GLN	variant	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	variant	UNP P0DTC2

- Molecule 2 is a protein called THC-2199 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	232	Total	C	N	O	S	0	0	0
			1760	1112	293	347	8			
2	D	228	Total	C	N	O	S	0	0	0
			1730	1096	288	339	7			

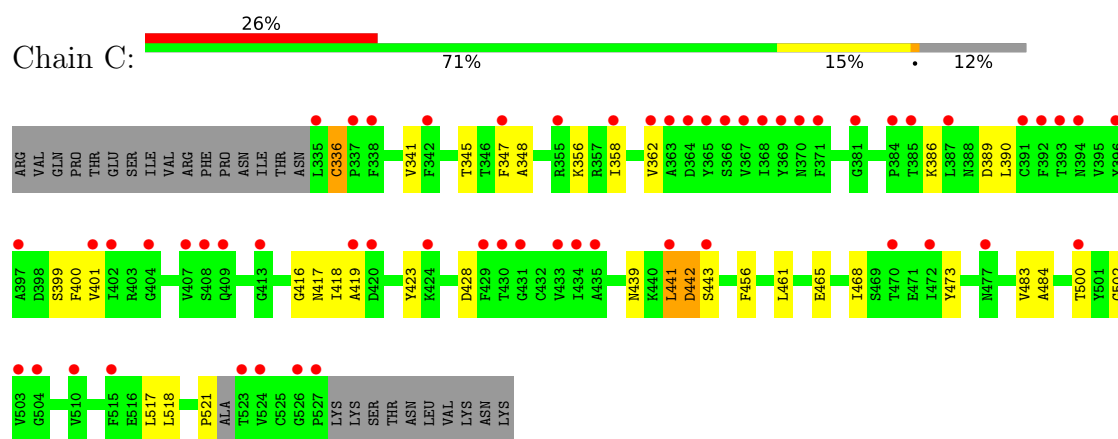
- Molecule 3 is a protein called THC-2199 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	219	Total	C	N	O	S	0	0	0
			1690	1054	290	339	7			
3	E	219	Total	C	N	O	S	0	0	0
			1690	1054	290	339	7			

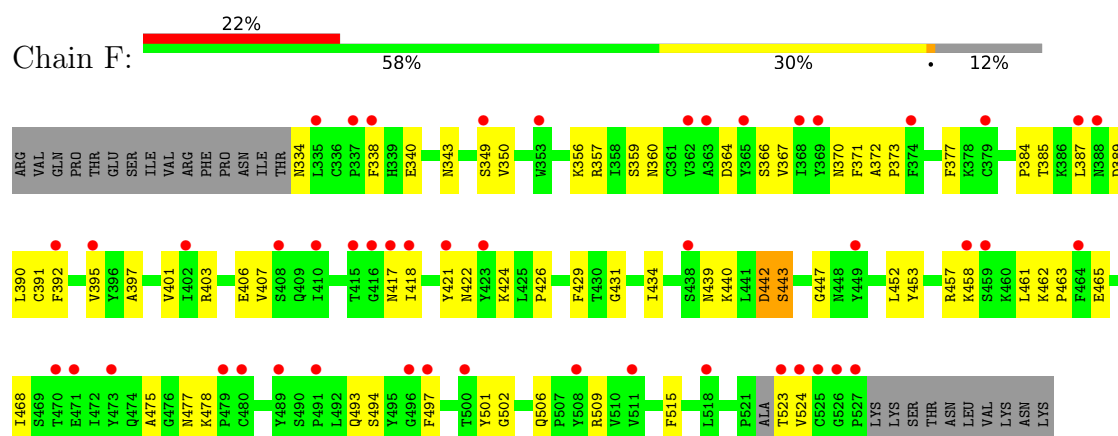
3 Residue-property plots [i](#)

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.

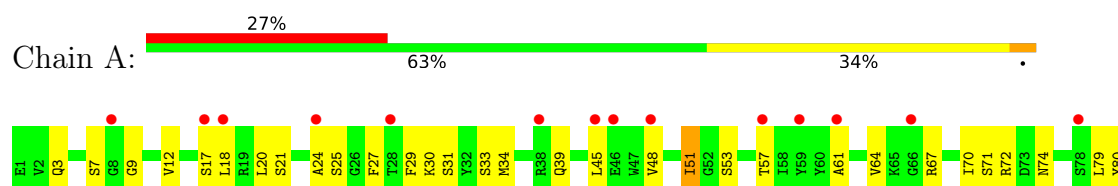
• Molecule 1: Spike protein S1

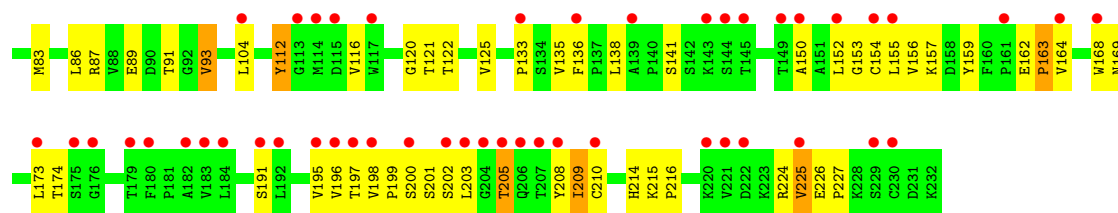


• Molecule 1: Spike protein S1

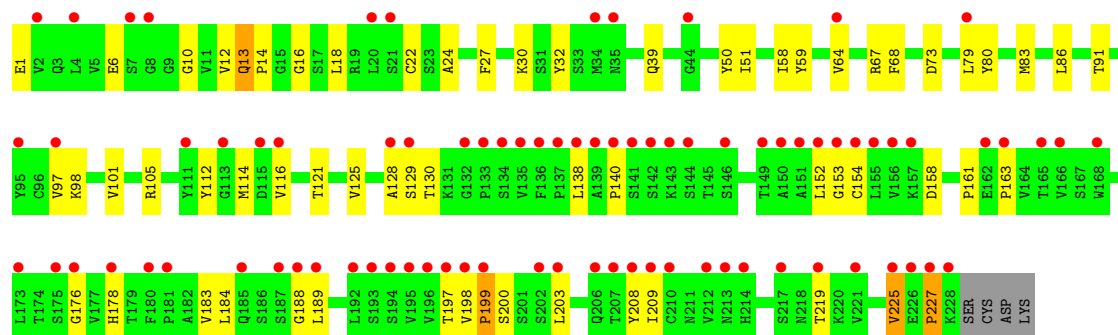


• Molecule 2: THC-2199 Heavy chain

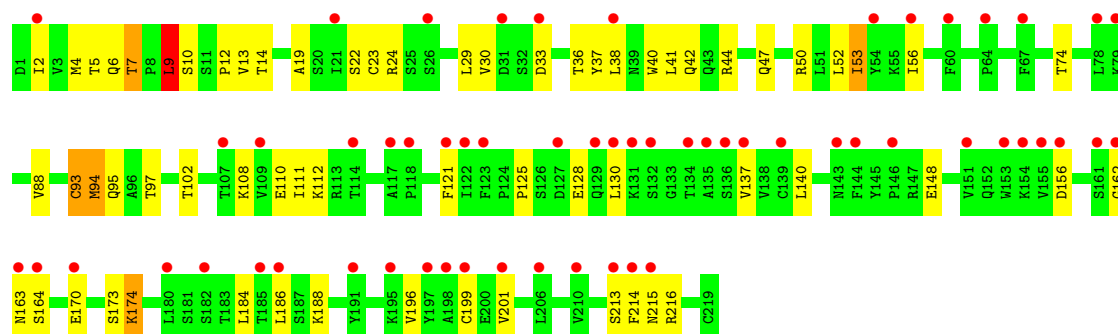




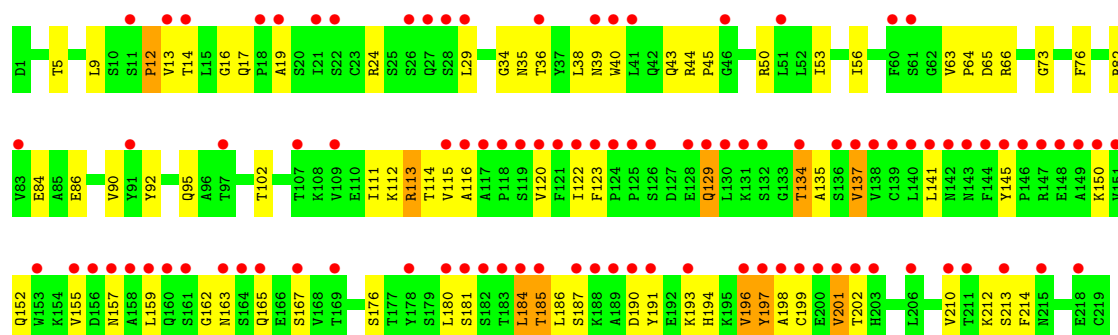
• Molecule 2: THC-2199 Heavy chain



• Molecule 3: THC-2199 Light chain



• Molecule 3: THC-2199 Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.79Å 120.30Å 317.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 2.91 48.89 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.89-2.91) 99.8 (48.89-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.300 , 0.351 0.351 , 0.353	Depositor DCC
R_{free} test set	2000 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	9932	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 4.76% 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	C	0.91	0/1575	1.23	3/2145 (0.1%)
1	F	0.93	0/1583	1.24	5/2156 (0.2%)
2	A	0.95	0/1803	1.24	2/2450 (0.1%)
2	D	0.97	1/1773 (0.1%)	1.28	5/2412 (0.2%)
3	B	0.95	1/1725 (0.1%)	1.27	3/2340 (0.1%)
3	E	0.97	0/1725	1.28	5/2340 (0.2%)
All	All	0.95	2/10184 (0.0%)	1.26	23/13843 (0.2%)

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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	199	PRO	N-CD	-7.90	1.36	1.47
3	B	9	LEU	CA-C	5.49	1.60	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	439	ASN	N-CA-C	-11.50	98.68	113.17
1	F	338	PHE	N-CA-C	-9.85	100.39	111.82
1	F	340	GLU	N-CA-C	8.56	121.69	111.33
3	B	164	SER	N-CA-C	8.19	122.60	108.76
3	E	137	VAL	N-CA-C	8.11	119.84	107.99
3	B	163	ASN	N-CA-C	7.30	126.35	110.80
3	B	162	GLY	N-CA-C	-7.06	105.57	115.32
1	C	441	LEU	N-CA-C	6.97	119.47	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	113	ARG	N-CA-C	6.66	116.84	108.45
2	D	225	VAL	N-CA-CB	6.19	120.56	111.52
2	D	129	SER	N-CA-C	6.09	118.39	110.53
1	C	345	THR	N-CA-C	-6.03	104.71	111.28
1	F	407	VAL	N-CA-C	-5.93	104.73	110.72
1	F	502	GLY	CA-C-O	-5.77	117.62	122.29
3	E	115	VAL	N-CA-C	-5.74	101.62	109.37
2	A	225	VAL	N-CA-CB	-5.70	104.15	110.99
2	D	128	ALA	N-CA-C	5.64	118.41	110.23
2	D	227	PRO	N-CA-C	-5.51	101.12	112.47
2	D	130	THR	N-CA-C	-5.46	101.78	109.96
3	E	29	LEU	N-CA-C	-5.34	106.54	113.16
1	F	443	SER	N-CA-C	-5.29	104.41	111.02
2	A	31	SER	N-CA-C	-5.18	106.81	112.72
3	E	134	THR	N-CA-C	5.02	117.08	108.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	7	THR	Peptide
3	B	9	LEU	Mainchain

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	C	1527	0	1454	58	4
1	F	1535	0	1460	56	24
2	A	1760	0	1719	75	59
2	D	1730	0	1692	58	0
3	B	1690	0	1653	52	0
3	E	1690	0	1653	80	83
All	All	9932	0	9631	356	87

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 18.

All (356) 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:C:347:PHE:HZ	1:C:400:PHE:N	1.09	1.50
3:E:191:TYR:HA	3:E:194:HIS:CE1	1.51	1.46
1:C:347:PHE:CD2	1:C:401:VAL:HG23	1.53	1.42
3:E:44:ARG:NH1	3:E:45:PRO:HG2	1.36	1.36
3:E:129:GLN:NE2	3:E:134:THR:HG22	1.38	1.34
3:E:129:GLN:HE21	3:E:134:THR:CG2	1.41	1.33
1:C:347:PHE:CZ	1:C:400:PHE:N	1.98	1.31
1:C:389:ASP:O	1:C:390:LEU:HD12	1.30	1.30
2:A:17:SER:O	2:A:18:LEU:HD12	1.31	1.30
3:E:44:ARG:NH1	3:E:45:PRO:CG	1.95	1.29
1:C:347:PHE:CE2	1:C:400:PHE:C	2.16	1.23
1:C:347:PHE:CZ	1:C:400:PHE:CA	2.25	1.19
3:E:44:ARG:HH11	3:E:45:PRO:CD	1.58	1.16
1:F:389:ASP:O	1:F:390:LEU:HD12	1.51	1.09
2:A:133:PRO:HB2	2:A:156:VAL:CG2	1.82	1.09
2:A:12:VAL:HG21	2:A:18:LEU:HD13	1.32	1.09
3:E:44:ARG:HH11	3:E:45:PRO:CG	1.59	1.08
2:A:12:VAL:CG2	2:A:18:LEU:HD22	1.83	1.08
2:D:140:PRO:HG3	2:D:152:LEU:HD13	1.36	1.05
1:C:483:VAL:HG23	1:C:484:ALA:H	1.18	1.05
2:A:12:VAL:HG21	2:A:18:LEU:CD1	1.86	1.04
2:A:12:VAL:CG2	2:A:18:LEU:CD2	2.36	1.03
3:E:44:ARG:HH11	3:E:45:PRO:HD2	1.22	1.03
1:C:347:PHE:HZ	1:C:400:PHE:CA	1.65	1.03
3:E:191:TYR:CA	3:E:194:HIS:CE1	2.41	1.02
1:F:364:ASP:OD2	1:F:367:VAL:CG2	2.08	1.02
3:E:129:GLN:HG2	3:E:134:THR:O	1.58	1.02
3:E:194:HIS:CD2	3:E:197:TYR:HE2	1.78	1.02
1:C:336:CYS:SG	1:C:358:ILE:CG2	2.48	1.01
3:E:44:ARG:HD2	3:E:45:PRO:HD2	1.39	1.01
1:C:347:PHE:CZ	1:C:400:PHE:C	2.39	1.00
2:A:133:PRO:HB2	2:A:156:VAL:HG23	1.41	0.99
1:C:347:PHE:CE2	1:C:400:PHE:CA	2.45	0.99
1:F:442:ASP:OD1	1:F:443:SER:N	1.95	0.98
3:E:191:TYR:HA	3:E:194:HIS:HE1	1.23	0.98
3:E:194:HIS:CD2	3:E:197:TYR:CE2	2.51	0.98
1:C:347:PHE:CD2	1:C:401:VAL:CG2	2.46	0.97
1:C:347:PHE:HE2	1:C:400:PHE:C	1.64	0.97
1:C:347:PHE:HE2	1:C:401:VAL:N	1.61	0.97
3:B:2:ILE:HG22	3:B:4:MET:HE2	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:6:GLN:OE1	3:B:93:CYS:SG	2.25	0.94
2:A:71:SER:HB2	2:A:80:TYR:HB2	1.45	0.94
1:C:347:PHE:HD2	1:C:401:VAL:HG23	1.25	0.94
1:C:389:ASP:C	1:C:390:LEU:HD12	1.96	0.91
2:D:140:PRO:CG	2:D:152:LEU:HD13	2.00	0.91
1:F:387:LEU:HD23	1:F:390:LEU:HD22	1.54	0.89
2:A:17:SER:C	2:A:18:LEU:HD12	1.95	0.89
3:E:44:ARG:HH12	3:E:45:PRO:HG2	1.12	0.89
2:A:12:VAL:HG23	2:A:18:LEU:HD22	1.53	0.89
1:C:347:PHE:CE2	1:C:401:VAL:HG23	2.06	0.89
1:C:441:LEU:HD12	1:C:442:ASP:N	1.90	0.87
3:E:129:GLN:HE21	3:E:134:THR:HG22	0.71	0.86
1:C:417:ASN:OD1	1:C:418:ILE:N	2.08	0.86
2:D:91:THR:HG22	2:D:125:VAL:H	1.40	0.85
1:C:336:CYS:SG	1:C:358:ILE:HG23	2.16	0.85
1:C:347:PHE:CE2	1:C:400:PHE:HA	2.10	0.85
3:E:113:ARG:HG2	3:E:114:THR:N	1.91	0.85
2:D:6:GLU:HB2	2:D:121:THR:HG23	1.57	0.84
2:A:12:VAL:HG21	2:A:18:LEU:CD2	2.07	0.83
1:F:389:ASP:C	1:F:390:LEU:HD12	2.03	0.82
1:F:417:ASN:OD1	1:F:418:ILE:HG12	1.79	0.82
3:E:113:ARG:HG2	3:E:114:THR:H	1.41	0.82
2:A:83:MET:HB3	2:A:86:LEU:HD21	1.62	0.82
2:A:138:LEU:HD11	2:A:155:LEU:HB2	1.62	0.81
2:A:12:VAL:HG21	2:A:18:LEU:HD22	1.60	0.81
2:D:198:VAL:HG22	2:D:199:PRO:HD2	1.61	0.81
2:A:133:PRO:CB	2:A:156:VAL:CG2	2.60	0.80
3:B:24:ARG:HE	3:B:74:THR:HB	1.44	0.80
1:C:347:PHE:CZ	1:C:399:SER:C	2.60	0.79
1:C:483:VAL:HG23	1:C:484:ALA:N	1.97	0.79
1:F:364:ASP:OD2	1:F:367:VAL:HB	1.82	0.79
1:C:347:PHE:CE1	1:C:399:SER:HB2	2.18	0.79
3:B:29:LEU:HB3	3:B:97:THR:HG21	1.64	0.79
1:C:347:PHE:HE1	1:C:399:SER:HB2	1.48	0.78
1:C:347:PHE:HZ	1:C:400:PHE:H	1.27	0.78
2:A:150:ALA:O	2:A:197:THR:HA	1.84	0.78
1:C:347:PHE:CE2	1:C:401:VAL:N	2.44	0.78
3:B:2:ILE:HG22	3:B:4:MET:CE	2.13	0.77
1:F:364:ASP:OD2	1:F:367:VAL:CB	2.33	0.76
3:B:9:LEU:HD12	3:B:10:SER:N	2.00	0.76
2:A:12:VAL:CG2	2:A:18:LEU:CD1	2.65	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:417:ASN:OD1	1:F:418:ILE:N	2.19	0.75
3:E:44:ARG:HH12	3:E:45:PRO:CG	1.81	0.75
3:E:129:GLN:CG	3:E:134:THR:O	2.34	0.75
2:D:183:VAL:HG11	3:E:165:GLN:HB3	1.65	0.75
3:E:50:ARG:HH12	3:E:63:VAL:HG22	1.50	0.75
2:A:91:THR:HG22	2:A:125:VAL:H	1.51	0.74
3:B:2:ILE:CG2	3:B:4:MET:CE	2.65	0.74
2:A:173:LEU:HD13	2:A:196:VAL:HG21	1.69	0.74
3:E:44:ARG:CD	3:E:45:PRO:HD2	2.16	0.74
3:E:13:VAL:HG11	3:E:19:ALA:HB2	1.69	0.73
2:D:116:VAL:HB	3:E:50:ARG:HG3	1.71	0.73
1:C:347:PHE:CZ	1:C:400:PHE:HA	2.20	0.73
1:C:500:THR:HG21	2:D:105:ARG:O	1.88	0.73
3:B:2:ILE:CG2	3:B:4:MET:HE2	2.18	0.73
1:F:364:ASP:OD2	1:F:367:VAL:HG23	1.89	0.72
3:E:141:LEU:HD21	3:E:201:VAL:HG11	1.71	0.72
1:C:347:PHE:CD2	1:C:348:ALA:N	2.57	0.72
2:A:198:VAL:HG22	2:A:199:PRO:HD2	1.72	0.71
2:A:116:VAL:HG12	2:A:116:VAL:O	1.91	0.71
2:D:12:VAL:HG11	2:D:86:LEU:HD22	1.71	0.71
2:A:9:GLY:HA3	2:A:121:THR:HG23	1.73	0.71
3:E:191:TYR:CA	3:E:194:HIS:HE1	1.94	0.70
1:C:347:PHE:CD2	1:C:348:ALA:O	2.45	0.69
3:E:113:ARG:CG	3:E:114:THR:H	2.06	0.69
2:A:173:LEU:HD13	2:A:196:VAL:CG2	2.22	0.69
1:F:403:ARG:HB2	1:F:406:GLU:OE1	1.92	0.69
3:B:184:LEU:CD2	3:B:186:LEU:HG	2.22	0.68
3:E:120:VAL:HG12	3:E:141:LEU:HG	1.76	0.68
3:B:5:THR:HB	3:B:24:ARG:HB3	1.76	0.68
2:A:116:VAL:HG11	3:B:50:ARG:HD2	1.76	0.68
3:E:44:ARG:NH1	3:E:45:PRO:CD	2.40	0.68
1:C:347:PHE:CE2	1:C:348:ALA:O	2.47	0.67
3:E:129:GLN:CG	3:E:134:THR:HB	2.24	0.67
2:A:12:VAL:CG2	2:A:18:LEU:HD21	2.24	0.67
2:D:198:VAL:CG2	2:D:199:PRO:HD2	2.25	0.67
1:F:364:ASP:OD2	1:F:367:VAL:HG21	1.93	0.67
1:C:441:LEU:CD1	1:C:443:SER:H	2.08	0.67
3:E:163:ASN:OD1	3:E:163:ASN:O	2.13	0.67
2:D:12:VAL:HG11	2:D:86:LEU:CD2	2.25	0.66
2:D:16:GLY:O	2:D:86:LEU:HD13	1.95	0.66
3:E:113:ARG:CG	3:E:114:THR:N	2.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:194:HIS:CD2	3:E:197:TYR:CD2	2.84	0.66
1:F:406:GLU:HG2	1:F:418:ILE:HG13	1.77	0.66
2:D:140:PRO:CD	2:D:152:LEU:HD13	2.25	0.66
2:D:176:GLY:HA3	2:D:197:THR:H	1.62	0.64
2:A:173:LEU:CD1	2:A:196:VAL:HG21	2.28	0.64
3:E:44:ARG:NH1	3:E:45:PRO:HD2	2.05	0.64
3:B:215:ASN:OD1	3:B:216:ARG:N	2.30	0.64
1:C:347:PHE:CG	1:C:348:ALA:N	2.58	0.63
3:E:129:GLN:HE21	3:E:134:THR:CB	2.07	0.63
3:E:38:LEU:HD22	3:E:76:PHE:CD2	2.33	0.63
1:C:441:LEU:HD12	1:C:443:SER:H	1.63	0.63
1:C:483:VAL:CG2	1:C:484:ALA:H	2.01	0.63
2:D:138:LEU:O	2:D:152:LEU:HD12	1.99	0.62
1:C:336:CYS:SG	1:C:358:ILE:HG22	2.39	0.62
1:C:417:ASN:OD1	1:C:418:ILE:HG12	1.99	0.62
2:A:9:GLY:CA	2:A:121:THR:HG23	2.30	0.62
1:F:439:ASN:HD21	1:F:506:GLN:HG2	1.65	0.62
1:F:424:LYS:HB3	1:F:463:PRO:HA	1.81	0.61
1:F:477:ASN:HD21	2:D:1:GLU:H1	1.47	0.61
2:A:12:VAL:HG21	2:A:18:LEU:CG	2.30	0.61
3:B:13:VAL:HG12	3:B:14:THR:N	2.14	0.61
1:F:461:LEU:HD21	1:F:465:GLU:O	2.00	0.61
1:F:461:LEU:HD23	1:F:462:LYS:O	2.01	0.61
2:A:224:ARG:NH1	2:A:226:GLU:OE2	2.31	0.61
1:C:500:THR:O	1:C:500:THR:HG22	2.00	0.60
2:A:12:VAL:CG2	2:A:18:LEU:HD13	2.19	0.60
2:A:116:VAL:CG1	3:B:50:ARG:HA	2.31	0.60
2:A:163:PRO:HG2	2:A:216:PRO:HD3	1.84	0.60
3:B:13:VAL:HG21	3:B:19:ALA:HB2	1.84	0.60
1:F:360:ASN:HA	1:F:523:THR:HB	1.82	0.60
2:A:83:MET:HE2	2:A:86:LEU:CD2	2.32	0.59
2:D:22:CYS:HB3	2:D:79:LEU:HB3	1.83	0.59
3:B:6:GLN:OE1	3:B:23:CYS:SG	2.60	0.59
3:B:42:GLN:HB2	3:B:52:LEU:HD11	1.84	0.59
1:F:406:GLU:HG2	1:F:418:ILE:CG1	2.33	0.59
3:E:191:TYR:HA	3:E:194:HIS:NE2	2.10	0.59
3:E:38:LEU:HD22	3:E:76:PHE:CG	2.38	0.58
2:A:135:VAL:HG13	2:A:154:CYS:HB3	1.85	0.58
2:D:140:PRO:HG3	2:D:152:LEU:CD1	2.23	0.58
3:E:129:GLN:NE2	3:E:134:THR:CG2	2.22	0.58
2:A:159:TYR:HE2	2:A:162:GLU:HG2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLU:CB	2:D:121:THR:HG23	2.31	0.58
2:D:154:CYS:SG	2:D:225:VAL:HG13	2.42	0.58
2:D:198:VAL:HG22	2:D:199:PRO:CD	2.33	0.58
2:D:152:LEU:CD2	2:D:225:VAL:HG23	2.34	0.58
2:A:198:VAL:HG22	2:A:199:PRO:CD	2.34	0.58
2:D:6:GLU:HB2	2:D:121:THR:CG2	2.30	0.58
2:A:136:PHE:O	2:A:138:LEU:HD12	2.04	0.58
1:F:477:ASN:ND2	2:D:1:GLU:N	2.51	0.58
1:F:377:PHE:HD1	1:F:434:ILE:HG12	1.69	0.58
1:F:458:LYS:HA	2:D:30:LYS:HZ3	1.69	0.58
2:A:12:VAL:HG22	2:A:18:LEU:HD21	1.86	0.57
2:D:154:CYS:SG	2:D:225:VAL:CG1	2.92	0.57
3:E:129:GLN:HG3	3:E:134:THR:HB	1.84	0.57
1:F:395:VAL:CG1	1:F:515:PHE:HD1	2.17	0.57
3:B:2:ILE:HG21	3:B:4:MET:CE	2.34	0.57
3:B:33:ASP:OD2	3:B:37:TYR:OH	2.19	0.57
3:B:40:TRP:C	3:B:41:LEU:HD12	2.29	0.56
1:F:421:TYR:CD1	1:F:457:ARG:HB3	2.40	0.56
3:E:38:LEU:CD2	3:E:76:PHE:CG	2.88	0.56
2:D:116:VAL:CB	3:E:50:ARG:HG3	2.36	0.56
3:E:111:ILE:HG21	3:E:176:SER:HB3	1.87	0.56
2:A:133:PRO:CB	2:A:156:VAL:HG22	2.36	0.56
3:B:14:THR:OG1	3:B:112:LYS:HB3	2.06	0.56
2:D:24:ALA:HB1	2:D:27:PHE:CE1	2.41	0.56
2:A:83:MET:HE2	2:A:86:LEU:HD21	1.88	0.55
3:E:137:VAL:HG23	3:E:137:VAL:O	2.06	0.55
1:C:347:PHE:CZ	1:C:400:PHE:O	2.58	0.55
2:A:136:PHE:HB2	2:A:155:LEU:HB3	1.89	0.55
2:D:138:LEU:O	2:D:152:LEU:CD1	2.55	0.54
3:E:5:THR:OG1	3:E:24:ARG:HB3	2.07	0.54
1:F:350:VAL:HG21	1:F:418:ILE:HG23	1.89	0.54
1:F:461:LEU:CD2	1:F:465:GLU:HB3	2.38	0.54
1:F:406:GLU:HB3	1:F:418:ILE:HG13	1.89	0.54
2:A:33:SER:HA	2:A:72:ARG:HH12	1.73	0.54
2:A:64:VAL:HA	2:A:67:ARG:HE	1.73	0.54
2:A:29:PHE:HZ	2:A:79:LEU:HB2	1.73	0.53
3:B:184:LEU:HD23	3:B:186:LEU:HG	1.90	0.53
2:A:133:PRO:HB2	2:A:156:VAL:HG22	1.82	0.53
1:C:473:TYR:OH	2:A:30:LYS:NZ	2.42	0.53
1:C:441:LEU:HD12	1:C:443:SER:N	2.24	0.53
2:D:184:LEU:HD11	2:D:188:GLY:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:VAL:CG2	2:D:199:PRO:CD	2.86	0.53
1:F:475:ALA:HB1	2:D:32:TYR:HE1	1.73	0.52
2:D:64:VAL:HA	2:D:67:ARG:HE	1.74	0.52
2:D:98:LYS:HE3	2:D:114:MET:HB3	1.92	0.52
2:A:48:VAL:HG13	2:A:64:VAL:HG21	1.92	0.52
3:B:9:LEU:HD12	3:B:9:LEU:C	2.34	0.52
2:A:196:VAL:HG11	2:A:208:TYR:CE1	2.45	0.52
1:F:391:CYS:HA	1:F:524:VAL:O	2.10	0.52
1:F:447:GLY:HA2	1:F:497:PHE:O	2.10	0.52
1:F:349:SER:HB3	1:F:452:LEU:O	2.10	0.52
3:E:194:HIS:HD2	3:E:197:TYR:CD2	2.27	0.52
1:F:461:LEU:HD21	1:F:465:GLU:HB3	1.91	0.52
1:F:477:ASN:HD21	2:D:1:GLU:N	2.07	0.52
2:A:17:SER:C	2:A:18:LEU:CD1	2.78	0.51
1:C:456:PHE:HZ	2:A:104:LEU:HD11	1.75	0.51
3:B:44:ARG:HB3	3:B:47:GLN:HB2	1.92	0.51
1:C:500:THR:HG22	3:E:35:ASN:ND2	2.25	0.51
2:D:51:ILE:HG13	2:D:58:ILE:HG12	1.92	0.51
3:E:194:HIS:NE2	3:E:197:TYR:CE2	2.77	0.51
3:E:190:ASP:O	3:E:194:HIS:CE1	2.63	0.51
3:B:36:THR:HB	3:B:56:ILE:HD11	1.92	0.51
1:C:500:THR:HG22	3:E:35:ASN:HD21	1.76	0.51
2:D:152:LEU:HD23	2:D:225:VAL:HG23	1.92	0.51
1:C:441:LEU:HD12	1:C:442:ASP:H	1.75	0.51
3:B:37:TYR:H	3:B:97:THR:HG22	1.75	0.51
2:A:29:PHE:HD2	2:A:74:ASN:HA	1.77	0.50
1:F:350:VAL:HG11	1:F:418:ILE:HD12	1.94	0.50
1:F:372:ALA:N	1:F:373:PRO:HD2	2.26	0.50
2:D:83:MET:O	2:D:86:LEU:HD11	2.11	0.50
1:C:389:ASP:C	1:C:390:LEU:CD1	2.78	0.50
2:A:93:VAL:HA	2:A:122:THR:HA	1.93	0.50
3:E:12:PRO:HB2	3:E:112:LYS:HD3	1.94	0.50
2:D:203:LEU:HD12	2:D:208:TYR:HE2	1.77	0.49
2:A:9:GLY:CA	2:A:121:THR:CG2	2.91	0.49
1:F:406:GLU:CG	1:F:418:ILE:HG13	2.42	0.49
1:C:416:GLY:H	1:C:419:ALA:HB3	1.77	0.49
3:E:36:THR:HB	3:E:56:ILE:HD11	1.94	0.49
1:C:336:CYS:HB2	1:C:362:VAL:O	2.12	0.49
3:B:13:VAL:CG1	3:B:14:THR:N	2.75	0.49
3:B:88:VAL:HG21	3:B:111:ILE:HG12	1.94	0.49
1:C:336:CYS:SG	1:C:358:ILE:HG21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:LEU:HG	1:C:465:GLU:HB3	1.95	0.48
2:A:3:GLN:HG3	2:A:25:SER:HB2	1.94	0.48
2:A:24:ALA:HB1	2:A:27:PHE:CZ	2.48	0.48
2:A:215:LYS:N	2:A:216:PRO:HD2	2.29	0.48
2:D:73:ASP:HB2	2:D:80:TYR:HE2	1.77	0.48
2:D:158:ASP:HA	2:D:189:LEU:HB3	1.95	0.48
2:A:164:VAL:HG22	2:A:214:HIS:CD2	2.48	0.48
3:B:7:THR:HB	3:B:22:SER:HB2	1.95	0.48
1:F:477:ASN:ND2	2:D:1:GLU:H2	2.12	0.48
3:E:129:GLN:HG2	3:E:134:THR:C	2.34	0.48
2:D:200:SER:O	2:D:203:LEU:HB3	2.14	0.48
2:A:157:LYS:HG3	2:A:191:SER:HB2	1.95	0.47
1:F:364:ASP:CG	1:F:367:VAL:HB	2.38	0.47
2:D:203:LEU:CD1	2:D:208:TYR:CE2	2.96	0.47
3:B:4:MET:HE3	3:B:95:GLN:HG2	1.96	0.47
2:D:138:LEU:HB3	3:E:123:PHE:HB3	1.97	0.47
1:F:442:ASP:O	1:F:443:SER:C	2.57	0.47
2:A:169:ASN:HA	2:A:209:ILE:HG13	1.97	0.47
1:F:442:ASP:CG	1:F:443:SER:N	2.68	0.47
1:C:419:ALA:HA	1:C:423:TYR:O	2.15	0.47
2:D:140:PRO:HG2	2:D:227:PRO:HA	1.96	0.47
2:A:87:ARG:HB3	2:A:89:GLU:HG2	1.97	0.46
3:B:174:LYS:H	3:B:174:LYS:HG2	1.50	0.46
1:F:401:VAL:HG22	1:F:509:ARG:HG2	1.97	0.46
1:C:347:PHE:HD2	1:C:401:VAL:CG2	2.06	0.46
2:A:153:GLY:HA2	2:A:168:TRP:CZ2	2.50	0.46
1:F:377:PHE:CD2	1:F:377:PHE:O	2.69	0.46
2:A:195:VAL:HG21	3:B:140:LEU:HD21	1.98	0.46
2:A:39:GLN:HB2	2:A:45:LEU:HD23	1.98	0.46
2:D:39:GLN:HE22	3:E:43:GLN:HE22	1.64	0.46
3:E:17:GLN:OE1	3:E:17:GLN:HA	2.16	0.46
3:E:113:ARG:CD	3:E:176:SER:HB2	2.46	0.46
2:D:140:PRO:HD3	2:D:152:LEU:HD13	1.97	0.46
3:E:116:ALA:H	3:E:145:TYR:HB3	1.80	0.46
2:A:163:PRO:HD2	2:A:214:HIS:CD2	2.50	0.46
1:F:377:PHE:HZ	1:F:384:PRO:CB	2.29	0.45
1:F:452:LEU:HD23	1:F:494:SER:HA	1.97	0.45
3:B:108:LYS:NZ	3:B:148:GLU:OE2	2.49	0.45
3:E:129:GLN:CD	3:E:134:THR:O	2.59	0.45
3:B:94:MET:HA	3:B:102:THR:O	2.17	0.45
1:F:392:PHE:O	1:F:523:THR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:130:LEU:O	3:B:188:LYS:HB2	2.16	0.45
2:D:203:LEU:CD1	2:D:208:TYR:HE2	2.30	0.45
1:F:453:TYR:CE1	1:F:493:GLN:HB3	2.52	0.45
3:E:38:LEU:C	3:E:39:ASN:HD22	2.24	0.45
2:D:83:MET:C	2:D:86:LEU:HD11	2.41	0.45
3:E:129:GLN:HG2	3:E:134:THR:HB	1.98	0.45
1:F:426:PRO:HD2	1:F:429:PHE:HB2	1.99	0.44
2:D:67:ARG:HG3	2:D:68:PHE:CD1	2.52	0.44
2:A:138:LEU:HD11	2:A:155:LEU:CB	2.38	0.44
2:A:34:MET:HB3	2:A:79:LEU:HD22	1.98	0.44
3:E:198:ALA:HB2	3:E:213:SER:HB3	1.99	0.44
2:A:9:GLY:HA3	2:A:121:THR:CG2	2.47	0.44
2:D:50:TYR:HD2	2:D:59:TYR:HD2	1.64	0.44
2:A:51:ILE:HD12	2:A:70:ILE:HG23	1.99	0.43
2:A:20:LEU:CD2	2:A:121:THR:HG21	2.48	0.43
2:A:159:TYR:CE2	2:A:162:GLU:HG2	2.51	0.43
2:D:24:ALA:HB1	2:D:27:PHE:HE1	1.81	0.43
3:E:9:LEU:HD23	3:E:9:LEU:HA	1.77	0.43
2:A:112:TYR:HD1	2:A:112:TYR:HA	1.74	0.43
3:B:4:MET:HB3	3:B:23:CYS:SG	2.58	0.43
3:E:113:ARG:HD2	3:E:176:SER:HB2	2.01	0.43
3:B:156:ASP:HB2	3:B:196:VAL:O	2.18	0.43
1:F:357:ARG:HE	1:F:359:SER:HB3	1.83	0.43
1:F:395:VAL:HG12	1:F:515:PHE:HD1	1.84	0.43
1:F:418:ILE:HA	1:F:422:ASN:HD22	1.83	0.43
2:D:6:GLU:CB	2:D:121:THR:CG2	2.94	0.43
3:E:180:LEU:HD23	3:E:181:SER:N	2.34	0.43
1:C:341:VAL:HG11	1:C:356:LYS:HB2	2.00	0.43
3:E:40:TRP:HB2	3:E:53:ILE:HB	2.00	0.43
3:B:121:PHE:HD2	3:B:140:LEU:HD23	1.84	0.43
1:C:417:ASN:OD1	1:C:417:ASN:C	2.62	0.43
1:F:431:GLY:HA2	1:F:515:PHE:CD2	2.53	0.43
3:E:191:TYR:N	3:E:194:HIS:HE1	2.15	0.43
3:E:190:ASP:C	3:E:194:HIS:HE1	2.26	0.42
3:B:13:VAL:CG2	3:B:19:ALA:HB2	2.49	0.42
3:E:95:GLN:HG3	3:E:102:THR:H	1.84	0.42
3:E:90:VAL:HG23	3:E:92:TYR:CE2	2.55	0.42
2:D:13:GLN:HG2	2:D:14:PRO:HD2	2.02	0.42
3:B:13:VAL:O	3:B:112:LYS:N	2.51	0.42
2:A:61:ALA:HB3	2:A:64:VAL:HG22	2.02	0.42
1:F:356:LYS:HB3	1:F:397:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:52:LEU:HB2	3:B:53:ILE:H	1.69	0.41
2:A:116:VAL:HG11	3:B:50:ARG:HA	2.02	0.41
3:B:121:PHE:CD2	3:B:140:LEU:HD23	2.56	0.41
2:D:10:GLY:H	2:D:18:LEU:HD21	1.85	0.41
3:E:14:THR:HB	3:E:17:GLN:HG3	2.02	0.41
1:C:428:ASP:OD1	1:C:428:ASP:O	2.38	0.41
3:B:7:THR:N	3:B:22:SER:O	2.52	0.41
3:B:12:PRO:HA	3:B:110:GLU:HB2	2.02	0.41
3:B:13:VAL:CG1	3:B:14:THR:H	2.34	0.41
3:E:150:LYS:HB2	3:E:202:THR:HB	2.02	0.41
3:E:155:VAL:HG22	3:E:197:TYR:HA	2.03	0.41
3:E:210:VAL:HG22	3:E:212:LYS:HG2	2.01	0.41
1:F:377:PHE:HD1	1:F:434:ILE:CG1	2.34	0.41
1:F:395:VAL:HG11	1:F:515:PHE:HD1	1.84	0.41
2:D:138:LEU:HB2	2:D:153:GLY:O	2.21	0.41
3:E:64:PRO:HB2	3:E:66:ARG:HG2	2.02	0.41
2:A:133:PRO:HD3	2:A:214:HIS:ND1	2.36	0.41
1:C:502:GLY:HA3	3:E:34:GLY:O	2.20	0.40
3:B:5:THR:O	3:B:23:CYS:SG	2.80	0.40
3:B:13:VAL:HG12	3:B:14:THR:H	1.84	0.40
3:B:29:LEU:CD1	3:B:38:LEU:HD12	2.51	0.40
1:F:477:ASN:OD1	1:F:478:LYS:N	2.54	0.40
2:A:195:VAL:HG21	3:B:140:LEU:HD11	2.03	0.40
3:B:125:PRO:HD3	3:B:137:VAL:HG22	2.02	0.40
1:C:347:PHE:HE2	1:C:400:PHE:CA	2.08	0.40
3:B:186:LEU:HD23	3:B:186:LEU:HA	1.83	0.40
2:D:183:VAL:CG1	3:E:165:GLN:HB3	2.43	0.40
3:E:86:GLU:H	3:E:86:GLU:HG2	1.69	0.40
3:E:50:ARG:NH1	3:E:63:VAL:HG22	2.26	0.40

All (87) 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:F:370:ASN:ND2	3:E:84:GLU:CD[5_545]	0.40	1.80
2:A:205:THR:O	3:E:194:HIS:CD2[4_555]	0.50	1.70
2:A:226:GLU:CB	3:E:159:LEU:CD1[4_555]	0.60	1.60
2:A:199:PRO:C	3:E:186:LEU:CG[4_555]	0.66	1.54
2:A:226:GLU:CA	3:E:159:LEU:CB[4_555]	0.69	1.51
2:A:199:PRO:CA	3:E:186:LEU:CD2[4_555]	0.74	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:199:PRO:O	3:E:186:LEU:CD1[4_555]	0.75	1.45
2:A:199:PRO:O	3:E:186:LEU:CG[4_555]	0.96	1.24
2:A:200:SER:O	3:E:184:LEU:CD2[4_555]	1.01	1.19
2:A:226:GLU:CB	3:E:159:LEU:CG[4_555]	1.07	1.13
2:A:201:SER:OG	3:E:135:ALA:O[4_555]	1.14	1.06
2:A:225:VAL:O	3:E:159:LEU:N[4_555]	1.18	1.02
1:F:370:ASN:ND2	3:E:84:GLU:OE2[5_545]	1.20	1.00
2:A:199:PRO:N	3:E:186:LEU:CD2[4_555]	1.23	0.97
2:A:198:VAL:CG2	3:E:190:ASP:OD1[4_555]	1.30	0.90
2:A:226:GLU:CG	3:E:159:LEU:CG[4_555]	1.33	0.87
2:A:199:PRO:C	3:E:186:LEU:CD2[4_555]	1.34	0.86
2:A:227:PRO:CG	3:E:152:GLN:OE1[4_555]	1.34	0.86
1:C:428:ASP:OD2	1:C:521:PRO:CD[3_555]	1.39	0.81
2:A:205:THR:CG2	3:E:197:TYR:CG[4_555]	1.41	0.79
1:F:370:ASN:ND2	3:E:84:GLU:CG[5_545]	1.44	0.76
2:A:201:SER:CB	3:E:135:ALA:O[4_555]	1.51	0.69
1:F:370:ASN:ND2	3:E:84:GLU:OE1[5_545]	1.51	0.69
2:A:205:THR:O	3:E:194:HIS:NE2[4_555]	1.55	0.65
2:A:226:GLU:CA	3:E:159:LEU:CG[4_555]	1.55	0.65
2:A:226:GLU:CG	3:E:159:LEU:CD1[4_555]	1.55	0.65
2:A:226:GLU:N	3:E:159:LEU:CB[4_555]	1.56	0.64
2:A:199:PRO:CB	3:E:186:LEU:CA[4_555]	1.57	0.63
1:F:385:THR:O	3:E:86:GLU:OE2[5_545]	1.58	0.62
2:A:205:THR:CB	3:E:197:TYR:CD2[4_555]	1.60	0.60
2:A:205:THR:C	3:E:194:HIS:CD2[4_555]	1.61	0.59
2:A:199:PRO:CG	3:E:187:SER:N[4_555]	1.62	0.58
2:A:201:SER:OG	3:E:135:ALA:C[4_555]	1.65	0.55
1:F:371:PHE:N	3:E:82:ARG:NH2[5_545]	1.66	0.54
2:A:202:SER:OG	3:E:190:ASP:CB[4_555]	1.68	0.52
1:F:370:ASN:CG	3:E:84:GLU:CD[5_545]	1.70	0.50
2:A:200:SER:N	3:E:186:LEU:CG[4_555]	1.74	0.46
1:F:370:ASN:O	3:E:82:ARG:NE[5_545]	1.75	0.45
1:F:371:PHE:CA	3:E:82:ARG:NE[5_545]	1.75	0.45
2:A:200:SER:C	3:E:184:LEU:CD2[4_555]	1.76	0.44
1:F:370:ASN:C	3:E:82:ARG:NE[5_545]	1.76	0.44
1:F:371:PHE:N	3:E:82:ARG:NE[5_545]	1.77	0.43
2:A:199:PRO:CA	3:E:186:LEU:CG[4_555]	1.78	0.42
2:A:225:VAL:O	3:E:159:LEU:CA[4_555]	1.79	0.41
2:A:205:THR:O	3:E:194:HIS:CG[4_555]	1.81	0.39
1:F:372:ALA:N	3:E:16:GLY:O[5_545]	1.82	0.38
2:A:199:PRO:O	3:E:186:LEU:CD2[4_555]	1.84	0.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:205:THR:C	3:E:194:HIS:NE2[4_555]	1.85	0.35
2:A:205:THR:CG2	3:E:197:TYR:CB[4_555]	1.86	0.34
2:A:141:SER:C	3:E:162:GLY:O[4_555]	1.87	0.33
1:C:386:LYS:NZ	1:C:389:ASP:OD2[3_555]	1.89	0.31
2:A:199:PRO:CB	3:E:186:LEU:C[4_555]	1.90	0.30
2:A:200:SER:N	3:E:185:THR:O[4_555]	1.90	0.30
2:A:224:ARG:NH2	3:E:157:ASN:O[4_555]	1.90	0.30
1:F:370:ASN:O	3:E:82:ARG:CB[5_545]	1.91	0.29
1:F:371:PHE:N	3:E:82:ARG:CZ[5_545]	1.91	0.29
2:A:199:PRO:C	3:E:186:LEU:CD1[4_555]	1.92	0.28
2:A:226:GLU:CB	3:E:159:LEU:CB[4_555]	1.92	0.28
2:A:199:PRO:CB	3:E:187:SER:N[4_555]	1.93	0.27
2:A:202:SER:CB	3:E:190:ASP:CB[4_555]	1.93	0.27
2:A:199:PRO:CB	3:E:186:LEU:CB[4_555]	1.95	0.25
2:A:203:LEU:CD1	3:E:163:ASN:ND2[4_555]	1.96	0.24
1:F:366:SER:O	3:E:84:GLU:OE2[5_545]	1.96	0.24
1:C:428:ASP:CG	1:C:521:PRO:CD[3_555]	1.98	0.22
1:C:517:LEU:O	1:C:517:LEU:O[3_555]	1.98	0.22
1:F:370:ASN:CG	3:E:84:GLU:OE2[5_545]	1.98	0.22
2:A:141:SER:O	3:E:162:GLY:O[4_555]	1.99	0.21
2:A:199:PRO:CB	3:E:186:LEU:CD2[4_555]	1.99	0.21
1:F:371:PHE:CB	3:E:82:ARG:CZ[5_545]	2.00	0.20
2:A:205:THR:CG2	3:E:197:TYR:CD2[4_555]	2.01	0.19
2:A:199:PRO:C	3:E:186:LEU:CB[4_555]	2.02	0.18
2:A:226:GLU:C	3:E:159:LEU:CB[4_555]	2.02	0.18
1:F:370:ASN:CG	3:E:84:GLU:CG[5_545]	2.03	0.17
1:F:371:PHE:C	3:E:16:GLY:CA[5_545]	2.03	0.17
2:A:205:THR:CA	3:E:197:TYR:CD2[4_555]	2.04	0.16
1:F:371:PHE:CB	3:E:82:ARG:NE[5_545]	2.09	0.11
2:A:226:GLU:CA	3:E:159:LEU:CD1[4_555]	2.10	0.10
2:A:198:VAL:C	3:E:186:LEU:CD2[4_555]	2.11	0.09
1:F:372:ALA:N	3:E:16:GLY:CA[5_545]	2.11	0.09
2:A:205:THR:CG2	3:E:197:TYR:CD1[4_555]	2.12	0.08
1:F:372:ALA:CB	3:E:16:GLY:O[5_545]	2.13	0.07
2:A:205:THR:CB	3:E:197:TYR:CG[4_555]	2.15	0.05
2:A:225:VAL:C	3:E:159:LEU:CB[4_555]	2.16	0.04
1:F:370:ASN:N	3:E:82:ARG:NH2[5_545]	2.17	0.03
2:A:199:PRO:CD	3:E:190:ASP:OD2[4_555]	2.18	0.02
2:A:226:GLU:CA	3:E:159:LEU:CA[4_555]	2.18	0.02
1:F:370:ASN:C	3:E:82:ARG:NH2[5_545]	2.19	0.01

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	C	188/219 (86%)	171 (91%)	16 (8%)	1 (0%)	24	53
1	F	189/219 (86%)	172 (91%)	16 (8%)	1 (0%)	24	53
2	A	230/232 (99%)	216 (94%)	12 (5%)	2 (1%)	14	40
2	D	226/232 (97%)	212 (94%)	11 (5%)	3 (1%)	9	30
3	B	217/219 (99%)	206 (95%)	9 (4%)	2 (1%)	14	40
3	E	217/219 (99%)	199 (92%)	13 (6%)	5 (2%)	5	18
All	All	1267/1340 (95%)	1176 (93%)	77 (6%)	14 (1%)	11	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	442	ASP
3	B	213	SER
1	F	442	ASP
3	E	129	GLN
3	B	214	PHE
2	D	163	PRO
3	E	214	PHE
2	A	163	PRO
2	A	120	GLY
2	D	178	HIS
3	E	73	GLY
3	E	12	PRO
3	E	196	VAL
2	D	161	PRO

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	C	166/192 (86%)	163 (98%)	3 (2%)	51	79
1	F	167/192 (87%)	162 (97%)	5 (3%)	36	68
2	A	200/200 (100%)	188 (94%)	12 (6%)	17	45
2	D	196/200 (98%)	190 (97%)	6 (3%)	35	67
3	B	194/194 (100%)	184 (95%)	10 (5%)	21	50
3	E	194/194 (100%)	184 (95%)	10 (5%)	21	50
All	All	1117/1172 (95%)	1071 (96%)	46 (4%)	27	60

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	336	CYS
1	C	468	ILE
1	C	518	LEU
2	A	7	SER
2	A	21	SER
2	A	51	ILE
2	A	53	SER
2	A	57	THR
2	A	93	VAL
2	A	112	TYR
2	A	152	LEU
2	A	174	THR
2	A	205	THR
2	A	209	ILE
2	A	210	CYS
3	B	30	VAL
3	B	53	ILE
3	B	93	CYS
3	B	94	MET
3	B	128	GLU
3	B	170	GLU
3	B	173	SER
3	B	174	LYS
3	B	199	CYS
3	B	201	VAL
1	F	334	ASN
1	F	343	ASN

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Mol	Chain	Res	Type
1	F	440	LYS
1	F	468	ILE
1	F	501	TYR
2	D	13	GLN
2	D	97	VAL
2	D	101	VAL
2	D	112	TYR
2	D	209	ILE
2	D	219	THR
3	E	65	ASP
3	E	122	ILE
3	E	167	SER
3	E	184	LEU
3	E	185	THR
3	E	193	LYS
3	E	196	VAL
3	E	197	TYR
3	E	199	CYS
3	E	201	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	354	ASN
1	C	439	ASN
1	C	448	ASN
2	A	82	GLN
2	A	84	ASN
3	B	6	GLN
3	B	171	GLN
1	F	437	ASN
1	F	477	ASN
2	D	3	GLN
2	D	39	GLN
2	D	206	GLN
2	D	213	ASN
3	E	35	ASN
3	E	39	ASN
3	E	129	GLN
3	E	152	GLN
3	E	157	ASN
3	E	163	ASN

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Mol	Chain	Res	Type
3	E	194	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	C	192/219 (87%)	1.56	57 (29%) 1 1	26, 58, 82, 92	0
1	F	193/219 (88%)	1.53	48 (24%) 2 1	30, 54, 82, 99	0
2	A	232/232 (100%)	1.55	62 (26%) 1 1	25, 50, 101, 106	0
2	D	228/232 (98%)	1.98	82 (35%) 1 1	28, 57, 111, 118	0
3	B	219/219 (100%)	1.51	59 (26%) 1 1	27, 59, 90, 100	0
3	E	219/219 (100%)	1.93	98 (44%) 0 0	27, 61, 104, 109	0
All	All	1283/1340 (95%)	1.68	406 (31%) 1 1	25, 57, 101, 118	0

All (406) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	195	VAL	8.5
2	D	208	TYR	8.5
3	E	124	PRO	6.8
2	D	137	PRO	6.6
2	D	226	GLU	6.3
1	F	417	ASN	6.2
3	E	188	LYS	6.2
3	E	130	LEU	6.1
1	F	369	TYR	6.1
2	D	209	ILE	6.1
2	A	113	GLY	5.9
2	D	194	SER	5.8
3	E	122	ILE	5.6
2	D	44	GLY	5.6
3	E	178	TYR	5.5
2	D	213	ASN	5.5
2	D	225	VAL	5.4
1	F	415	THR	5.4
3	E	139	CYS	5.4

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Mol	Chain	Res	Type	RSRZ
1	F	335	LEU	5.3
2	D	113	GLY	5.3
3	E	26	SER	5.3
2	D	178	HIS	5.3
2	D	151	ALA	5.2
3	B	201	VAL	5.2
2	A	204	GLY	5.2
1	F	387	LEU	5.0
1	F	374	PHE	4.9
2	A	210	CYS	4.8
3	E	144	PHE	4.8
2	D	115	ASP	4.8
2	D	139	ALA	4.8
3	E	125	PRO	4.8
3	E	201	VAL	4.7
3	E	141	LEU	4.7
2	A	195	VAL	4.7
2	A	149	THR	4.6
3	B	198	ALA	4.6
2	D	193	SER	4.5
3	E	121	PHE	4.5
2	D	152	LEU	4.5
3	E	60	PHE	4.5
2	A	179	THR	4.5
1	C	397	ALA	4.4
1	C	429	PHE	4.4
2	D	198	VAL	4.4
2	A	205	THR	4.3
2	D	133	PRO	4.2
3	E	115	VAL	4.2
2	A	152	LEU	4.2
2	D	138	LEU	4.2
2	D	4	LEU	4.2
3	E	153	TRP	4.2
1	C	369	TYR	4.2
2	A	145	THR	4.1
1	C	370	ASN	4.1
1	C	335	LEU	4.1
3	E	120	VAL	4.1
3	E	148	GLU	4.1
2	A	180	PHE	4.1
2	A	208	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
3	E	97	THR	4.0
3	E	191	TYR	4.0
1	C	342	PHE	4.0
2	A	154	CYS	4.0
3	E	196	VAL	4.0
1	C	435	ALA	4.0
3	B	170	GLU	4.0
3	E	118	PRO	4.0
1	F	471	GLU	3.9
3	B	121	PHE	3.9
3	B	213	SER	3.9
2	D	168	TRP	3.8
2	D	197	THR	3.8
1	C	477	ASN	3.8
3	B	118	PRO	3.8
3	B	135	ALA	3.8
2	A	225	VAL	3.8
3	E	160	GLN	3.8
3	B	54	TYR	3.8
2	D	180	PHE	3.8
2	D	140	PRO	3.7
3	E	187	SER	3.7
3	E	158	ALA	3.7
2	D	212	VAL	3.7
3	E	140	LEU	3.6
3	E	61	SER	3.6
3	B	31	ASP	3.6
2	D	163	PRO	3.6
1	F	464	PHE	3.6
3	E	126	SER	3.6
2	D	196	VAL	3.6
2	D	206	GLN	3.6
1	C	365	TYR	3.6
2	D	165	THR	3.6
1	F	508	TYR	3.5
1	F	362	VAL	3.5
2	A	221	VAL	3.5
3	E	138	VAL	3.5
2	A	203	LEU	3.5
3	E	136	SER	3.5
3	E	190	ASP	3.5
2	D	173	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
3	E	147	ARG	3.4
2	A	168	TRP	3.4
2	A	222	ASP	3.4
2	A	18	LEU	3.4
3	E	146	PRO	3.4
2	A	114	MET	3.4
3	B	151	VAL	3.4
1	F	470	THR	3.4
1	F	480	CYS	3.3
2	D	128	ALA	3.3
3	E	180	LEU	3.3
2	A	207	THR	3.3
3	E	21	ILE	3.3
3	E	123	PHE	3.3
3	B	210	VAL	3.3
2	A	202	SER	3.3
1	C	391	CYS	3.3
1	C	394	ASN	3.2
2	A	183	VAL	3.2
2	D	132	GLY	3.2
3	E	210	VAL	3.2
2	D	155	LEU	3.2
3	B	214	PHE	3.2
3	E	203	HIS	3.2
1	C	393	THR	3.2
2	D	35	ASN	3.1
1	C	503	VAL	3.1
1	C	355	ARG	3.1
3	E	51	LEU	3.1
3	E	197	TYR	3.1
2	D	214	HIS	3.1
2	D	136	PHE	3.1
1	F	523	THR	3.1
2	A	150	ALA	3.1
3	E	189	ALA	3.1
1	C	392	PHE	3.1
1	C	510	VAL	3.1
2	D	142	SER	3.1
3	E	107	THR	3.1
2	D	141	SER	3.1
2	D	175	SER	3.1
2	D	21	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	129	SER	3.0
2	D	162	GLU	3.0
3	E	218	GLU	3.0
3	B	143	ASN	3.0
1	C	434	ILE	3.0
3	B	191	TYR	3.0
2	A	115	ASP	3.0
3	B	182	SER	3.0
3	E	132	SER	3.0
1	C	524	VAL	3.0
2	A	192	LEU	3.0
3	B	199	CYS	3.0
1	C	523	THR	3.0
2	D	97	VAL	3.0
3	B	122	ILE	2.9
2	D	20	LEU	2.9
3	B	186	LEU	2.9
3	E	165	GLN	2.9
3	B	144	PHE	2.9
3	E	151	VAL	2.9
2	A	173	LEU	2.9
2	A	24	ALA	2.9
2	A	191	SER	2.9
2	D	166	VAL	2.9
2	D	203	LEU	2.9
2	D	153	GLY	2.9
2	A	161	PRO	2.9
2	D	146	SER	2.9
2	D	202	SER	2.9
3	E	169	THR	2.9
2	A	176	GLY	2.8
2	D	2	VAL	2.8
3	B	163	ASN	2.8
3	E	213	SER	2.8
1	F	368	ILE	2.8
3	E	193	LYS	2.8
3	E	155	VAL	2.8
1	F	338	PHE	2.8
3	E	36	THR	2.8
1	F	491	PRO	2.8
2	A	45	LEU	2.8
1	C	430	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	404	GLY	2.8
3	E	198	ALA	2.8
3	E	163	ASN	2.8
1	F	458	LYS	2.7
2	A	133	PRO	2.7
2	A	139	ALA	2.7
2	A	184	LEU	2.7
2	D	154	CYS	2.7
2	D	207	THR	2.7
1	C	358	ILE	2.7
3	B	130	LEU	2.7
3	B	79	LYS	2.7
1	F	479	PRO	2.7
3	E	156	ASP	2.7
2	A	206	GLN	2.7
3	E	128	GLU	2.7
1	C	424	LYS	2.7
3	E	131	LYS	2.7
3	E	91	TYR	2.7
1	F	337	PRO	2.7
3	E	185	THR	2.7
1	C	443	SER	2.7
2	D	116	VAL	2.6
2	D	135	VAL	2.6
3	E	137	VAL	2.6
2	D	176	GLY	2.6
3	B	134	THR	2.6
3	B	123	PHE	2.6
1	F	459	SER	2.6
3	E	164	SER	2.6
3	E	181	SER	2.6
3	B	153	TRP	2.6
1	F	423	TYR	2.6
1	F	473	TYR	2.6
2	D	143	LYS	2.6
3	E	183	THR	2.6
3	B	164	SER	2.6
1	C	368	ILE	2.6
3	E	14	THR	2.6
3	E	129	GLN	2.6
3	B	117	ALA	2.6
2	A	78	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	46	GLU	2.5
2	D	185	GLN	2.5
3	E	200	GLU	2.5
2	D	150	ALA	2.5
3	B	33	ASP	2.5
2	D	144	SER	2.5
1	F	526	GLY	2.5
2	D	192	LEU	2.5
1	C	402	ILE	2.5
2	A	59	TYR	2.5
2	D	111	TYR	2.5
1	C	385	THR	2.5
3	B	107	THR	2.5
1	C	419	ALA	2.5
3	E	199	CYS	2.5
2	D	228	LYS	2.5
3	B	154	LYS	2.5
2	D	217	SER	2.5
1	C	337	PRO	2.5
3	B	38	LEU	2.5
3	B	78	LEU	2.5
2	A	164	VAL	2.5
2	A	136	PHE	2.5
2	D	210	CYS	2.5
1	C	366	SER	2.5
1	C	413	GLY	2.5
2	A	182	ALA	2.5
1	F	518	LEU	2.4
2	A	17	SER	2.4
2	A	144	SER	2.4
2	A	38	ARG	2.4
3	E	116	ALA	2.4
3	E	134	THR	2.4
3	E	202	THR	2.4
1	C	472	ILE	2.4
1	F	527	PRO	2.4
2	D	181	PRO	2.4
1	C	381	GLY	2.4
1	F	524	VAL	2.4
1	F	438	SER	2.4
2	A	200	SER	2.4
1	C	409	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	117	ALA	2.4
1	F	449	TYR	2.4
1	F	500	THR	2.4
2	A	104	LEU	2.4
2	D	79	LEU	2.4
3	B	215	ASN	2.4
2	D	188	GLY	2.4
1	F	363	ALA	2.4
3	E	149	ALA	2.4
1	F	402	ILE	2.4
1	C	362	VAL	2.4
2	D	64	VAL	2.4
3	E	119	SER	2.4
2	A	57	THR	2.4
3	E	206	LEU	2.4
1	F	418	ILE	2.4
1	C	515	PHE	2.3
1	C	408	SER	2.3
2	D	187	SER	2.3
3	E	28	SER	2.3
1	C	387	LEU	2.3
3	B	206	LEU	2.3
1	C	527	PRO	2.3
3	B	155	VAL	2.3
1	C	420	ASP	2.3
2	A	155	LEU	2.3
1	C	470	THR	2.3
1	F	496	GLY	2.3
3	E	46	GLY	2.3
3	E	215	ASN	2.3
1	F	497	PHE	2.3
1	C	441	LEU	2.3
3	B	139	CYS	2.3
2	A	175	SER	2.3
3	B	56	ILE	2.3
2	A	197	THR	2.3
3	E	211	THR	2.3
2	D	95	TYR	2.3
3	B	197	TYR	2.3
2	A	198	VAL	2.3
3	E	18	PRO	2.3
1	C	526	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	8	GLY	2.3
1	C	338	PHE	2.3
3	E	143	ASN	2.3
2	D	189	LEU	2.3
1	F	379	CYS	2.3
3	B	161	SER	2.3
3	E	167	SER	2.3
1	F	421	TYR	2.3
1	C	407	VAL	2.3
3	B	60	PHE	2.2
3	E	184	LEU	2.2
2	A	220	LYS	2.2
1	C	367	VAL	2.2
1	F	349	SER	2.2
1	F	511	VAL	2.2
2	D	7	SER	2.2
3	B	136	SER	2.2
3	B	146	PRO	2.2
1	F	388	ASN	2.2
1	F	410	ILE	2.2
3	B	21	ILE	2.2
3	E	40	TRP	2.2
2	D	34	MET	2.2
1	C	401	VAL	2.2
1	F	525	CYS	2.2
2	A	8	GLY	2.2
2	A	66	GLY	2.2
2	A	229	SER	2.2
3	E	182	SER	2.2
2	D	157	LYS	2.2
3	B	195	LYS	2.2
1	F	395	VAL	2.2
1	C	500	THR	2.2
2	A	28	THR	2.2
3	E	150	LYS	2.2
1	F	365	TYR	2.2
3	B	26	SER	2.2
3	E	27	GLN	2.1
3	B	131	LYS	2.1
1	F	353	TRP	2.1
3	E	41	LEU	2.1
3	E	145	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	61	ALA	2.1
3	B	132	SER	2.1
3	B	2	ILE	2.1
1	C	384	PRO	2.1
3	B	137	VAL	2.1
3	E	83	VAL	2.1
1	C	431	GLY	2.1
1	F	416	GLY	2.1
3	B	185	THR	2.1
1	C	371	PHE	2.1
3	E	159	LEU	2.1
1	C	396	TYR	2.1
1	F	489	TYR	2.1
2	A	230	CYS	2.1
2	D	199	PRO	2.1
3	E	157	ASN	2.1
1	C	347	PHE	2.1
2	D	149	THR	2.1
3	B	114	THR	2.1
3	B	156	ASP	2.1
2	A	117	TRP	2.1
3	E	11	SER	2.1
3	E	161	SER	2.1
2	A	196	VAL	2.1
3	E	13	VAL	2.1
2	D	227	PRO	2.1
3	B	180	LEU	2.1
1	C	504	GLY	2.1
3	B	127	ASP	2.1
1	F	408	SER	2.0
2	A	143	LYS	2.0
2	D	134	SER	2.0
1	C	433	VAL	2.0
3	E	109	VAL	2.0
3	E	29	LEU	2.0
3	E	39	ASN	2.0
3	E	142	ASN	2.0
3	B	67	PHE	2.0
2	D	156	VAL	2.0
3	B	129	GLN	2.0
3	E	22	SER	2.0
3	B	64	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	392	PHE	2.0
3	B	162	GLY	2.0
1	C	363	ALA	2.0
2	D	219	THR	2.0
3	E	19	ALA	2.0
1	C	364	ASP	2.0
2	A	48	VAL	2.0
2	D	221	VAL	2.0
3	B	109	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 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.