



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:26 AM UTC

PDB ID : 3M0C / pdb_00003m0c
Title : The X-ray Crystal Structure of PCSK9 in Complex with the LDL receptor
Authors : Spraggon, G.; Hampton, E.N.
Deposited on : 2010-03-02
Resolution : 7.01 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

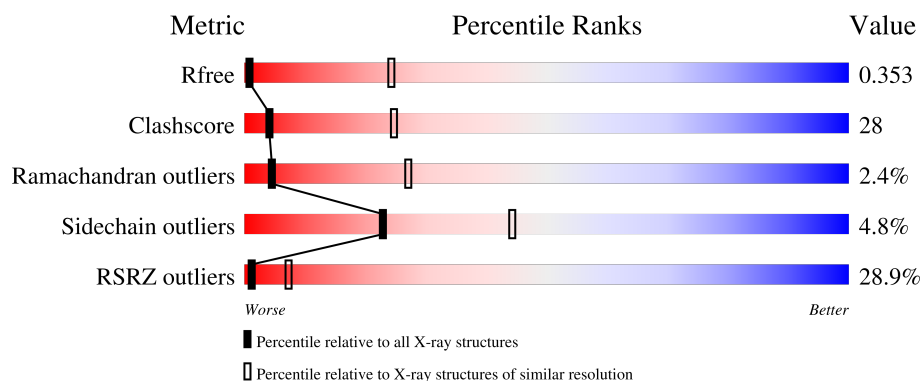
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.01 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	1167 (10.00-4.00)
Clashscore	190562	1009 (10.00-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	124	26% 70% 26%
2	B	546	21% 71% 17% 11%
3	C	791	18% 34% 13% 5% 46%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7705 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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	1	0
			748	479	136	131	2			

- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	486	Total	C	N	O	S	0	1	0
			3618	2234	668	684	32			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	374	TYR	ASP	engineered mutation	UNP Q8NBP7
B	693	HIS	-	expression tag	UNP Q8NBP7
B	694	HIS	-	expression tag	UNP Q8NBP7
B	695	HIS	-	expression tag	UNP Q8NBP7
B	696	HIS	-	expression tag	UNP Q8NBP7
B	697	HIS	-	expression tag	UNP Q8NBP7
B	698	HIS	-	expression tag	UNP Q8NBP7

- Molecule 3 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	430	Total	C	N	O	S	0	0	0
			3336	2079	578	647	32			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	768	HIS	-	expression tag	UNP P01130
C	769	HIS	-	expression tag	UNP P01130
C	770	HIS	-	expression tag	UNP P01130

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Chain	Residue	Modelled	Actual	Comment	Reference
C	771	HIS	-	expression tag	UNP P01130
C	772	HIS	-	expression tag	UNP P01130
C	773	HIS	-	expression tag	UNP P01130

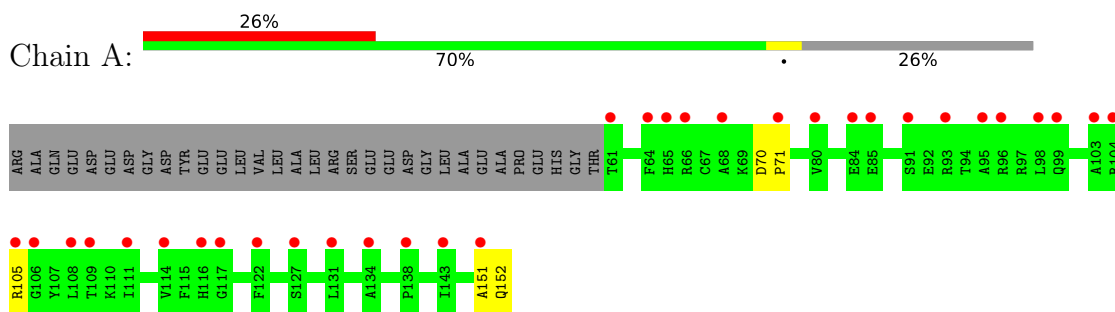
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total 3	Ca 3	0	0

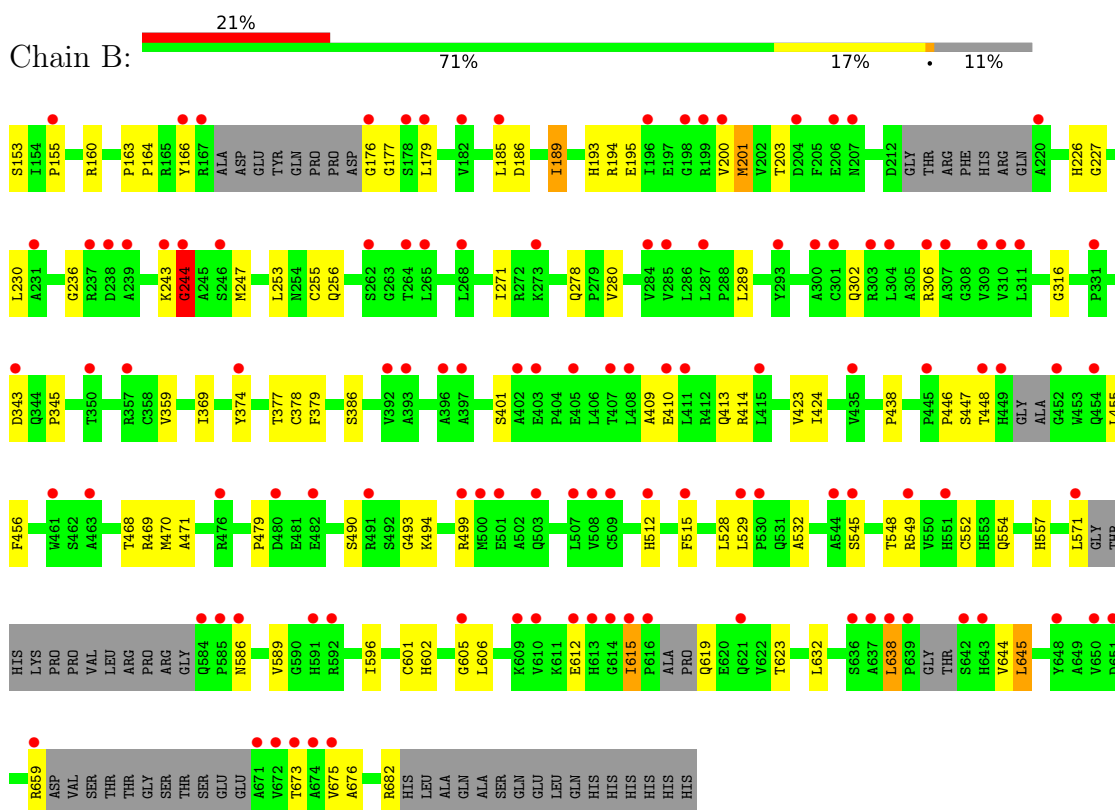
3 Residue-property plots [i](#)

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.

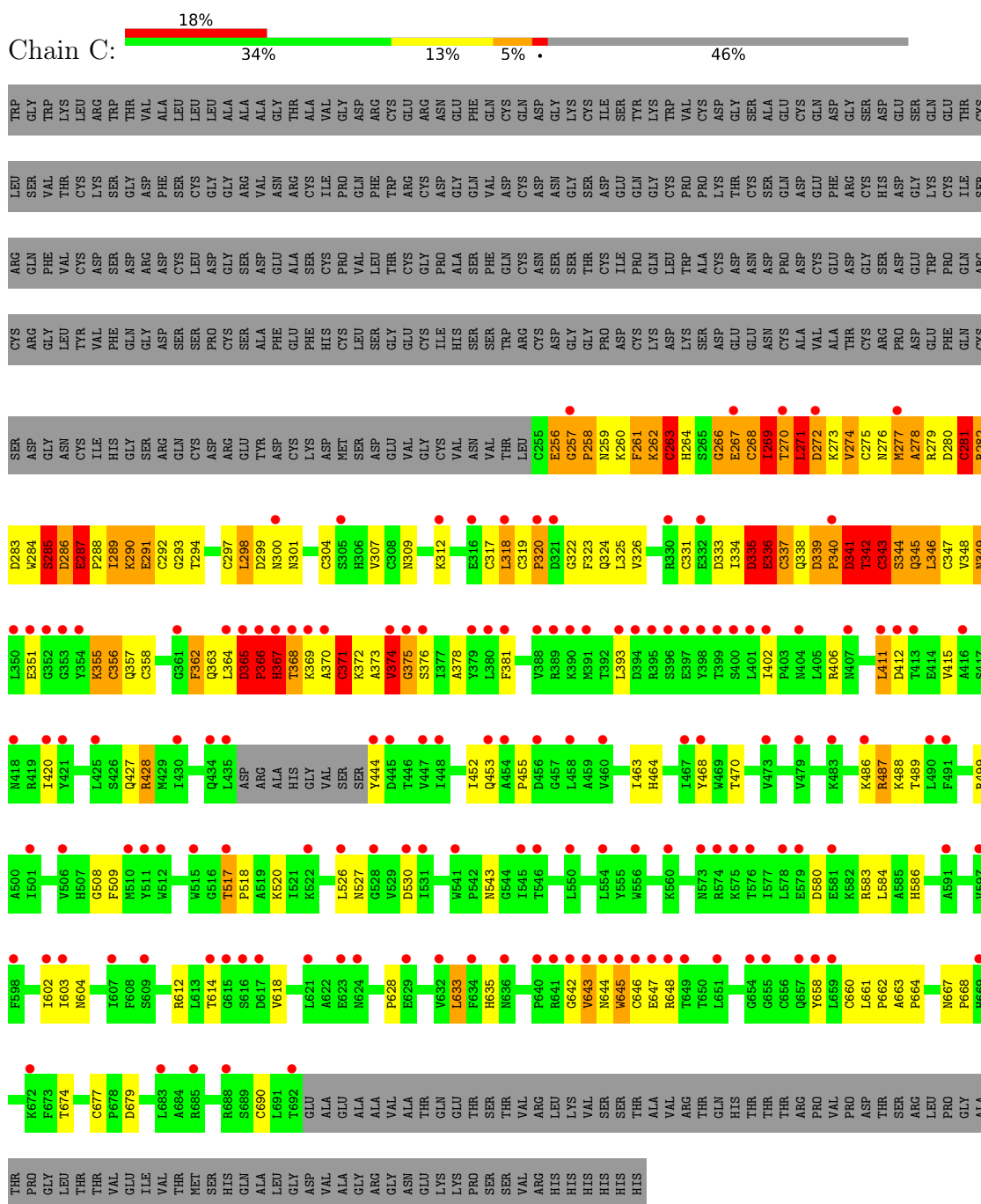
- Molecule 1: Proprotein convertase subtilisin/kexin type 9



- Molecule 2: Proprotein convertase subtilisin/kexin type 9



- Molecule 3: Low-density lipoprotein receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	322.91Å 322.91Å 76.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	279.64 – 7.01 279.64 – 7.01	Depositor EDS
% Data completeness (in resolution range)	82.2 (279.64-7.01) 97.6 (279.64-7.01)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 6.74Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.341 , 0.362 0.339 , 0.353	Depositor DCC
R_{free} test set	339 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	247.1	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 410.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	0.189 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	7705	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.97	0/768	0.87	0/1037
2	B	0.92	4/3687 (0.1%)	0.88	0/5003
3	C	0.79	4/3405 (0.1%)	1.44	43/4628 (0.9%)
All	All	0.87	8/7860 (0.1%)	1.15	43/10668 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	2
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	487	ARG	CD-NE	-20.75	1.17	1.46
3	C	444	TYR	N-CA	-17.89	1.12	1.46
2	B	255	CYS	C-N	-8.67	1.21	1.33
2	B	256	GLN	C-N	-7.61	1.23	1.33
3	C	487	ARG	CA-CB	5.45	1.63	1.53
2	B	189	ILE	C-N	-5.14	1.26	1.33
3	C	343	CYS	N-CA	-5.02	1.40	1.46
2	B	236	GLY	C-O	-5.02	1.18	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	517	THR	CA-C-O	-17.83	102.01	120.38
3	C	365	ASP	CA-C-N	15.30	138.97	119.84
3	C	365	ASP	C-N-CA	15.30	138.97	119.84
3	C	367	HIS	N-CA-C	-14.52	93.00	112.03
3	C	346	LEU	N-CA-C	14.37	130.68	111.28
3	C	272	ASP	N-CA-C	-12.57	94.77	111.74
3	C	287	GLU	CA-C-N	-10.85	107.95	120.11
3	C	287	GLU	C-N-CA	-10.85	107.95	120.11
3	C	518	PRO	N-CA-CB	10.06	113.67	102.60
3	C	336	GLU	N-CA-C	8.22	122.10	110.68
3	C	274	VAL	N-CA-C	7.98	125.94	109.34
3	C	368	THR	N-CA-C	7.94	118.37	107.73
3	C	270	THR	N-CA-C	7.92	120.18	108.14
3	C	281	CYS	N-CA-C	-7.79	94.21	110.80
3	C	366	PRO	N-CA-C	7.37	127.64	112.47
3	C	285	SER	N-CA-C	-7.23	100.67	111.81
3	C	444	TYR	N-CA-CB	7.14	122.63	110.50
3	C	342	THR	N-CA-C	-7.02	97.98	107.88
3	C	263	CYS	N-CA-C	-7.01	95.86	110.80
3	C	262	LYS	N-CA-C	-6.96	95.98	110.80
3	C	268	CYS	N-CA-C	-6.90	97.28	108.52
3	C	344	SER	N-CA-C	-6.66	100.45	110.24
3	C	261	PHE	N-CA-C	6.65	120.34	109.24
3	C	518	PRO	CA-N-CD	-6.61	102.25	111.50
3	C	518	PRO	N-CD-CG	6.55	111.66	103.80
3	C	345	GLN	CA-C-N	6.53	132.03	122.63
3	C	345	GLN	C-N-CA	6.53	132.03	122.63
3	C	371	CYS	N-CA-C	-6.20	99.53	109.39
3	C	267	GLU	N-CA-C	6.13	116.17	108.45
3	C	287	GLU	N-CA-C	6.12	123.33	109.81
3	C	355	LYS	N-CA-C	6.02	117.55	108.46
3	C	271	LEU	N-CA-C	-5.84	98.36	110.80
3	C	286	ASP	N-CA-C	-5.79	95.45	107.67
3	C	349	ASN	N-CA-C	5.65	117.58	107.80
3	C	365	ASP	N-CA-C	5.60	121.30	108.81
3	C	487	ARG	N-CA-CB	-5.60	102.31	111.66
3	C	604	ASN	CA-CB-CG	5.56	118.16	112.60
3	C	381	PHE	CA-CB-CG	5.49	119.29	113.80
3	C	269	ILE	N-CA-C	5.28	115.32	108.35
3	C	278	ALA	N-CA-C	5.28	116.43	108.46
3	C	343	CYS	N-CA-CB	-5.13	102.23	110.69
3	C	415	VAL	N-CA-C	5.06	115.28	110.42
3	C	660	CYS	CA-C-O	-5.04	114.91	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	GLY	Peptide
2	B	494	LYS	Peptide
3	C	517	THR	Mainchain,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	748	0	763	5	2
2	B	3618	0	3529	98	6
3	C	3336	0	3186	339	8
4	C	3	0	0	0	0
All	All	7705	0	7478	415	8

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 28.

All (415) 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:C:527:ASN:HA	3:C:661:LEU:CD1	1.32	1.52
3:C:340:PRO:O	3:C:342:THR:N	1.58	1.35
3:C:339:ASP:HA	3:C:340:PRO:O	1.35	1.25
3:C:323:PHE:CZ	3:C:351:GLU:OE2	1.94	1.21
3:C:339:ASP:OD1	3:C:342:THR:HG21	1.41	1.20
3:C:463:ILE:CG2	3:C:644:ASN:HB2	1.71	1.19
3:C:486:LYS:HD3	3:C:658:TYR:CE1	1.79	1.18
3:C:463:ILE:HG23	3:C:644:ASN:HB2	1.23	1.16
3:C:342:THR:HG23	3:C:347:CYS:CB	1.76	1.15
3:C:527:ASN:CA	3:C:661:LEU:HD13	1.78	1.14
2:B:155:PRO:HD3	3:C:298:LEU:HD22	1.21	1.14
2:B:378:CYS:HB3	3:C:307:VAL:CG1	1.76	1.13
2:B:369:ILE:HD11	3:C:301:ASN:OD1	1.46	1.13
3:C:463:ILE:CG2	3:C:644:ASN:CB	2.25	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:527:ASN:CA	3:C:661:LEU:CD1	2.27	1.12
3:C:374:VAL:HG22	3:C:375:GLY:N	1.54	1.12
3:C:527:ASN:HA	3:C:661:LEU:HD12	1.30	1.12
3:C:643:VAL:HG12	3:C:644:ASN:C	1.74	1.12
3:C:526:LEU:HD12	3:C:662:PRO:HG2	1.21	1.10
3:C:275:CYS:HA	3:C:287:GLU:HG2	1.22	1.09
3:C:275:CYS:HA	3:C:287:GLU:CG	1.83	1.09
3:C:486:LYS:HD3	3:C:658:TYR:CD1	1.88	1.08
3:C:643:VAL:HG11	3:C:648:ARG:HB2	1.35	1.08
3:C:643:VAL:HA	3:C:644:ASN:HB3	1.25	1.08
2:B:378:CYS:HB3	3:C:307:VAL:HG13	1.32	1.07
3:C:486:LYS:HB3	3:C:658:TYR:CZ	1.91	1.04
3:C:358:CYS:HB3	3:C:362:PHE:HB3	1.33	1.04
3:C:374:VAL:CG2	3:C:375:GLY:H	1.66	1.04
2:B:377:THR:OG1	3:C:309:ASN:ND2	1.91	1.03
3:C:270:THR:CG2	3:C:272:ASP:H	1.71	1.02
3:C:289:ILE:HB	3:C:292:CYS:HB3	1.38	1.02
3:C:342:THR:HG23	3:C:347:CYS:HB2	1.05	1.02
3:C:488:LYS:HD2	3:C:677:CYS:O	1.59	1.01
3:C:270:THR:HG22	3:C:272:ASP:H	1.25	1.00
3:C:364:LEU:HD11	3:C:369:LYS:HA	1.44	1.00
3:C:643:VAL:HA	3:C:644:ASN:CB	1.87	1.00
3:C:323:PHE:CE2	3:C:351:GLU:OE2	2.14	1.00
2:B:201:MET:HE1	2:B:203:THR:HG22	1.44	0.99
3:C:339:ASP:OD1	3:C:342:THR:CG2	2.11	0.99
3:C:374:VAL:HG22	3:C:375:GLY:H	0.81	0.98
3:C:264:HIS:HB3	3:C:285:SER:HB3	1.45	0.98
3:C:508:GLY:HA2	3:C:662:PRO:HB2	1.45	0.98
3:C:286:ASP:C	3:C:287:GLU:HG3	1.84	0.98
3:C:333:ASP:HB3	3:C:351:GLU:HG3	1.45	0.98
2:B:153:SER:O	3:C:298:LEU:O	1.82	0.96
2:B:155:PRO:HD3	3:C:298:LEU:CD2	1.97	0.95
2:B:153:SER:O	3:C:298:LEU:HB3	1.67	0.94
3:C:527:ASN:HB3	3:C:661:LEU:HB2	1.46	0.94
3:C:342:THR:CG2	3:C:343:CYS:N	2.28	0.93
3:C:508:GLY:CA	3:C:662:PRO:HB2	1.99	0.92
3:C:263:CYS:SG	3:C:266:GLY:HA3	2.09	0.92
3:C:342:THR:HG22	3:C:343:CYS:N	1.81	0.92
3:C:643:VAL:HG12	3:C:644:ASN:O	1.67	0.92
3:C:463:ILE:HG21	3:C:644:ASN:N	1.85	0.91
3:C:275:CYS:CA	3:C:287:GLU:HG2	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:375:GLY:O	3:C:635:HIS:NE2	2.04	0.91
2:B:369:ILE:CD1	3:C:301:ASN:OD1	2.19	0.90
3:C:527:ASN:HA	3:C:661:LEU:HD13	0.89	0.89
2:B:615:ILE:HD12	2:B:619:GLN:HE21	1.34	0.88
3:C:342:THR:CG2	3:C:347:CYS:HB2	1.98	0.88
3:C:261:PHE:HD2	3:C:262:LYS:N	1.72	0.88
3:C:339:ASP:HA	3:C:340:PRO:C	1.90	0.88
3:C:486:LYS:CD	3:C:658:TYR:CE1	2.57	0.88
3:C:259:ASN:O	3:C:270:THR:HB	1.73	0.87
3:C:339:ASP:N	3:C:342:THR:HB	1.90	0.87
3:C:527:ASN:CA	3:C:661:LEU:HD12	2.00	0.87
3:C:526:LEU:O	3:C:661:LEU:HD13	1.74	0.87
3:C:374:VAL:CG2	3:C:375:GLY:N	2.30	0.86
3:C:644:ASN:O	3:C:646:CYS:N	2.08	0.86
2:B:378:CYS:CB	3:C:307:VAL:CG1	2.52	0.86
3:C:526:LEU:CD1	3:C:662:PRO:HG2	2.05	0.86
3:C:342:THR:CG2	3:C:343:CYS:H	1.87	0.85
3:C:337:CYS:C	3:C:342:THR:OG1	2.19	0.85
3:C:269:ILE:HD13	3:C:280:ASP:O	1.75	0.85
3:C:463:ILE:CG2	3:C:644:ASN:CA	2.54	0.85
3:C:488:LYS:HG3	3:C:679:ASP:OD1	1.75	0.85
3:C:263:CYS:HB3	3:C:267:GLU:H	1.40	0.85
3:C:464:HIS:CD2	3:C:646:CYS:SG	2.70	0.85
3:C:486:LYS:HB3	3:C:658:TYR:CE1	2.11	0.85
3:C:346:LEU:HD23	3:C:357:GLN:HB3	1.58	0.85
3:C:509:PHE:CZ	3:C:664:PRO:HB3	2.12	0.84
3:C:335:ASP:CA	3:C:349:ASN:HD21	1.89	0.84
3:C:452:ILE:HD11	3:C:455:PRO:HG3	1.60	0.84
3:C:463:ILE:HG23	3:C:644:ASN:CB	1.95	0.83
3:C:463:ILE:HG21	3:C:644:ASN:CA	2.08	0.83
3:C:292:CYS:C	3:C:294:THR:H	1.85	0.82
3:C:283:ASP:C	3:C:285:SER:H	1.85	0.82
3:C:643:VAL:CG1	3:C:648:ARG:HB2	2.09	0.82
3:C:280:ASP:N	3:C:286:ASP:OD2	2.13	0.81
3:C:263:CYS:CB	3:C:267:GLU:H	1.93	0.81
3:C:270:THR:HG22	3:C:271:LEU:N	1.96	0.81
3:C:677:CYS:HG	3:C:690:CYS:HG	0.95	0.81
3:C:343:CYS:H	3:C:347:CYS:HB2	1.43	0.81
3:C:261:PHE:HD2	3:C:262:LYS:H	1.28	0.81
2:B:615:ILE:HD12	2:B:619:GLN:NE2	1.95	0.80
3:C:260:LYS:HA	3:C:270:THR:OG1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:HIS:HB3	3:C:285:SER:CB	2.12	0.79
3:C:323:PHE:HZ	3:C:351:GLU:OE2	1.64	0.79
2:B:446:PRO:HB2	2:B:448:THR:HG22	1.63	0.79
3:C:263:CYS:HB3	3:C:267:GLU:O	1.83	0.79
1:A:152:GLN:C	2:B:386:SER:OG	2.26	0.78
2:B:185:LEU:HD11	2:B:271:ILE:HD11	1.65	0.78
2:B:378:CYS:SG	3:C:307:VAL:HG11	2.23	0.78
3:C:487:ARG:N	3:C:658:TYR:OH	2.17	0.77
3:C:486:LYS:HB3	3:C:658:TYR:OH	1.85	0.77
2:B:186:ASP:OD2	2:B:230:LEU:HD12	1.85	0.77
3:C:339:ASP:CA	3:C:342:THR:HB	2.15	0.76
2:B:409:ALA:CB	2:B:528:LEU:HD21	2.15	0.76
3:C:262:LYS:O	3:C:264:HIS:N	2.20	0.75
2:B:378:CYS:HB3	3:C:307:VAL:HG11	1.68	0.75
3:C:340:PRO:O	3:C:341:ASP:C	2.30	0.75
3:C:463:ILE:HG21	3:C:644:ASN:HB2	1.67	0.74
3:C:509:PHE:CZ	3:C:664:PRO:CB	2.69	0.74
3:C:340:PRO:C	3:C:342:THR:N	2.40	0.74
3:C:342:THR:HG23	3:C:343:CYS:H	1.49	0.74
3:C:337:CYS:SG	3:C:349:ASN:HB2	2.27	0.74
2:B:413:GLN:OE1	2:B:456:PHE:HB3	1.88	0.73
3:C:256:GLU:O	3:C:258:PRO:N	2.21	0.73
2:B:302:GLN:HE21	2:B:306:ARG:HH21	1.34	0.73
3:C:488:LYS:CG	3:C:679:ASP:OD1	2.35	0.73
3:C:281:CYS:C	3:C:283:ASP:H	1.97	0.73
3:C:337:CYS:SG	3:C:348:VAL:C	2.72	0.73
3:C:344:SER:O	3:C:345:GLN:OE1	2.07	0.73
3:C:270:THR:HG22	3:C:272:ASP:N	2.03	0.72
3:C:340:PRO:O	3:C:342:THR:CA	2.38	0.71
3:C:489:THR:H	3:C:679:ASP:CG	1.97	0.71
3:C:270:THR:CG2	3:C:271:LEU:H	2.03	0.71
3:C:643:VAL:CG1	3:C:644:ASN:C	2.60	0.71
3:C:263:CYS:SG	3:C:267:GLU:N	2.63	0.71
3:C:286:ASP:OD1	3:C:287:GLU:HG3	1.91	0.71
1:A:152:GLN:C	2:B:386:SER:HG	1.96	0.71
3:C:644:ASN:C	3:C:646:CYS:H	1.99	0.70
2:B:378:CYS:SG	3:C:307:VAL:CG1	2.80	0.70
3:C:325:LEU:HA	3:C:331:CYS:HB3	1.74	0.70
3:C:335:ASP:C	3:C:349:ASN:HD21	2.00	0.70
3:C:273:LYS:O	3:C:273:LYS:HG2	1.92	0.69
3:C:297:CYS:C	3:C:299:ASP:H	1.98	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:256:GLU:C	3:C:258:PRO:HD2	2.18	0.69
3:C:269:ILE:O	3:C:270:THR:OG1	2.10	0.69
2:B:201:MET:HE1	2:B:203:THR:CG2	2.23	0.68
3:C:333:ASP:CB	3:C:351:GLU:HG3	2.21	0.68
3:C:337:CYS:HB2	3:C:349:ASN:HB3	1.74	0.68
2:B:529:LEU:HG	2:B:532:ALA:HB2	1.76	0.68
3:C:337:CYS:SG	3:C:349:ASN:CB	2.83	0.67
3:C:269:ILE:O	3:C:269:ILE:HG13	1.94	0.67
3:C:362:PHE:CE1	3:C:373:ALA:HB2	2.30	0.67
3:C:335:ASP:CB	3:C:349:ASN:HD21	2.08	0.67
3:C:270:THR:CG2	3:C:271:LEU:N	2.56	0.67
3:C:292:CYS:C	3:C:294:THR:N	2.51	0.67
2:B:343:ASP:HB3	2:B:423:VAL:HG12	1.76	0.67
2:B:409:ALA:HB1	2:B:528:LEU:HD21	1.76	0.67
3:C:348:VAL:HG22	3:C:355:LYS:O	1.94	0.66
3:C:289:ILE:HG12	3:C:289:ILE:O	1.94	0.66
3:C:261:PHE:CD2	3:C:262:LYS:N	2.60	0.66
3:C:463:ILE:CG2	3:C:644:ASN:CG	2.67	0.66
3:C:346:LEU:O	3:C:346:LEU:HG	1.93	0.66
3:C:259:ASN:O	3:C:270:THR:CB	2.43	0.66
3:C:367:HIS:O	3:C:368:THR:HG23	1.96	0.65
3:C:527:ASN:CB	3:C:661:LEU:HD12	2.26	0.65
3:C:270:THR:HG22	3:C:271:LEU:H	1.57	0.65
3:C:261:PHE:C	3:C:263:CYS:N	2.54	0.65
2:B:410:GLU:HA	2:B:528:LEU:CD1	2.27	0.65
3:C:274:VAL:HG21	3:C:312:LYS:HG3	1.78	0.65
3:C:271:LEU:HB2	3:C:273:LYS:HB2	1.79	0.65
2:B:378:CYS:CB	3:C:307:VAL:HG11	2.23	0.65
3:C:256:GLU:O	3:C:258:PRO:HD2	1.97	0.65
3:C:644:ASN:C	3:C:646:CYS:N	2.51	0.65
3:C:274:VAL:CG2	3:C:312:LYS:HG3	2.27	0.64
3:C:464:HIS:HD2	3:C:646:CYS:HB2	1.62	0.64
3:C:527:ASN:ND2	3:C:674:THR:OG1	2.29	0.64
3:C:275:CYS:HA	3:C:287:GLU:CB	2.26	0.64
3:C:643:VAL:HB	3:C:645:TRP:N	2.12	0.64
3:C:283:ASP:C	3:C:285:SER:N	2.54	0.64
3:C:508:GLY:HA2	3:C:662:PRO:CB	2.25	0.64
3:C:270:THR:HG23	3:C:272:ASP:H	1.59	0.64
3:C:256:GLU:O	3:C:258:PRO:CD	2.46	0.64
3:C:263:CYS:HB3	3:C:267:GLU:N	2.13	0.64
3:C:346:LEU:HD23	3:C:357:GLN:CB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:261:PHE:O	3:C:267:GLU:O	2.16	0.63
3:C:289:ILE:CB	3:C:292:CYS:HB3	2.23	0.63
3:C:463:ILE:HG22	3:C:644:ASN:CB	2.26	0.63
3:C:276:ASN:O	3:C:277:MET:C	2.42	0.63
3:C:261:PHE:O	3:C:263:CYS:N	2.28	0.62
2:B:612:GLU:HG2	2:B:675:VAL:HG22	1.81	0.62
3:C:292:CYS:O	3:C:294:THR:N	2.33	0.62
2:B:176:GLY:O	2:B:244:GLY:HA3	2.00	0.62
3:C:464:HIS:NE2	3:C:644:ASN:HA	2.15	0.62
3:C:260:LYS:CA	3:C:270:THR:OG1	2.48	0.61
3:C:286:ASP:C	3:C:287:GLU:CG	2.63	0.61
2:B:343:ASP:OD2	2:B:423:VAL:HG11	2.00	0.61
3:C:333:ASP:HB3	3:C:351:GLU:CG	2.27	0.61
2:B:374:TYR:CE2	3:C:318:LEU:HB3	2.36	0.61
2:B:306:ARG:HH12	2:B:479:PRO:CG	2.14	0.61
2:B:409:ALA:HB3	2:B:528:LEU:HD21	1.81	0.61
3:C:334:ILE:O	3:C:335:ASP:C	2.43	0.61
3:C:374:VAL:O	3:C:376:SER:N	2.33	0.61
3:C:262:LYS:O	3:C:263:CYS:C	2.44	0.61
3:C:358:CYS:HB3	3:C:362:PHE:CB	2.21	0.61
3:C:643:VAL:HG12	3:C:645:TRP:N	2.14	0.61
2:B:343:ASP:CB	2:B:423:VAL:HG12	2.31	0.61
3:C:363:GLN:HA	3:C:363:GLN:OE1	2.01	0.61
3:C:509:PHE:CE1	3:C:664:PRO:HB3	2.36	0.61
3:C:367:HIS:O	3:C:368:THR:CG2	2.48	0.60
3:C:358:CYS:CB	3:C:362:PHE:HB3	2.22	0.60
3:C:643:VAL:CG1	3:C:645:TRP:HA	2.31	0.60
3:C:643:VAL:HG11	3:C:645:TRP:HA	1.84	0.60
3:C:274:VAL:HG23	3:C:274:VAL:O	2.02	0.60
1:A:151:ALA:HB2	2:B:253:LEU:HD13	1.83	0.59
3:C:261:PHE:C	3:C:263:CYS:H	2.10	0.59
3:C:342:THR:HG23	3:C:347:CYS:HB3	1.81	0.59
3:C:346:LEU:HB3	3:C:357:GLN:O	2.01	0.59
3:C:463:ILE:HD13	3:C:642:GLY:O	2.03	0.59
3:C:338:GLN:N	3:C:342:THR:OG1	2.36	0.59
3:C:356:CYS:O	3:C:371:CYS:SG	2.60	0.59
3:C:464:HIS:CE1	3:C:644:ASN:HA	2.36	0.59
3:C:278:ALA:O	3:C:286:ASP:OD2	2.21	0.59
3:C:463:ILE:HG22	3:C:644:ASN:HA	1.85	0.58
2:B:638:LEU:HD13	2:B:675:VAL:HG21	1.86	0.58
3:C:333:ASP:CB	3:C:351:GLU:CG	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:GLN:CD	2:B:456:PHE:HB3	2.27	0.58
3:C:464:HIS:CD2	3:C:646:CYS:HG	2.19	0.58
3:C:583:ARG:HD3	3:C:618:VAL:HG11	1.86	0.58
3:C:281:CYS:O	3:C:283:ASP:N	2.35	0.58
3:C:486:LYS:CB	3:C:658:TYR:CE1	2.84	0.58
3:C:289:ILE:O	3:C:289:ILE:CG1	2.52	0.57
3:C:362:PHE:O	3:C:363:GLN:CD	2.48	0.57
3:C:428:ARG:HD2	3:C:453:GLN:O	2.04	0.57
3:C:464:HIS:CD2	3:C:646:CYS:HB2	2.38	0.57
3:C:335:ASP:C	3:C:349:ASN:ND2	2.62	0.57
3:C:602:ILE:HD13	3:C:628:PRO:HD2	1.87	0.57
3:C:526:LEU:C	3:C:661:LEU:HD13	2.29	0.57
3:C:286:ASP:O	3:C:287:GLU:HG3	2.02	0.57
3:C:488:LYS:CD	3:C:677:CYS:O	2.45	0.57
3:C:463:ILE:HG22	3:C:644:ASN:CG	2.28	0.57
2:B:552:CYS:HB3	2:B:557[B]:HIS:CE1	2.39	0.56
3:C:463:ILE:HG23	3:C:644:ASN:CG	2.30	0.56
2:B:409:ALA:C	2:B:528:LEU:HD11	2.30	0.56
3:C:297:CYS:O	3:C:299:ASP:N	2.38	0.56
3:C:464:HIS:NE2	3:C:646:CYS:SG	2.76	0.56
3:C:339:ASP:CA	3:C:340:PRO:O	2.30	0.56
3:C:297:CYS:C	3:C:299:ASP:N	2.62	0.56
3:C:643:VAL:CG1	3:C:645:TRP:N	2.69	0.56
3:C:463:ILE:HG22	3:C:644:ASN:CA	2.34	0.55
3:C:284:TRP:C	3:C:286:ASP:H	2.14	0.55
3:C:411:LEU:HD12	3:C:412:ASP:N	2.21	0.55
3:C:486:LYS:CG	3:C:658:TYR:CE1	2.88	0.55
2:B:155:PRO:CD	3:C:298:LEU:HD22	2.15	0.55
3:C:643:VAL:CB	3:C:645:TRP:N	2.70	0.55
3:C:259:ASN:C	3:C:260:LYS:HG2	2.32	0.55
3:C:362:PHE:CD1	3:C:373:ALA:HB2	2.42	0.55
3:C:259:ASN:O	3:C:260:LYS:HG2	2.06	0.55
3:C:508:GLY:HA3	3:C:662:PRO:HB2	1.89	0.55
2:B:189:ILE:CD1	2:B:200:VAL:HG11	2.37	0.54
3:C:455:PRO:HA	3:C:470:THR:O	2.07	0.54
3:C:463:ILE:HG21	3:C:644:ASN:CB	2.18	0.54
2:B:413:GLN:HB3	2:B:456:PHE:HB3	1.89	0.54
3:C:370:ALA:C	3:C:372:LYS:N	2.66	0.54
2:B:638:LEU:HD22	2:B:673:THR:HG21	1.90	0.53
3:C:322:GLY:O	3:C:333:ASP:CG	2.51	0.53
3:C:370:ALA:O	3:C:372:LYS:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:358:CYS:HB3	3:C:362:PHE:C	2.33	0.53
3:C:378:ALA:HB1	3:C:633:LEU:HD11	1.89	0.53
3:C:644:ASN:O	3:C:647:GLU:N	2.32	0.53
2:B:410:GLU:HG2	2:B:528:LEU:HD13	1.91	0.53
3:C:663:ALA:HB1	3:C:664:PRO:HD2	1.90	0.53
2:B:615:ILE:CD1	2:B:619:GLN:HE21	2.13	0.53
3:C:402:ILE:HD11	3:C:420:ILE:HG21	1.89	0.53
3:C:344:SER:C	3:C:345:GLN:OE1	2.52	0.53
3:C:269:ILE:CD1	3:C:280:ASP:O	2.52	0.52
2:B:201:MET:CE	2:B:203:THR:HG22	2.29	0.52
2:B:469:ARG:HD2	2:B:515:PHE:CD1	2.44	0.52
3:C:586:HIS:HB2	3:C:603:ILE:HD12	1.91	0.52
3:C:527:ASN:HB3	3:C:661:LEU:CB	2.30	0.52
3:C:580:ASP:OD2	3:C:583:ARG:HD2	2.10	0.52
2:B:549:ARG:HG2	2:B:589:VAL:HG22	1.90	0.52
3:C:289:ILE:HG13	3:C:292:CYS:H	1.74	0.52
3:C:335:ASP:HA	3:C:349:ASN:HD21	1.74	0.52
3:C:263:CYS:HB3	3:C:267:GLU:C	2.33	0.52
3:C:643:VAL:CA	3:C:644:ASN:CB	2.70	0.52
2:B:345:PRO:HD3	2:B:424:ILE:HG23	1.91	0.52
3:C:276:ASN:O	3:C:276:ASN:OD1	2.27	0.52
3:C:463:ILE:CG2	3:C:644:ASN:HA	2.36	0.51
2:B:179:LEU:HD22	2:B:401:SER:HA	1.93	0.51
3:C:281:CYS:C	3:C:283:ASP:N	2.61	0.51
3:C:643:VAL:CG1	3:C:645:TRP:CA	2.88	0.51
2:B:186:ASP:OD1	2:B:226:HIS:ND1	2.36	0.51
3:C:339:ASP:HA	3:C:342:THR:HB	1.90	0.51
3:C:367:HIS:C	3:C:368:THR:HG23	2.36	0.51
3:C:337:CYS:SG	3:C:349:ASN:N	2.84	0.51
2:B:468:THR:OG1	2:B:471:ALA:HB2	2.11	0.51
3:C:486:LYS:CD	3:C:658:TYR:CD1	2.80	0.50
2:B:343:ASP:CB	2:B:423:VAL:CG1	2.89	0.50
3:C:263:CYS:SG	3:C:266:GLY:CA	2.93	0.50
3:C:527:ASN:CB	3:C:661:LEU:HB2	2.31	0.50
3:C:289:ILE:C	3:C:291:GLU:N	2.70	0.50
3:C:667:ASN:HB2	3:C:668:PRO:HD2	1.94	0.50
2:B:410:GLU:CG	2:B:528:LEU:HD13	2.42	0.50
2:B:306:ARG:HH12	2:B:479:PRO:HG2	1.76	0.50
3:C:338:GLN:O	3:C:341:ASP:C	2.55	0.49
3:C:428:ARG:HD2	3:C:453:GLN:HA	1.94	0.49
3:C:284:TRP:O	3:C:288:PRO:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:644:ASN:O	3:C:645:TRP:C	2.54	0.49
2:B:378:CYS:SG	3:C:318:LEU:HD23	2.53	0.49
3:C:256:GLU:C	3:C:258:PRO:CD	2.85	0.49
3:C:338:GLN:C	3:C:342:THR:HB	2.36	0.49
2:B:155:PRO:CD	3:C:298:LEU:CD2	2.82	0.49
3:C:261:PHE:H	3:C:269:ILE:H	1.60	0.49
3:C:340:PRO:O	3:C:342:THR:HB	2.12	0.49
2:B:177:GLY:HA2	2:B:401:SER:OG	2.12	0.48
3:C:667:ASN:HB2	3:C:668:PRO:CD	2.43	0.48
3:C:464:HIS:HD2	3:C:646:CYS:CB	2.26	0.48
2:B:632:LEU:HD13	2:B:676:ALA:HB1	1.95	0.48
3:C:364:LEU:HG	3:C:365:ASP:N	2.27	0.48
2:B:193:HIS:HD2	2:B:195:GLU:H	1.61	0.48
2:B:409:ALA:O	2:B:528:LEU:HD11	2.13	0.48
2:B:632:LEU:CD1	2:B:676:ALA:HB1	2.43	0.48
2:B:410:GLU:HA	2:B:528:LEU:HD11	1.95	0.48
3:C:464:HIS:CD2	3:C:646:CYS:CB	2.96	0.48
2:B:306:ARG:NH1	2:B:479:PRO:HG2	2.29	0.48
2:B:379:PHE:O	3:C:307:VAL:HA	2.14	0.47
3:C:270:THR:CG2	3:C:272:ASP:N	2.57	0.47
3:C:489:THR:N	3:C:679:ASP:OD1	2.47	0.47
2:B:374:TYR:CE1	3:C:320:PRO:HA	2.49	0.47
3:C:283:ASP:HB3	3:C:285:SER:HB2	1.96	0.47
2:B:374:TYR:CZ	3:C:319:CYS:O	2.67	0.47
2:B:414:ARG:NH2	2:B:456:PHE:CE2	2.83	0.47
3:C:337:CYS:HB2	3:C:349:ASN:CB	2.44	0.47
3:C:286:ASP:OD1	3:C:287:GLU:CG	2.62	0.47
3:C:406:ARG:NH2	3:C:427:GLN:OE1	2.48	0.47
3:C:463:ILE:HG23	3:C:644:ASN:ND2	2.30	0.47
2:B:413:GLN:HG3	2:B:528:LEU:CD1	2.45	0.46
2:B:469:ARG:C	2:B:470:MET:HE2	2.40	0.46
3:C:322:GLY:O	3:C:333:ASP:CB	2.63	0.46
3:C:333:ASP:OD1	3:C:334:ILE:N	2.48	0.46
2:B:369:ILE:HD11	3:C:301:ASN:CG	2.32	0.46
3:C:468:TYR:OH	3:C:661:LEU:HD22	2.15	0.46
2:B:455:LEU:HD22	2:B:606:LEU:HD11	1.96	0.46
3:C:339:ASP:CA	3:C:340:PRO:C	2.72	0.46
3:C:290:LYS:HA	3:C:290:LYS:HD3	1.68	0.46
3:C:289:ILE:C	3:C:291:GLU:H	2.24	0.46
3:C:290:LYS:O	3:C:291:GLU:HB2	2.15	0.46
2:B:289:LEU:C	2:B:289:LEU:HD12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:LYS:O	2:B:244:GLY:C	2.58	0.45
3:C:268:CYS:C	3:C:269:ILE:HG23	2.42	0.45
2:B:469:ARG:O	2:B:470:MET:HE2	2.16	0.45
2:B:554:GLN:HB2	2:B:557[B]:HIS:CE1	2.51	0.45
3:C:612:ARG:NH1	3:C:612:ARG:HG3	2.31	0.45
2:B:201:MET:CE	2:B:203:THR:CG2	2.91	0.45
3:C:290:LYS:O	3:C:291:GLU:CB	2.64	0.45
3:C:337:CYS:C	3:C:342:THR:HG1	2.23	0.45
1:A:152:GLN:OE1	2:B:316:GLY:HA2	2.16	0.45
3:C:488:LYS:HG2	3:C:679:ASP:OD1	2.16	0.45
2:B:557[A]:HIS:CE1	2:B:602:HIS:HB2	2.52	0.45
3:C:273:LYS:NZ	3:C:280:ASP:CG	2.76	0.44
3:C:337:CYS:CB	3:C:349:ASN:HB3	2.43	0.44
3:C:373:ALA:O	3:C:374:VAL:O	2.36	0.44
2:B:200:VAL:HG22	2:B:247:MET:HB2	1.99	0.44
3:C:276:ASN:H	3:C:287:GLU:CD	2.24	0.44
3:C:322:GLY:O	3:C:333:ASP:HA	2.17	0.44
3:C:333:ASP:HB2	3:C:351:GLU:CG	2.47	0.44
3:C:286:ASP:O	3:C:287:GLU:CB	2.65	0.44
3:C:287:GLU:O	3:C:288:PRO:C	2.52	0.44
3:C:336:GLU:N	3:C:349:ASN:CG	2.76	0.44
2:B:493:GLY:HA3	2:B:645:LEU:HD12	1.99	0.44
3:C:365:ASP:HA	3:C:366:PRO:HD2	1.60	0.44
3:C:527:ASN:N	3:C:661:LEU:HD13	2.28	0.44
3:C:486:LYS:CB	3:C:658:TYR:OH	2.59	0.44
3:C:336:GLU:N	3:C:349:ASN:ND2	2.66	0.44
3:C:344:SER:C	3:C:345:GLN:CD	2.86	0.43
3:C:486:LYS:CD	3:C:658:TYR:HE1	2.26	0.43
3:C:362:PHE:CZ	3:C:373:ALA:HB2	2.53	0.43
3:C:271:LEU:C	3:C:273:LYS:N	2.70	0.43
3:C:526:LEU:O	3:C:661:LEU:HD22	2.17	0.43
3:C:334:ILE:O	3:C:334:ILE:HG13	2.18	0.43
2:B:493:GLY:CA	2:B:645:LEU:HD12	2.48	0.43
3:C:378:ALA:O	3:C:393:LEU:HG	2.19	0.43
3:C:337:CYS:CB	3:C:349:ASN:CB	2.97	0.43
3:C:642:GLY:O	3:C:643:VAL:C	2.62	0.42
2:B:194:ARG:HG3	2:B:377:THR:HG22	2.02	0.42
3:C:286:ASP:O	3:C:287:GLU:CG	2.64	0.42
3:C:340:PRO:O	3:C:342:THR:CB	2.67	0.42
3:C:486:LYS:CG	3:C:658:TYR:HE1	2.30	0.42
2:B:302:GLN:O	2:B:306:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ILE:CD1	3:C:301:ASN:CG	2.90	0.42
3:C:333:ASP:HB2	3:C:351:GLU:HG2	2.02	0.42
3:C:272:ASP:C	3:C:274:VAL:HG13	2.43	0.42
3:C:338:GLN:O	3:C:340:PRO:C	2.62	0.42
2:B:359:VAL:O	2:B:438:PRO:HG2	2.20	0.42
3:C:580:ASP:O	3:C:584:LEU:HB2	2.20	0.42
3:C:612:ARG:HG3	3:C:612:ARG:HH11	1.84	0.42
2:B:189:ILE:HG22	2:B:227:GLY:C	2.44	0.41
3:C:273:LYS:CE	3:C:280:ASP:OD2	2.67	0.41
3:C:277:MET:O	3:C:278:ALA:HB2	2.20	0.41
1:A:70:ASP:N	1:A:71:PRO:CD	2.83	0.41
2:B:557[B]:HIS:HB2	2:B:601:CYS:O	2.20	0.41
3:C:452:ILE:CD1	3:C:455:PRO:HG3	2.39	0.41
3:C:428:ARG:NH1	3:C:428:ARG:HB2	2.35	0.41
2:B:166:TYR:HA	2:B:447:SER:OG	2.20	0.41
2:B:490:SER:OG	2:B:493:GLY:N	2.51	0.41
3:C:586:HIS:HB2	3:C:603:ILE:CD1	2.51	0.41
3:C:256:GLU:O	3:C:257:GLY:C	2.63	0.41
3:C:335:ASP:CB	3:C:349:ASN:ND2	2.82	0.41
3:C:301:ASN:O	3:C:304:CYS:HB2	2.21	0.41
2:B:306:ARG:NH1	2:B:479:PRO:CG	2.84	0.41
3:C:272:ASP:C	3:C:274:VAL:H	2.28	0.41
3:C:276:ASN:N	3:C:287:GLU:CD	2.79	0.41
2:B:548:THR:HG22	2:B:596:ILE:HG22	2.03	0.41
3:C:269:ILE:C	3:C:270:THR:OG1	2.64	0.41
2:B:499:ARG:HD3	2:B:512:HIS:NE2	2.36	0.40
3:C:279:ARG:HH11	3:C:282:ARG:HA	1.85	0.40
3:C:324:GLN:O	3:C:331:CYS:HA	2.22	0.40
3:C:337:CYS:SG	3:C:348:VAL:N	2.94	0.40
2:B:605:GLY:O	2:B:682:ARG:N	2.54	0.40
3:C:463:ILE:O	3:C:644:ASN:ND2	2.55	0.40
2:B:552:CYS:HB2	2:B:586:ASN:HB3	2.02	0.40

All (8) 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:B:164:PRO:CA	3:C:284:TRP:CA[3_655]	1.95	0.25
2:B:164:PRO:CA	3:C:284:TRP:CB[3_655]	1.98	0.22
2:B:164:PRO:CB	3:C:286:ASP:O[3_655]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105[A]:ARG:CZ	3:C:530:ASP:OD1[4_545]	2.07	0.13
2:B:164:PRO:C	3:C:284:TRP:CB[3_655]	2.08	0.12
2:B:163:PRO:O	3:C:284:TRP:CB[3_655]	2.10	0.10
1:A:105[A]:ARG:NE	3:C:530:ASP:OD1[4_545]	2.15	0.05
2:B:160:ARG:NE	3:C:282:ARG:CB[3_655]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	91/124 (73%)	90 (99%)	1 (1%)	0	100	100
2	B	471/546 (86%)	459 (98%)	9 (2%)	3 (1%)	21	59
3	C	426/791 (54%)	362 (85%)	43 (10%)	21 (5%)	1	16
All	All	988/1461 (68%)	911 (92%)	53 (5%)	24 (2%)	4	27

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	257	GLY
3	C	271	LEU
3	C	287	GLU
3	C	291	GLU
3	C	340	PRO
3	C	341	ASP
3	C	366	PRO
3	C	374	VAL
3	C	645	TRP
2	B	244	GLY
3	C	293	GLY
3	C	298	LEU
3	C	335	ASP
3	C	375	GLY

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Mol	Chain	Res	Type
2	B	545	SER
3	C	263	CYS
3	C	281	CYS
3	C	282	ARG
3	C	300	ASN
3	C	258	PRO
3	C	277	MET
3	C	320	PRO
3	C	266	GLY
2	B	280	VAL

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	80/104 (77%)	80 (100%)	0	100	100
2	B	389/437 (89%)	380 (98%)	9 (2%)	44	64
3	C	374/691 (54%)	343 (92%)	31 (8%)	10	30
All	All	843/1232 (68%)	803 (95%)	40 (5%)	23	45

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	201	MET
2	B	278	GLN
2	B	571	LEU
2	B	615	ILE
2	B	623	THR
2	B	638	LEU
2	B	644	VAL
2	B	645	LEU
2	B	659	ARG
3	C	256	GLU
3	C	263	CYS
3	C	269	ILE

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Mol	Chain	Res	Type
3	C	285	SER
3	C	289	ILE
3	C	290	LYS
3	C	317	CYS
3	C	318	LEU
3	C	326	VAL
3	C	335	ASP
3	C	336	GLU
3	C	337	CYS
3	C	339	ASP
3	C	341	ASP
3	C	342	THR
3	C	343	CYS
3	C	356	CYS
3	C	362	PHE
3	C	365	ASP
3	C	366	PRO
3	C	367	HIS
3	C	371	CYS
3	C	374	VAL
3	C	411	LEU
3	C	428	ARG
3	C	499	ARG
3	C	520	LYS
3	C	543	ASN
3	C	614	THR
3	C	633	LEU
3	C	643	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	116	HIS
2	B	193	HIS
2	B	207	ASN
2	B	302	GLN
2	B	449	HIS
2	B	464	HIS
2	B	551	HIS
2	B	602	HIS
2	B	619	GLN

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Mol	Chain	Res	Type
3	C	264	HIS
3	C	309	ASN
3	C	324	GLN
3	C	349	ASN
3	C	453	GLN
3	C	543	ASN
3	C	573	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	92/124 (74%)	1.61	32 (34%) 1 6	97, 181, 209, 231	1 (1%)
2	B	486/546 (89%)	1.15	115 (23%) 2 9	81, 178, 253, 349	1 (0%)
3	C	430/791 (54%)	1.70	144 (33%) 1 6	79, 170, 278, 322	1 (0%)
All	All	1008/1461 (68%)	1.43	291 (28%) 1 7	79, 176, 268, 349	3 (0%)

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	642	GLY	39.2
3	C	473	VAL	12.0
3	C	453	GLN	10.8
3	C	641	ARG	10.7
3	C	648	ARG	10.6
3	C	512	TRP	10.2
2	B	350	THR	10.1
3	C	649	THR	9.9
3	C	643	VAL	9.5
3	C	458	LEU	8.6
1	A	122	PHE	8.4
3	C	645	TRP	8.2
3	C	629	GLU	7.6
2	B	393	ALA	7.6
3	C	381	PHE	7.5
2	B	671	ALA	7.4
3	C	412	ASP	7.4
2	B	673	THR	7.2
2	B	639	PRO	7.1
2	B	449	HIS	7.0
2	B	642	SER	6.5
3	C	556	TRP	6.2
2	B	491	ARG	6.1

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Mol	Chain	Res	Type	RSRZ
2	B	396	ALA	6.0
2	B	304	LEU	5.9
2	B	311	LEU	5.9
2	B	301	CYS	5.8
2	B	303	ARG	5.8
3	C	380	LEU	5.8
1	A	95	ALA	5.8
3	C	510	MET	5.8
2	B	405	GLU	5.8
2	B	529	LEU	5.6
2	B	651	ASP	5.5
3	C	468	TYR	5.4
3	C	647	GLU	5.3
3	C	644	ASN	5.3
2	B	284	VAL	5.2
1	A	111	ILE	5.2
3	C	624	ASN	5.2
2	B	638	LEU	5.2
3	C	597	VAL	5.1
2	B	585	PRO	5.1
2	B	264	THR	5.1
3	C	490	LEU	5.1
3	C	394	ASP	5.0
3	C	545	ILE	5.0
2	B	621	GLN	4.9
1	A	68	ALA	4.9
2	B	612	GLU	4.9
2	B	530	PRO	4.9
3	C	483	LYS	4.9
3	C	316	GLU	4.9
3	C	651	LEU	4.9
2	B	637	ALA	4.8
3	C	416	ALA	4.8
3	C	614	THR	4.8
3	C	398	TYR	4.7
1	A	103	ALA	4.7
3	C	685	ARG	4.7
3	C	435	LEU	4.7
2	B	285	VAL	4.6
2	B	584	GLN	4.6
3	C	421	TYR	4.6
2	B	268	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
3	C	367	HIS	4.4
3	C	654	GLY	4.4
3	C	581	GLU	4.4
2	B	675	VAL	4.4
3	C	550	LEU	4.4
3	C	369	LYS	4.4
2	B	310	VAL	4.3
3	C	528	GLY	4.3
3	C	366	PRO	4.3
3	C	598	PHE	4.3
3	C	411	LEU	4.1
2	B	454	GLN	4.1
3	C	467	ILE	4.1
1	A	80	VAL	4.1
1	A	143	ILE	4.1
1	A	91	SER	4.0
3	C	354	TYR	4.0
3	C	374	VAL	4.0
3	C	632	VAL	4.0
2	B	306	ARG	4.0
3	C	352	GLY	4.0
3	C	376	SER	4.0
3	C	397	GLU	4.0
3	C	603	ILE	4.0
3	C	602	ILE	4.0
1	A	134	ALA	4.0
2	B	231	ALA	4.0
2	B	176	GLY	3.9
2	B	307	ALA	3.9
1	A	116	HIS	3.9
2	B	591	HIS	3.9
3	C	456	ASP	3.9
1	A	85	GLU	3.9
1	A	104	ARG	3.8
2	B	415	LEU	3.8
2	B	402	ALA	3.8
3	C	616	SER	3.8
2	B	309	VAL	3.7
3	C	621	LEU	3.7
2	B	220	ALA	3.7
2	B	199	ARG	3.7
1	A	64	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	388	VAL	3.6
2	B	300	ALA	3.6
2	B	610	VAL	3.6
2	B	515	PHE	3.6
2	B	672	VAL	3.6
3	C	390	LYS	3.5
2	B	331	PRO	3.5
3	C	277	MET	3.5
2	B	182	VAL	3.5
2	B	178	SER	3.5
2	B	273	LYS	3.5
2	B	571	LEU	3.5
2	B	167	ARG	3.4
2	B	198	GLY	3.4
2	B	461	TRP	3.4
3	C	560	LYS	3.4
3	C	413	THR	3.4
2	B	605	GLY	3.4
2	B	551	HIS	3.4
3	C	579	GLU	3.4
2	B	452	GLY	3.4
3	C	365	ASP	3.4
3	C	399	THR	3.4
2	B	650	VAL	3.4
2	B	643	HIS	3.3
3	C	305	SER	3.3
3	C	300	ASN	3.3
3	C	318	LEU	3.3
2	B	615	ILE	3.3
3	C	655	GLY	3.3
3	C	350	LEU	3.3
3	C	511	TYR	3.3
2	B	204	ASP	3.3
3	C	425	LEU	3.2
3	C	657	GLN	3.2
3	C	479	VAL	3.2
3	C	396	SER	3.2
2	B	374	TYR	3.2
3	C	506	VAL	3.2
3	C	370	ALA	3.2
3	C	517	THR	3.2
3	C	575	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	692	THR	3.1
1	A	106	GLY	3.1
2	B	500	MET	3.1
2	B	238	ASP	3.1
1	A	117	GLY	3.1
1	A	127	SER	3.1
2	B	287	LEU	3.1
3	C	541	TRP	3.1
3	C	267	GLU	3.1
2	B	410	GLU	3.1
2	B	179	LEU	3.0
2	B	343	ASP	3.0
1	A	114	VAL	3.0
3	C	460	VAL	3.0
3	C	640	PRO	3.0
3	C	364	LEU	3.0
1	A	151	ALA	3.0
2	B	435	VAL	3.0
3	C	401	LEU	3.0
3	C	257	GLY	3.0
3	C	351	GLU	3.0
3	C	353	GLY	3.0
2	B	244	GLY	3.0
3	C	434	GLN	3.0
3	C	402	ILE	2.9
2	B	616	PRO	2.9
3	C	617	ASP	2.9
3	C	683	LEU	2.9
3	C	361	GLY	2.9
3	C	609	SER	2.9
3	C	636	ASN	2.9
3	C	554	LEU	2.9
3	C	615	GLY	2.9
1	A	66	ARG	2.9
3	C	389	ARG	2.9
3	C	368	THR	2.9
3	C	491	PHE	2.9
2	B	243	LYS	2.8
3	C	445	ASP	2.8
3	C	400	SER	2.8
3	C	623	GLU	2.8
2	B	166	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	138	PRO	2.8
3	C	515	TRP	2.8
2	B	648	TYR	2.8
3	C	591	ALA	2.8
3	C	391	MET	2.8
3	C	444	TYR	2.8
3	C	375	GLY	2.8
3	C	546	THR	2.8
2	B	507	LEU	2.8
2	B	674	ALA	2.7
1	A	71	PRO	2.7
2	B	448	THR	2.7
1	A	93	ARG	2.7
2	B	549	ARG	2.7
3	C	672	LYS	2.7
2	B	397	ALA	2.7
2	B	503	GLN	2.7
2	B	293	TYR	2.6
2	B	206	GLU	2.6
3	C	530	ASP	2.6
1	A	105[A]	ARG	2.6
1	A	131	LEU	2.6
2	B	609	LYS	2.6
3	C	501	ILE	2.6
3	C	688	ARG	2.6
1	A	109	THR	2.6
2	B	545	SER	2.6
3	C	607	ILE	2.6
3	C	578	LEU	2.6
2	B	508	VAL	2.6
2	B	445	PRO	2.6
3	C	634	PHE	2.6
3	C	404	ASN	2.6
3	C	418	ASN	2.6
2	B	200	VAL	2.5
2	B	659	ARG	2.5
2	B	636	SER	2.5
2	B	357	ARG	2.5
3	C	574	ARG	2.5
3	C	312	LYS	2.5
2	B	499	ARG	2.5
3	C	272	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	586	ASN	2.4
3	C	646	CYS	2.4
3	C	448	ILE	2.4
3	C	393	LEU	2.4
2	B	544	ALA	2.4
3	C	379	TYR	2.4
3	C	395	ARG	2.4
3	C	430	ILE	2.4
2	B	207	ASN	2.4
3	C	340	PRO	2.3
1	A	84	GLU	2.3
3	C	526	LEU	2.3
2	B	613	HIS	2.3
2	B	185	LEU	2.3
3	C	320	PRO	2.3
2	B	262	SER	2.3
2	B	614	GLY	2.3
3	C	486	LYS	2.3
2	B	512	HIS	2.3
3	C	522	LYS	2.3
1	A	99	GLN	2.3
1	A	108	LEU	2.2
2	B	392	VAL	2.2
2	B	463	ALA	2.2
3	C	407	ASN	2.2
3	C	420	ILE	2.2
2	B	403	GLU	2.2
1	A	96	ARG	2.2
3	C	576	THR	2.2
2	B	408	LEU	2.2
2	B	501	GLU	2.2
3	C	531	ILE	2.2
3	C	659	LEU	2.2
2	B	246	SER	2.2
2	B	509	CYS	2.2
3	C	330	ARG	2.2
2	B	239	ALA	2.1
2	B	480	ASP	2.1
2	B	476	ARG	2.1
1	A	98	LEU	2.1
2	B	407	THR	2.1
2	B	592	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	669	HIS	2.1
3	C	573	ASN	2.1
3	C	270	THR	2.1
2	B	196	ILE	2.1
3	C	332	GLU	2.1
2	B	237	ARG	2.1
3	C	658	TYR	2.1
1	A	65	HIS	2.1
1	A	61	THR	2.1
3	C	447	VAL	2.1
2	B	411	LEU	2.0
3	C	321	ASP	2.0
2	B	265	LEU	2.0
3	C	454	ALA	2.0
2	B	482	GLU	2.0
2	B	155	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	C	1002	1/1	0.97	0.15	153,153,153,153	0
4	CA	C	1001	1/1	1.00	0.09	136,136,136,136	0
4	CA	C	1003	1/1	1.00	0.07	170,170,170,170	0

6.5 Other polymers [i](#)

There are no such residues in this entry.