



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 02:48 PM EDT

PDB ID : 3M0C
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

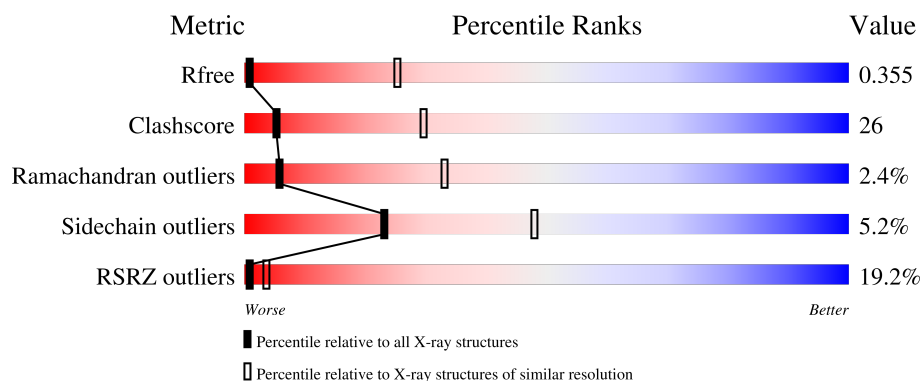
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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	<div> <div>10%</div> <div>69%</div> <div>5%</div> <div>26%</div> </div>
2	B	546	<div> <div>17%</div> <div>71%</div> <div>16%</div> <div>• 11%</div> </div>
3	C	791	<div> <div>11%</div> <div>35%</div> <div>14%</div> <div>5%</div> <div>• 46%</div> </div>

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

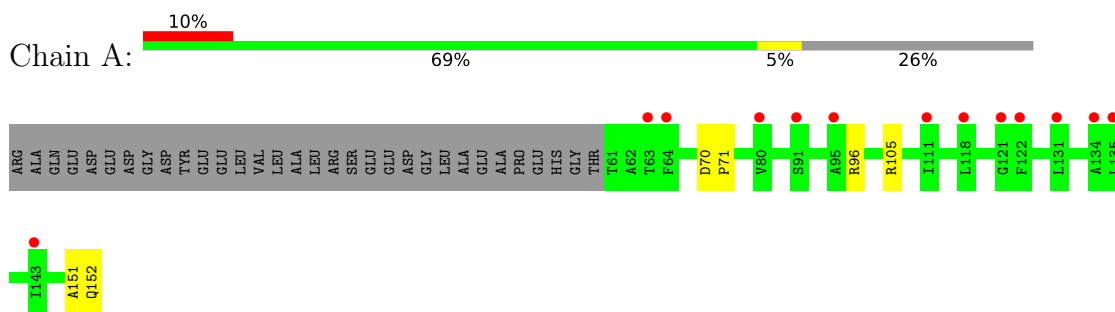
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

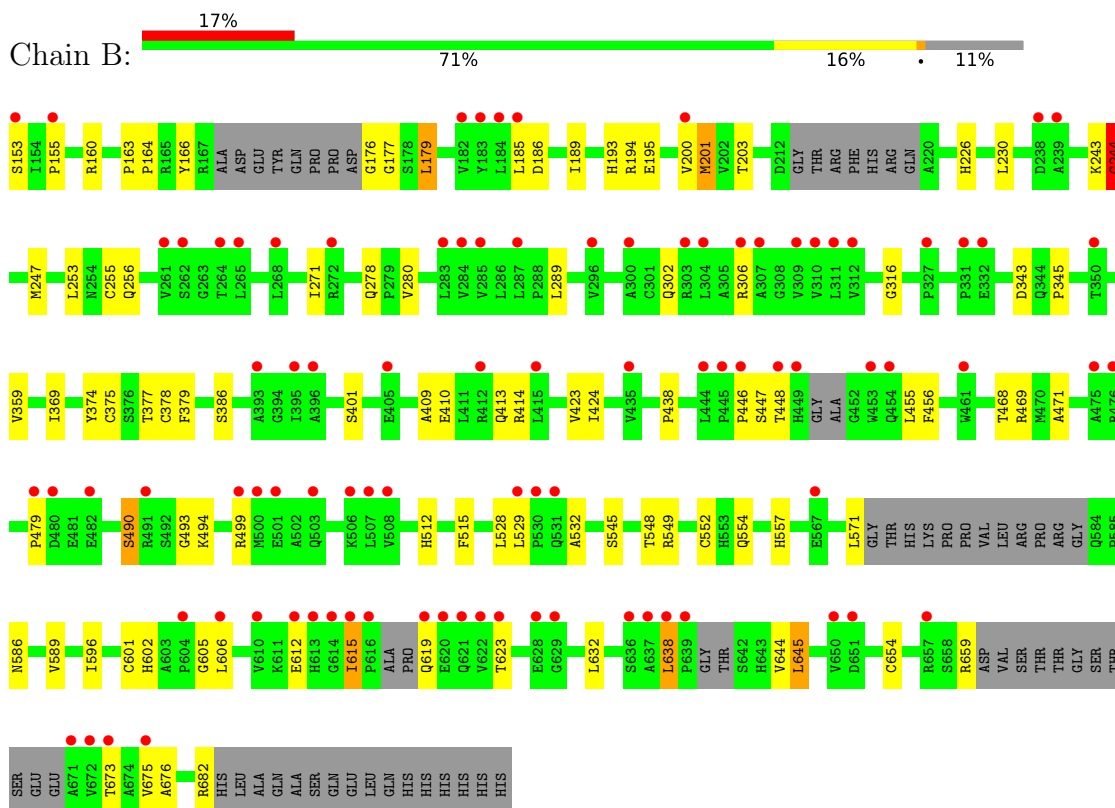
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

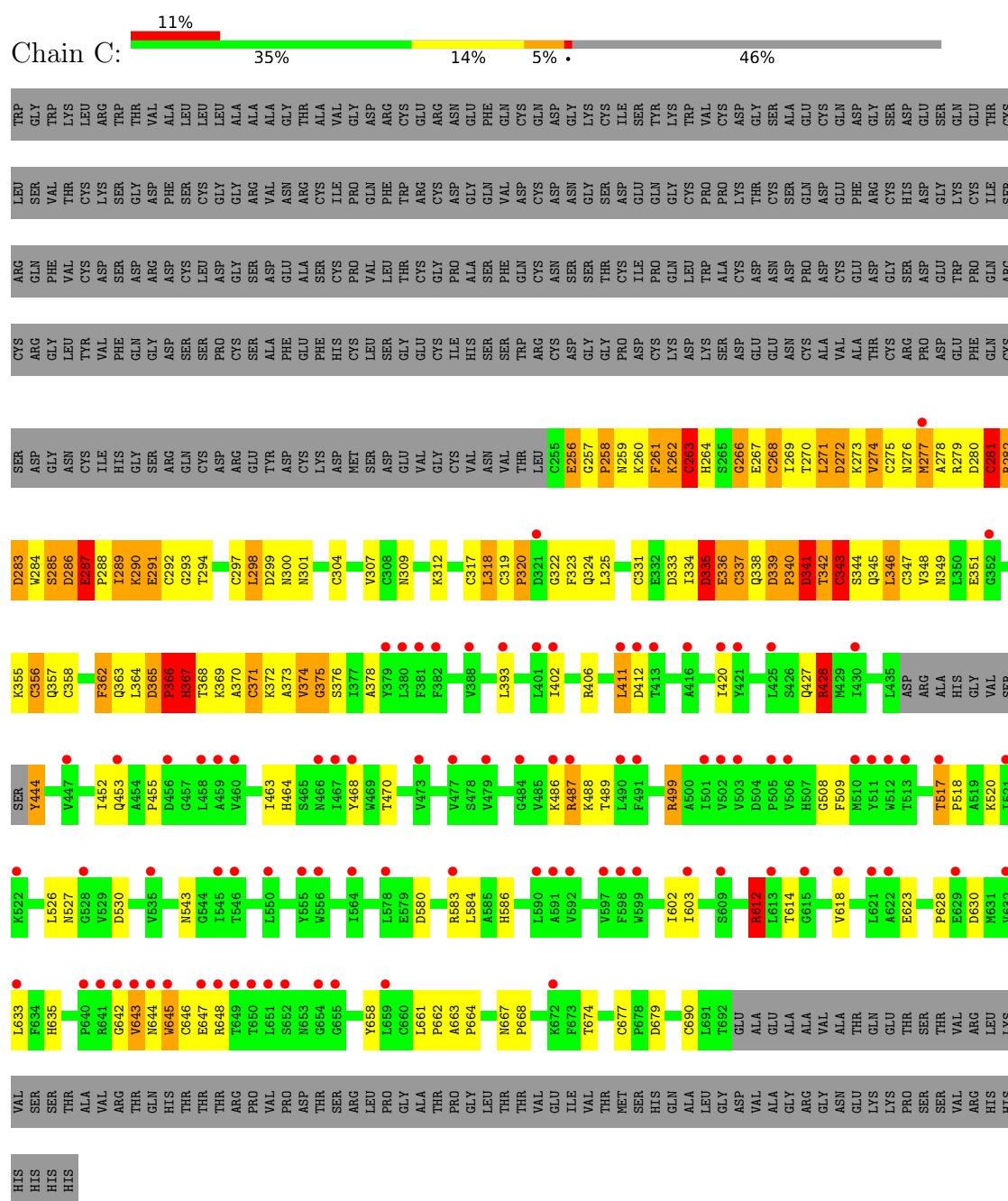
- Molecule 1: Proprotein convertase subtilisin/kexin type 9



- 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 , 0.355	Depositor DCC
R_{free} test set	339 reflections (4.64%)	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 , 199.2	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	0.72	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	0.80	0/768	0.77	0/1037
2	B	0.73	3/3687 (0.1%)	0.75	1/5003 (0.0%)
3	C	0.65	3/3405 (0.1%)	1.09	21/4628 (0.5%)
All	All	0.70	6/7860 (0.1%)	0.91	22/10668 (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
2	B	0	2
3	C	0	2
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	487	ARG	CD-NE	-17.20	1.17	1.46
3	C	444	TYR	N-CA	-17.05	1.12	1.46
3	C	343	CYS	CB-SG	-8.72	1.67	1.82
2	B	654	CYS	CB-SG	-6.39	1.71	1.82
2	B	255	CYS	C-N	-5.59	1.21	1.34
2	B	256	GLN	C-N	-5.31	1.23	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	428	ARG	NE-CZ-NH2	-9.01	115.80	120.30
3	C	518	PRO	N-CA-CB	8.64	113.67	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	517	THR	CA-C-O	-8.61	102.01	120.10
3	C	346	LEU	N-CA-C	7.29	130.68	111.00
3	C	444	TYR	N-CA-CB	6.68	122.63	110.60
3	C	367	HIS	N-CA-C	-6.67	93.00	111.00
3	C	518	PRO	CA-N-CD	-6.61	102.25	111.50
2	B	179	LEU	CA-CB-CG	6.42	130.07	115.30
3	C	499	ARG	NE-CZ-NH1	6.34	123.47	120.30
3	C	281	CYS	N-CA-C	-6.22	94.21	111.00
3	C	272	ASP	N-CA-C	-6.01	94.77	111.00
3	C	366	PRO	N-CA-C	5.98	127.64	112.10
3	C	287	GLU	C-N-CD	5.77	140.52	128.40
3	C	286	ASP	N-CA-C	-5.76	95.45	111.00
3	C	612	ARG	NE-CZ-NH1	5.76	123.18	120.30
3	C	518	PRO	N-CD-CG	5.64	111.66	103.20
3	C	263	CYS	N-CA-C	-5.61	95.86	111.00
3	C	262	LYS	N-CA-C	-5.56	95.98	111.00
3	C	274	VAL	N-CA-C	5.53	125.94	111.00
3	C	630	ASP	CB-CG-OD2	-5.33	113.50	118.30
3	C	263	CYS	CA-CB-SG	5.32	123.57	114.00
3	C	268	CYS	N-CA-C	-5.08	97.28	111.00

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	Peptide,Mainchain

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	93	6
3	C	3336	0	3186	326	8
4	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7705	0	7478	399	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 26.

All (399) 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
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: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
3:C:643:VAL:HG12	3:C:644:ASN:C	1.74	1.07
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:333:ASP:HB3	3:C:351:GLU:HG3	1.45	0.98
2:B:201:MET:HE1	2:B:203:THR:HG22	1.45	0.97
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:286:ASP:C	3:C:287:GLU:HG3	1.84	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:339:ASP:HA	3:C:340:PRO:C	1.90	0.83
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	0.88	0.81
3:C:343:CYS:H	3:C:347:CYS:HB2	1.43	0.81
3:C:337:CYS:C	3:C:342:THR:OG1	2.19	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
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
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:283:ASP:C	3:C:285:SER:H	1.85	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
3:C:292:CYS:C	3:C:294:THR:H	1.85	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: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: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
1:A:152:GLN:C	2:B:386:SER:OG	2.26	0.73
2:B:413:GLN:OE1	2:B:456:PHE:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:270:THR:CG2	3:C:271:LEU:H	2.03	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
2:B:378:CYS:SG	3:C:307:VAL:CG1	2.80	0.70
3:C:340:PRO:C	3:C:342:THR:N	2.40	0.70
3:C:325:LEU:HA	3:C:331:CYS:HB3	1.74	0.70
3:C:273:LYS:O	3:C:273:LYS:HG2	1.92	0.69
3:C:269:ILE:O	3:C:270:THR:OG1	2.10	0.69
3:C:281:CYS:C	3:C:283:ASP:H	1.97	0.68
3:C:333:ASP:CB	3:C:351:GLU:HG3	2.21	0.68
3:C:337:CYS:SG	3:C:348:VAL:C	2.72	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
2:B:201:MET:HE1	2:B:203:THR:CG2	2.24	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
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:489:THR:H	3:C:679:ASP:CG	1.97	0.67
3:C:643:VAL:CG1	3:C:644:ASN:C	2.60	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: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:644:ASN:C	3:C:646:CYS:H	1.99	0.65
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:340:PRO:O	3:C:341:ASP:C	2.30	0.65
3:C:297:CYS:C	3:C:299:ASP:H	1.98	0.65
2:B:410:GLU:HA	2:B:528:LEU:CD1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:256:GLU:C	3:C:258:PRO:HD2	2.18	0.64
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:643:VAL:CA	3:C:644:ASN:CB	2.70	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:508:GLY:HA2	3:C:662:PRO:CB	2.25	0.64
3:C:292:CYS:C	3:C:294:THR:N	2.51	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:335:ASP:C	3:C:349:ASN:HD21	2.00	0.63
3:C:346:LEU:HD23	3:C:357:GLN:CB	2.29	0.63
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: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
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
3:C:463:ILE:CG2	3:C:644:ASN:CG	2.67	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:374:VAL:O	3:C:376:SER:N	2.33	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:261:PHE:C	3:C:263:CYS:N	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:644:ASN:C	3:C:646:CYS:N	2.51	0.60
1:A:151:ALA:HB2	2:B:253:LEU:HD13	1.83	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:286:ASP:O	3:C:287:GLU:HG3	2.02	0.58
3:C:333:ASP:CB	3:C:351:GLU:CG	2.81	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:276:ASN:O	3:C:277:MET:C	2.42	0.58
3:C:289:ILE:O	3:C:289:ILE:CG1	2.52	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:337:CYS:C	3:C:342:THR:HG1	2.08	0.57
3:C:602:ILE:HD13	3:C:628:PRO:HD2	1.87	0.57
2:B:201:MET:CE	2:B:203:THR:HG22	2.29	0.57
3:C:488:LYS:CD	3:C:677:CYS:O	2.45	0.57
2:B:552:CYS:HB3	2:B:557[B]:HIS:CE1	2.39	0.56
3:C:334:ILE:O	3:C:335:ASP:C	2.43	0.56
3:C:262:LYS:O	3:C:263:CYS:C	2.44	0.56
3:C:283:ASP:C	3:C:285:SER:N	2.54	0.56
3:C:286:ASP:C	3:C:287:GLU:CG	2.63	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: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:339:ASP:CA	3:C:340:PRO:C	2.72	0.55
3:C:411:LEU:HD12	3:C:412:ASP:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:413:GLN:CD	2:B:456:PHE:HB3	2.27	0.54
1:A:152:GLN:C	2:B:386:SER:HG	2.09	0.54
2:B:638:LEU:HD22	2:B:673:THR:HG21	1.90	0.53
3:C:370:ALA:O	3:C:372:LYS:N	2.39	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
3:C:281:CYS:C	3:C:283:ASP:N	2.61	0.53
3:C:463:ILE:HG22	3:C:644:ASN:CG	2.28	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:362:PHE:O	3:C:363:GLN:CD	2.48	0.53
3:C:269:ILE:CD1	3:C:280:ASP:O	2.52	0.52
3:C:335:ASP:C	3:C:349:ASN:ND2	2.62	0.52
3:C:526:LEU:C	3:C:661:LEU:HD13	2.29	0.52
3:C:297:CYS:C	3:C:299:ASP:N	2.62	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:463:ILE:HG23	3:C:644:ASN:CG	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:339:ASP:HA	3:C:342:THR:HB	1.90	0.51
2:B:409:ALA:C	2:B:528:LEU:HD11	2.30	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:284:TRP:C	3:C:286:ASP:H	2.14	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: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:259:ASN:C	3:C:260:LYS:HG2	2.32	0.50
3:C:364:LEU:HG	3:C:365:ASP:N	2.27	0.50
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
3:C:370:ALA:C	3:C:372:LYS:N	2.66	0.49
2:B:378:CYS:SG	3:C:318:LEU:HD23	2.53	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
3:C:322:GLY:O	3:C:333:ASP:CG	2.51	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:358:CYS:HB3	3:C:362:PHE:C	2.33	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
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:344:SER:C	3:C:345:GLN:OE1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:263:CYS:HB3	3:C:267:GLU:C	2.33	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
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
3:C:367:HIS:C	3:C:368:THR:HG23	2.36	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:290:LYS:HA	3:C:290:LYS:HD3	1.68	0.46
3:C:290:LYS:O	3:C:291:GLU:HB2	2.15	0.46
2:B:554:GLN:HB2	2:B:557[B]:HIS:CE1	2.51	0.45
3:C:289:ILE:C	3:C:291:GLU:N	2.70	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:338:GLN:O	3:C:341:ASP:C	2.55	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:337:CYS:CB	3:C:349:ASN:HB3	2.43	0.44
3:C:338:GLN:C	3:C:342:THR:HB	2.36	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: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:256:GLU:C	3:C:258:PRO:CD	2.85	0.44
3:C:286:ASP:O	3:C:287:GLU:CB	2.65	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:337:CYS:CB	3:C:349:ASN:CB	2.97	0.43
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
3:C:468:TYR:HH	3:C:661:LEU:HD22	1.85	0.42
3:C:333:ASP:HB2	3:C:351:GLU:HG2	2.02	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
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:289:ILE:C	3:C:291:GLU:H	2.24	0.41
3:C:586:HIS:HB2	3:C:603:ILE:CD1	2.51	0.41
3:C:335:ASP:CB	3:C:349:ASN:ND2	2.82	0.41
3:C:287:GLU:O	3:C:288:PRO:C	2.52	0.41
3:C:301:ASN:O	3:C:304:CYS:HB2	2.21	0.41
2:B:289:LEU:C	2:B:289:LEU:HD12	2.41	0.41
2:B:243:LYS:O	2:B:244:GLY:C	2.58	0.41
2:B:306:ARG:NH1	2:B:479:PRO:CG	2.84	0.41
3:C:268:CYS:C	3:C:269:ILE:HG23	2.42	0.41
2:B:548:THR:HG22	2:B:596:ILE:HG22	2.03	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:644:ASN:O	3:C:645:TRP:C	2.54	0.40
3:C:261:PHE:C	3:C:263:CYS:H	2.10	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
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 ⓘ

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	91/124 (73%)	90 (99%)	1 (1%)	0	100	100
2	B	471/546 (86%)	459 (98%)	9 (2%)	3 (1%)	25	66
3	C	426/791 (54%)	362 (85%)	43 (10%)	21 (5%)	2	20
All	All	988/1461 (68%)	911 (92%)	53 (5%)	24 (2%)	6	33

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

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Mol	Chain	Res	Type
3	C	335	ASP
3	C	375	GLY
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%)	79 (99%)	1 (1%)	69	81
2	B	389/437 (89%)	378 (97%)	11 (3%)	43	65
3	C	374/691 (54%)	342 (91%)	32 (9%)	10	32
All	All	843/1232 (68%)	799 (95%)	44 (5%)	23	48

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
2	B	201	MET
2	B	278	GLN
2	B	375	CYS
2	B	490	SER
2	B	571	LEU
2	B	615	ILE
2	B	623	THR
2	B	638	LEU
2	B	644	VAL

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Mol	Chain	Res	Type
2	B	645	LEU
2	B	659	ARG
3	C	256	GLU
3	C	261	PHE
3	C	263	CYS
3	C	283	ASP
3	C	285	SER
3	C	289	ILE
3	C	290	LYS
3	C	317	CYS
3	C	318	LEU
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	411	LEU
3	C	428	ARG
3	C	444	TYR
3	C	499	ARG
3	C	520	LYS
3	C	543	ASN
3	C	612	ARG
3	C	614	THR
3	C	623	GLU
3	C	643	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	193	HIS
2	B	302	GLN
2	B	449	HIS
2	B	537	HIS

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Mol	Chain	Res	Type
2	B	619	GLN
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
3	C	586	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

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%)	0.85	13 (14%) 2 6	106, 181, 209, 231	0
2	B	486/546 (89%)	0.77	91 (18%) 1 4	81, 178, 253, 349	0
3	C	430/791 (54%)	1.06	90 (20%) 1 3	79, 170, 278, 322	1 (0%)
All	All	1008/1461 (68%)	0.90	194 (19%) 1 3	79, 176, 268, 349	1 (0%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	642	GLY	10.1
3	C	649	THR	8.7
3	C	648	ARG	8.0
3	C	412	ASP	7.9
3	C	641	ARG	7.7
2	B	449	HIS	7.1
2	B	530	PRO	7.0
2	B	529	LEU	6.7
2	B	448	THR	6.4
3	C	512	TRP	6.3
3	C	643	VAL	6.2
3	C	546	THR	5.4
3	C	645	TRP	5.3
3	C	632	VAL	5.3
3	C	633	LEU	5.2
3	C	591	ALA	5.2
2	B	311	LEU	4.9
2	B	671	ALA	4.9
3	C	578	LEU	4.8
2	B	507	LEU	4.7
3	C	556	TRP	4.6
2	B	651	ASP	4.6
3	C	458	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
3	C	413	THR	4.5
2	B	616	PRO	4.5
3	C	510	MET	4.5
3	C	380	LEU	4.5
1	A	118	LEU	4.5
2	B	672	VAL	4.3
3	C	651	LEU	4.3
3	C	468	TYR	4.3
2	B	638	LEU	4.3
3	C	545	ILE	4.2
2	B	304	LEU	4.2
2	B	476	ARG	4.2
2	B	393	ALA	4.2
1	A	80	VAL	4.2
3	C	459	ALA	4.1
2	B	615	ILE	4.1
2	B	284	VAL	4.1
3	C	598	PHE	4.1
2	B	310	VAL	4.1
3	C	621	LEU	4.0
3	C	502	VAL	4.0
3	C	503	VAL	4.0
2	B	621	GLN	3.9
2	B	454	GLN	3.9
3	C	381	PHE	3.9
3	C	453	GLN	3.9
2	B	415	LEU	3.9
2	B	285	VAL	3.9
3	C	473	VAL	3.8
3	C	411	LEU	3.8
3	C	456	ASP	3.8
2	B	306	ARG	3.7
2	B	567	GLU	3.7
2	B	619	GLN	3.7
3	C	511	TYR	3.6
2	B	332	GLU	3.6
3	C	647	GLU	3.5
2	B	479	PRO	3.5
2	B	309	VAL	3.5
3	C	528	GLY	3.5
3	C	644	ASN	3.5
3	C	590	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	491	ARG	3.5
3	C	522	LYS	3.5
1	A	122	PHE	3.5
2	B	303	ARG	3.5
2	B	350	THR	3.4
3	C	652	SER	3.4
1	A	111	ILE	3.4
2	B	623	THR	3.4
2	B	637	ALA	3.4
2	B	396	ALA	3.4
3	C	479	VAL	3.4
2	B	673	THR	3.4
3	C	506	VAL	3.3
3	C	672	LYS	3.3
3	C	517	THR	3.3
2	B	435	VAL	3.3
2	B	183	TYR	3.3
2	B	182	VAL	3.3
2	B	264	THR	3.3
2	B	480	ASP	3.3
3	C	460	VAL	3.3
3	C	640	PRO	3.3
2	B	612	GLU	3.2
3	C	393	LEU	3.2
2	B	508	VAL	3.1
3	C	402	ILE	3.1
2	B	155	PRO	3.1
2	B	300	ALA	3.1
2	B	268	LEU	3.1
3	C	501	ILE	3.1
1	A	64	PHE	3.1
2	B	500	MET	3.1
2	B	445	PRO	3.0
2	B	307	ALA	3.0
3	C	592	VAL	3.0
3	C	277	MET	2.9
2	B	604	PRO	2.9
3	C	484	GLY	2.9
3	C	521	ILE	2.9
2	B	639	PRO	2.9
2	B	620	GLU	2.9
3	C	486	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	564	ILE	2.8
3	C	650	THR	2.8
2	B	185	LEU	2.8
2	B	287	LEU	2.8
2	B	283	LEU	2.8
2	B	453	TRP	2.8
3	C	487	ARG	2.8
2	B	501	GLU	2.7
3	C	477	VAL	2.7
2	B	153	SER	2.7
2	B	636	SER	2.7
3	C	467	ILE	2.7
3	C	490	LEU	2.7
3	C	535	VAL	2.7
2	B	239	ALA	2.6
3	C	491	PHE	2.6
2	B	327	PRO	2.6
3	C	597	VAL	2.6
1	A	121	GLY	2.6
2	B	446	PRO	2.6
3	C	401	LEU	2.6
2	B	272	ARG	2.6
1	A	143	ILE	2.5
3	C	599	TRP	2.5
3	C	382	PHE	2.5
2	B	312	VAL	2.5
2	B	405	GLU	2.5
1	A	95	ALA	2.5
1	A	135	LEU	2.5
3	C	352	GLY	2.4
3	C	655	GLY	2.4
3	C	555	TYR	2.4
2	B	610	VAL	2.4
3	C	629	GLU	2.4
2	B	650	VAL	2.4
1	A	134	ALA	2.4
3	C	618	VAL	2.4
3	C	421	TYR	2.4
3	C	416	ALA	2.4
3	C	654	GLY	2.4
2	B	622	VAL	2.4
3	C	447	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	466	ASN	2.4
2	B	482	GLU	2.4
3	C	603	ILE	2.4
2	B	657	ARG	2.3
3	C	388	VAL	2.3
2	B	238	ASP	2.3
2	B	475	ALA	2.3
3	C	583	ARG	2.3
3	C	622	ALA	2.3
2	B	331	PRO	2.3
2	B	506	LYS	2.3
2	B	629	GLY	2.3
2	B	444	LEU	2.3
3	C	609	SER	2.3
1	A	91	SER	2.3
2	B	614	GLY	2.3
2	B	296	VAL	2.3
3	C	659	LEU	2.2
3	C	613	LEU	2.2
2	B	503	GLN	2.2
2	B	606	LEU	2.2
2	B	613	HIS	2.2
3	C	425	LEU	2.2
2	B	261	VAL	2.2
2	B	262	SER	2.2
3	C	420	ILE	2.2
2	B	461	TRP	2.2
2	B	395	ILE	2.2
2	B	265	LEU	2.2
3	C	505	PRO	2.1
2	B	675	VAL	2.1
3	C	615	GLY	2.1
2	B	412	ARG	2.1
2	B	499	ARG	2.1
2	B	184	LEU	2.1
2	B	628	GLU	2.1
3	C	513	THR	2.1
2	B	200	VAL	2.1
3	C	321	ASP	2.1
2	B	531	GLN	2.1
1	A	131	LEU	2.1
1	A	63	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	430	ILE	2.1
3	C	550	LEU	2.0
3	C	379	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 monosaccharides 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(\AA^2)	Q<0.9
4	CA	C	1002	1/1	0.74	0.34	153,153,153,153	0
4	CA	C	1001	1/1	0.87	0.32	136,136,136,136	0
4	CA	C	1003	1/1	0.94	0.25	170,170,170,170	0

6.5 Other polymers [i](#)

There are no such residues in this entry.