



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:34 AM UTC

PDB ID : 2GH8 / pdb_00002gh8
Title : X-ray structure of a native calicivirus
Authors : Chen, R.
Deposited on : 2006-03-26
Resolution : 3.20 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

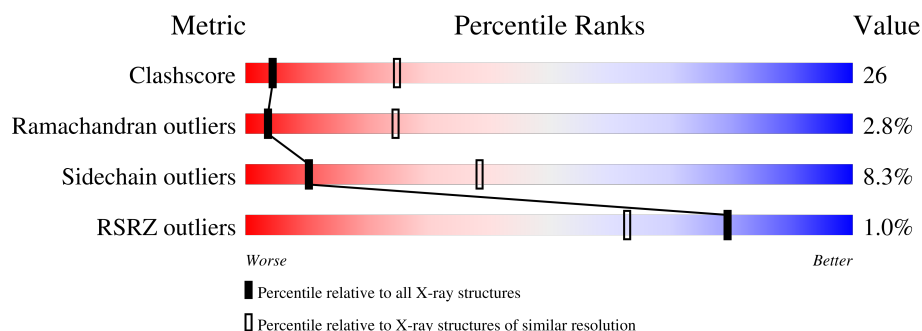
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	558	2% 49% 40% 8% ••
1	B	558	% 51% 40% 6% •
1	C	558	% 54% 38% 5% ••

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12747 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4257	2719	698	828	12			
1	B	541	Total	C	N	O	S	0	0	0
			4233	2703	695	823	12			
1	C	544	Total	C	N	O	S	0	0	0
			4257	2719	698	828	12			

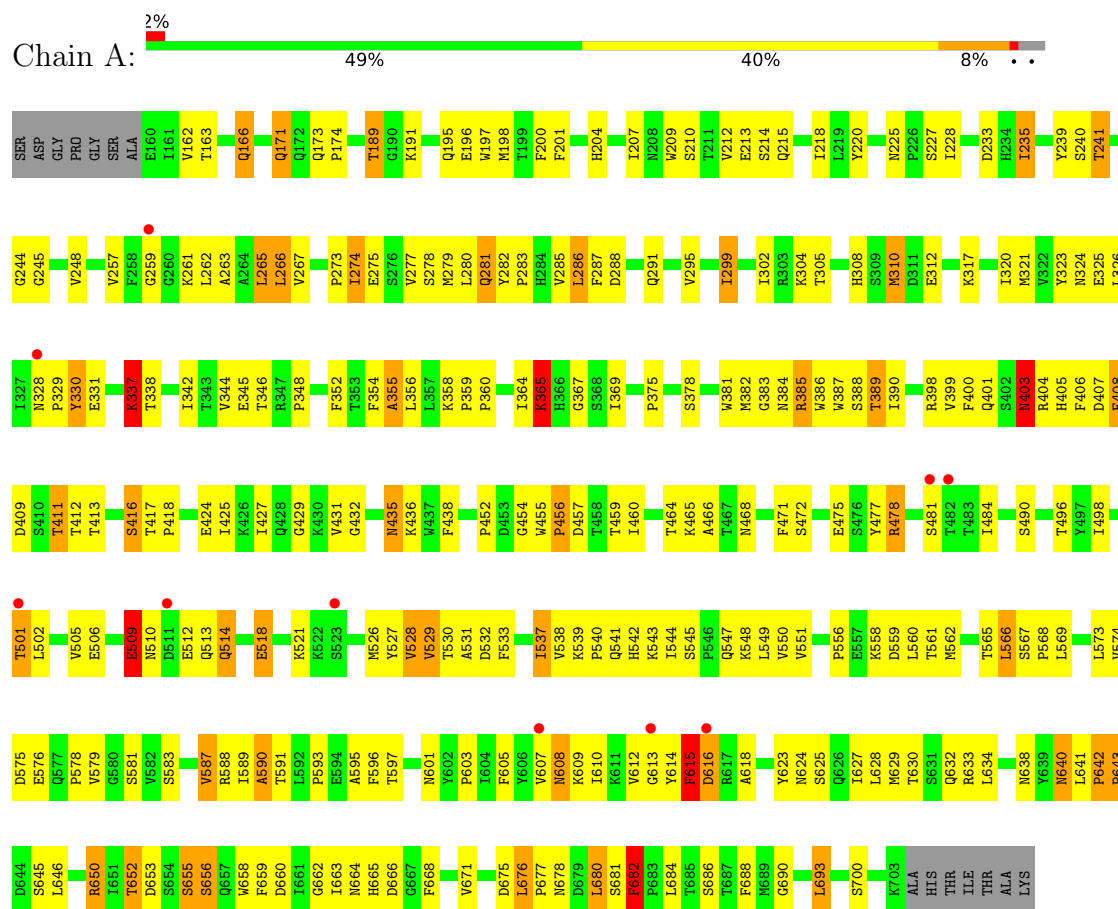
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	ILE	-	SEE REMARK 999	UNP P36285
A	321	MET	-	SEE REMARK 999	UNP P36285
A	322	VAL	-	SEE REMARK 999	UNP P36285
A	323	TYR	-	SEE REMARK 999	UNP P36285
A	324	ASN	-	SEE REMARK 999	UNP P36285
A	325	GLU	-	SEE REMARK 999	UNP P36285
A	326	LEU	-	SEE REMARK 999	UNP P36285
B	320	ILE	-	SEE REMARK 999	UNP P36285
B	321	MET	-	SEE REMARK 999	UNP P36285
B	322	VAL	-	SEE REMARK 999	UNP P36285
B	323	TYR	-	SEE REMARK 999	UNP P36285
B	324	ASN	-	SEE REMARK 999	UNP P36285
B	325	GLU	-	SEE REMARK 999	UNP P36285
B	326	LEU	-	SEE REMARK 999	UNP P36285
C	320	ILE	-	SEE REMARK 999	UNP P36285
C	321	MET	-	SEE REMARK 999	UNP P36285
C	322	VAL	-	SEE REMARK 999	UNP P36285
C	323	TYR	-	SEE REMARK 999	UNP P36285
C	324	ASN	-	SEE REMARK 999	UNP P36285
C	325	GLU	-	SEE REMARK 999	UNP P36285
C	326	LEU	-	SEE REMARK 999	UNP P36285

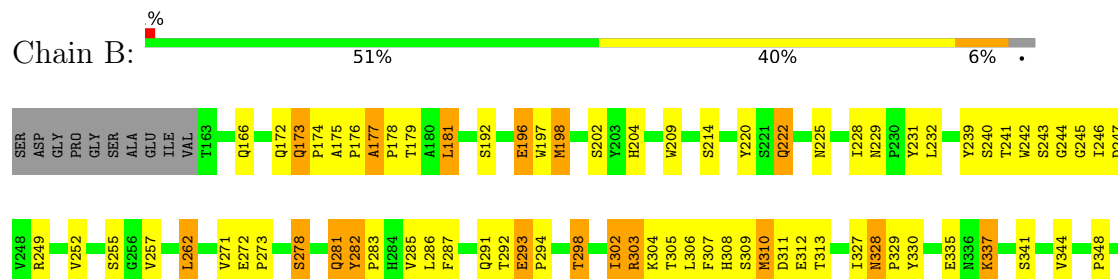
3 Residue-property plots [i](#)

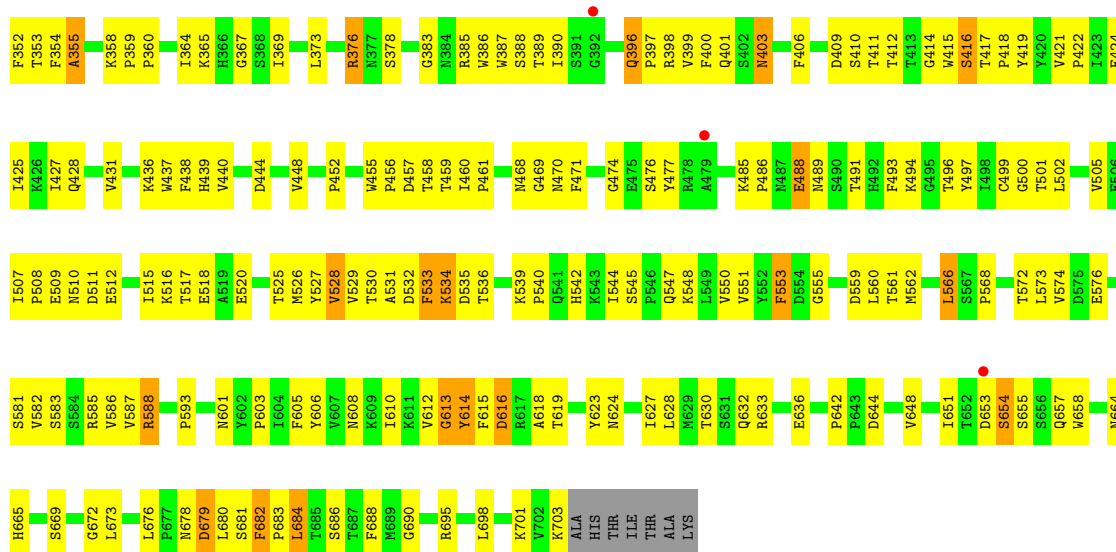
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Capsid protein

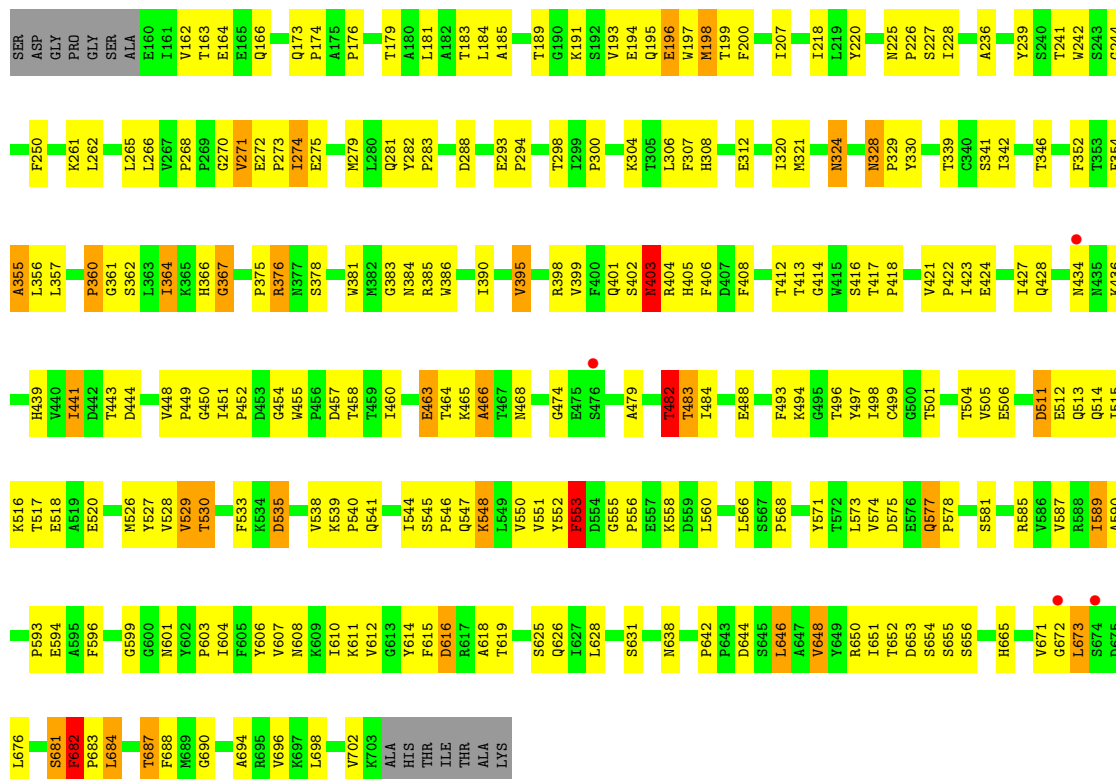


• Molecule 1: Capsid protein





• Molecule 1: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	457.55Å 457.55Å 457.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	86.1 (50.00-3.20) 86.1 (50.00-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.260 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 121.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.44	EDS
Total number of atoms	12747	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	0/4371	1.04	18/5967 (0.3%)
1	B	0.64	1/4347 (0.0%)	1.04	19/5934 (0.3%)
1	C	0.64	1/4371 (0.0%)	1.01	15/5967 (0.3%)
All	All	0.64	2/13089 (0.0%)	1.03	52/17868 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	MET	SD-CE	5.23	1.92	1.79
1	B	302	ILE	CA-CB	-5.04	1.48	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	ALA	N-CA-C	9.81	116.83	108.78
1	B	682	PHE	N-CA-C	7.83	127.11	109.81
1	B	282	TYR	N-CA-C	-7.64	101.34	108.22
1	B	179	THR	N-CA-C	-7.20	104.75	113.97
1	B	281	GLN	N-CA-C	-7.02	101.93	111.55
1	A	501	THR	N-CA-C	6.97	119.76	109.24
1	B	684	LEU	N-CA-C	6.50	120.15	110.52
1	C	682	PHE	N-CA-C	6.45	124.06	109.81
1	B	293	GLU	CA-C-N	6.44	126.46	119.89
1	B	293	GLU	C-N-CA	6.44	126.46	119.89
1	B	648	VAL	N-CA-C	6.27	117.61	108.58
1	A	299	ILE	N-CA-C	-6.17	101.95	107.56
1	C	682	PHE	CA-C-N	-6.02	112.31	119.84
1	C	682	PHE	C-N-CA	-6.02	112.31	119.84
1	C	607	VAL	N-CA-C	5.92	117.28	108.23
1	C	281	GLN	N-CA-C	-5.87	103.36	111.81
1	A	607	VAL	N-CA-C	5.87	117.03	108.58
1	C	355	ALA	N-CA-C	5.87	123.29	110.80
1	A	682	PHE	N-CA-C	5.76	122.55	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	PHE	N-CA-C	5.73	118.99	107.41
1	C	479	ALA	N-CA-C	-5.69	105.73	114.16
1	A	528	VAL	N-CA-C	5.61	117.30	109.55
1	C	298	THR	CA-C-N	-5.57	118.81	122.60
1	C	298	THR	C-N-CA	-5.57	118.81	122.60
1	A	281	GLN	N-CA-C	-5.56	105.64	113.20
1	B	173	GLN	CA-C-N	-5.55	112.90	119.84
1	B	173	GLN	C-N-CA	-5.55	112.90	119.84
1	B	682	PHE	CA-C-N	-5.54	112.91	119.84
1	B	682	PHE	C-N-CA	-5.54	112.91	119.84
1	A	369	ILE	CA-C-N	5.49	126.70	119.84
1	A	369	ILE	C-N-CA	5.49	126.70	119.84
1	B	528	VAL	N-CA-C	5.45	117.73	109.12
1	B	550	VAL	N-CA-C	5.42	115.92	108.12
1	C	648	VAL	N-CA-C	5.35	117.00	108.87
1	C	577	GLN	CA-C-N	5.34	125.63	119.92
1	C	577	GLN	C-N-CA	5.34	125.63	119.92
1	A	365	LYS	CA-C-N	-5.33	114.28	122.60
1	A	365	LYS	C-N-CA	-5.33	114.28	122.60
1	B	355	ALA	N-CA-C	5.33	122.16	110.80
1	A	266	LEU	CA-C-N	-5.33	118.14	123.04
1	A	266	LEU	C-N-CA	-5.33	118.14	123.04
1	C	684	LEU	N-CA-C	5.30	117.37	110.43
1	A	676	LEU	CA-C-N	5.19	125.47	119.92
1	A	676	LEU	C-N-CA	5.19	125.47	119.92
1	C	199	THR	N-CA-C	5.17	118.61	112.72
1	A	359	PRO	CA-C-N	5.13	126.25	119.84
1	A	359	PRO	C-N-CA	5.13	126.25	119.84
1	B	214	SER	N-CA-C	5.12	118.30	110.36
1	B	534	LYS	N-CA-C	-5.11	100.18	108.41
1	C	395	VAL	CB-CA-C	-5.07	106.42	111.80
1	B	196	GLU	N-CA-C	5.06	117.45	111.33
1	A	310	MET	N-CA-C	5.04	118.52	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4257	0	4164	253	0
1	B	4233	0	4138	222	0
1	C	4257	0	4164	206	1
All	All	12747	0	12466	666	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (666) 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:B:241:THR:HB	1:B:355:ALA:HB3	1.22	1.16
1:C:241:THR:HB	1:C:355:ALA:HB3	1.11	1.05
1:C:412:THR:HG22	1:C:414:GLY:H	1.21	1.02
1:A:228:ILE:HG22	1:A:346:THR:HG21	1.43	0.99
1:A:459:THR:HG22	1:A:460:ILE:H	1.26	0.97
1:C:241:THR:CB	1:C:355:ALA:HB3	1.95	0.97
1:C:225:ASN:HD22	1:C:227:SER:H	1.00	0.96
1:A:286:LEU:H	1:B:166:GLN:HE22	1.18	0.92
1:C:577:GLN:HE21	1:C:585:ARG:HH12	1.18	0.92
1:B:412:THR:HG22	1:B:414:GLY:H	1.32	0.91
1:C:428:GLN:HB2	1:C:441:ILE:HD11	1.53	0.91
1:C:364:ILE:HD12	1:C:364:ILE:H	1.35	0.91
1:C:611:LYS:HA	1:C:619:THR:HG22	1.53	0.91
1:B:496:THR:HG21	1:B:527:TYR:HB3	1.52	0.90
1:B:241:THR:CB	1:B:355:ALA:HB3	2.01	0.90
1:A:163:THR:HG23	1:A:166:GLN:NE2	1.86	0.90
1:A:496:THR:HA	1:A:529:VAL:HG13	1.55	0.89
1:A:526:MET:HE2	1:A:551:VAL:HG11	1.52	0.89
1:C:416:SER:HB3	1:C:454:GLY:H	1.36	0.89
1:C:376:ARG:H	1:C:376:ARG:HD2	1.36	0.89
1:B:529:VAL:HG12	1:B:530:THR:H	1.39	0.88
1:A:431:VAL:HG13	1:A:432:GLY:H	1.37	0.88
1:A:459:THR:HG23	1:A:530:THR:O	1.74	0.86
1:C:499:CYS:HB3	1:C:568:PRO:HA	1.57	0.85
1:C:225:ASN:ND2	1:C:227:SER:H	1.74	0.85
1:A:435:ASN:HD21	1:A:466:ALA:HB1	1.42	0.83
1:B:378:SER:HB3	1:B:684:LEU:HB2	1.60	0.83
1:B:496:THR:HG23	1:B:529:VAL:HG23	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:H	1:A:624:ASN:HD22	1.24	0.82
1:C:193:VAL:HG12	1:C:194:GLU:H	1.42	0.82
1:B:657:GLN:HE21	1:B:703:LYS:H	1.27	0.82
1:B:601:ASN:HD21	1:B:698:LEU:H	1.27	0.81
1:B:282:TYR:CG	1:B:283:PRO:HD2	2.16	0.81
1:B:553:PHE:HZ	1:B:562:MET:HE1	1.43	0.81
1:A:496:THR:HA	1:A:529:VAL:CG1	2.11	0.80
1:C:654:SER:HB2	1:C:681:SER:HB2	1.62	0.79
1:A:459:THR:HG22	1:A:460:ILE:N	1.97	0.78
1:B:460:ILE:HG23	1:B:529:VAL:HG11	1.66	0.78
1:B:176:PRO:C	1:B:178:PRO:HD2	2.08	0.78
1:C:436:LYS:HE3	1:C:468:ASN:HB3	1.64	0.78
1:A:228:ILE:CG2	1:A:346:THR:HG21	2.14	0.78
1:C:455:TRP:CZ2	1:C:528:VAL:HG13	2.19	0.77
1:B:303:ARG:NH1	1:B:306:LEU:O	2.17	0.77
1:B:427:ILE:HD12	1:B:562:MET:HE3	1.67	0.77
1:C:406:PHE:H	1:C:626:GLN:HE22	1.31	0.76
1:B:529:VAL:HG12	1:B:530:THR:N	1.98	0.76
1:A:652:THR:HG23	1:A:658:TRP:HB3	1.66	0.76
1:A:680:LEU:HD23	1:A:680:LEU:H	1.51	0.76
1:B:531:ALA:HB1	1:B:539:LYS:O	1.85	0.76
1:A:427:ILE:HD11	1:A:562:MET:SD	2.26	0.75
1:B:505:VAL:HG13	1:B:560:LEU:HD11	1.69	0.75
1:C:573:LEU:HD12	1:C:574:VAL:H	1.51	0.75
1:A:526:MET:CE	1:A:551:VAL:HG11	2.17	0.75
1:C:328:ASN:ND2	1:C:330:TYR:H	1.86	0.74
1:C:193:VAL:HG12	1:C:194:GLU:N	2.00	0.74
1:A:218:ILE:HG13	1:A:275:GLU:HG2	1.68	0.73
1:C:578:PRO:HG2	1:C:581:SER:HB3	1.69	0.73
1:B:496:THR:HA	1:B:529:VAL:HG22	1.70	0.73
1:A:541:GLN:HG2	1:A:548:LYS:HG2	1.69	0.73
1:C:218:ILE:HG13	1:C:275:GLU:HG3	1.70	0.73
1:A:567:SER:O	1:A:569:LEU:HD12	1.89	0.73
1:A:207:ILE:HD13	1:A:220:TYR:HB2	1.68	0.73
1:B:282:TYR:CD1	1:B:283:PRO:HD2	2.24	0.73
1:C:189:THR:HG23	1:C:191:LYS:H	1.55	0.72
1:B:328:ASN:C	1:B:328:ASN:HD22	1.96	0.72
1:C:185:ALA:O	1:C:189:THR:HG22	1.89	0.72
1:A:496:THR:HG22	1:A:529:VAL:HG21	1.70	0.72
1:A:650:ARG:HD3	1:A:660:ASP:OD1	1.89	0.72
1:A:408:PHE:HA	1:A:634:LEU:HD22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:H	1:A:624:ASN:ND2	1.89	0.71
1:A:583:SER:OG	1:A:588:ARG:NH2	2.24	0.71
1:B:328:ASN:HD22	1:B:329:PRO:N	1.88	0.71
1:C:395:VAL:HA	1:C:604:ILE:HG22	1.73	0.71
1:A:460:ILE:HG13	1:A:540:PRO:HB3	1.72	0.71
1:C:375:PRO:HG2	1:C:381:TRP:CD1	2.25	0.71
1:A:367:GLY:HA3	1:A:640:ASN:HB3	1.72	0.70
1:A:531:ALA:HB1	1:A:539:LYS:O	1.91	0.70
1:A:262:LEU:HD21	1:A:342:ILE:HD13	1.72	0.70
1:A:244:GLY:HA3	1:A:352:PHE:HA	1.72	0.70
1:A:288:ASP:HB3	1:A:291:GLN:HG3	1.73	0.70
1:A:431:VAL:HB	1:A:559:ASP:HB3	1.73	0.70
1:B:455:TRP:CZ2	1:B:528:VAL:HG13	2.27	0.70
1:C:328:ASN:HD22	1:C:329:PRO:N	1.88	0.70
1:B:232:LEU:HD11	1:B:348:PRO:HB3	1.75	0.69
1:B:376:ARG:H	1:B:376:ARG:HD2	1.57	0.69
1:A:641:LEU:HD21	1:A:646:LEU:HA	1.75	0.69
1:C:384:ASN:HB2	1:C:626:GLN:O	1.92	0.68
1:A:225:ASN:HD22	1:A:227:SER:H	1.42	0.68
1:A:241:THR:HG23	1:A:355:ALA:HB3	1.74	0.68
1:C:529:VAL:HG22	1:C:530:THR:N	2.08	0.68
1:A:501:THR:HG22	1:A:502:LEU:N	2.07	0.68
1:A:459:THR:CG2	1:A:460:ILE:H	2.06	0.68
1:B:328:ASN:HD22	1:B:329:PRO:CD	2.06	0.68
1:B:612:VAL:HG22	1:B:618:ALA:O	1.94	0.68
1:A:541:GLN:HE21	1:A:542:HIS:N	1.91	0.67
1:B:526:MET:HE2	1:B:566:LEU:HD22	1.75	0.67
1:A:171:GLN:H	1:A:171:GLN:NE2	1.93	0.67
1:A:556:PRO:HG3	1:A:560:LEU:HD11	1.76	0.67
1:A:285:VAL:HG11	1:A:295:VAL:HG11	1.76	0.67
1:C:328:ASN:HD22	1:C:328:ASN:C	2.00	0.66
1:C:577:GLN:NE2	1:C:585:ARG:HH12	1.92	0.66
1:B:427:ILE:HG22	1:B:428:GLN:N	2.11	0.66
1:C:385:ARG:NH1	1:C:457:ASP:OD2	2.28	0.66
1:C:228:ILE:HG21	1:C:346:THR:HG21	1.76	0.66
1:A:282:TYR:CG	1:A:283:PRO:HD2	2.31	0.66
1:A:413:THR:O	1:A:589:ILE:HG21	1.96	0.65
1:A:628:LEU:HG	1:A:632:GLN:HE21	1.61	0.65
1:B:566:LEU:N	1:B:566:LEU:HD23	2.11	0.65
1:C:228:ILE:CG2	1:C:346:THR:HG21	2.25	0.65
1:C:383:GLY:HA3	1:C:608:ASN:HD21	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:PHE:H	1:C:626:GLN:NE2	1.93	0.65
1:A:431:VAL:HG13	1:A:432:GLY:N	2.11	0.65
1:A:573:LEU:HD12	1:A:574:VAL:H	1.62	0.65
1:B:403:ASN:ND2	1:B:415:TRP:H	1.95	0.65
1:A:399:VAL:HG13	1:A:605:PHE:CZ	2.32	0.65
1:C:225:ASN:HD22	1:C:227:SER:N	1.85	0.65
1:A:378:SER:HB3	1:A:684:LEU:HB2	1.77	0.64
1:A:308:HIS:HA	1:A:312:GLU:OE2	1.97	0.64
1:A:225:ASN:ND2	1:A:227:SER:H	1.96	0.64
1:B:431:VAL:HG23	1:B:559:ASP:HB2	1.78	0.64
1:B:469:GLY:C	1:B:470:ASN:HD22	2.05	0.64
1:C:412:THR:HG22	1:C:414:GLY:N	2.03	0.64
1:C:424:GLU:O	1:C:443:THR:HG23	1.97	0.64
1:C:528:VAL:HG21	1:C:566:LEU:HD13	1.79	0.64
1:B:293:GLU:HG3	1:B:294:PRO:HD2	1.80	0.64
1:B:281:GLN:HB2	1:C:360:PRO:HG2	1.79	0.63
1:A:241:THR:CG2	1:A:355:ALA:HB3	2.28	0.63
1:B:474:GLY:HA3	1:B:488:GLU:HB3	1.78	0.63
1:C:529:VAL:HG22	1:C:530:THR:H	1.64	0.63
1:A:560:LEU:HD12	1:A:560:LEU:C	2.24	0.63
1:B:507:ILE:HD12	1:B:507:ILE:H	1.64	0.63
1:B:303:ARG:HD2	1:B:305:THR:O	1.98	0.62
1:A:680:LEU:HD23	1:A:680:LEU:N	2.13	0.62
1:B:328:ASN:C	1:B:328:ASN:ND2	2.54	0.62
1:B:417:THR:HB	1:B:418:PRO:HD2	1.81	0.62
1:B:534:LYS:O	1:B:536:THR:N	2.33	0.62
1:A:189:THR:HG22	1:A:191:LYS:H	1.65	0.62
1:A:567:SER:O	1:A:569:LEU:CD1	2.46	0.62
1:C:646:LEU:N	1:C:646:LEU:HD23	2.15	0.62
1:B:376:ARG:H	1:B:376:ARG:CD	2.12	0.62
1:C:448:VAL:HG13	1:C:449:PRO:HD2	1.81	0.62
1:A:204:HIS:HB3	1:A:344:VAL:O	2.00	0.61
1:C:460:ILE:O	1:C:540:PRO:HB3	2.00	0.61
1:C:518:GLU:HG3	1:C:560:LEU:HD11	1.81	0.61
1:B:616:ASP:C	1:B:618:ALA:H	2.07	0.61
1:A:676:LEU:HD12	1:A:677:PRO:HD2	1.82	0.61
1:A:399:VAL:HG23	1:A:603:PRO:HB2	1.81	0.61
1:A:496:THR:HG22	1:A:529:VAL:CG2	2.31	0.61
1:A:615:PHE:HD2	1:A:615:PHE:N	1.99	0.61
1:C:364:ILE:H	1:C:364:ILE:CD1	2.07	0.60
1:C:197:TRP:HA	1:C:200:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:GLU:HG3	1:C:294:PRO:HD2	1.83	0.60
1:C:376:ARG:H	1:C:376:ARG:CD	2.00	0.60
1:B:664:ASN:ND2	1:B:665:HIS:H	2.00	0.60
1:A:273:PRO:HB3	1:A:279:MET:HE1	1.84	0.60
1:B:385:ARG:H	1:B:624:ASN:HD22	1.50	0.60
1:C:463:GLU:HB2	1:C:539:LYS:HG2	1.84	0.59
1:B:271:VAL:HG13	1:C:362:SER:HB2	1.84	0.59
1:B:654:SER:HB2	1:B:683:PRO:HG2	1.82	0.59
1:B:682:PHE:O	1:B:684:LEU:N	2.35	0.59
1:B:529:VAL:CG1	1:B:530:THR:H	2.11	0.59
1:C:434:ASN:HD21	1:C:466:ALA:HB1	1.68	0.59
1:A:282:TYR:CD1	1:A:283:PRO:HD2	2.38	0.59
1:A:286:LEU:H	1:B:166:GLN:NE2	1.97	0.59
1:B:398:ARG:HH12	1:B:583:SER:HB2	1.67	0.59
1:B:493:PHE:O	1:B:572:THR:HG21	2.02	0.59
1:B:329:PRO:HG2	1:B:330:TYR:H	1.67	0.59
1:C:376:ARG:HD2	1:C:376:ARG:N	2.15	0.59
1:C:501:THR:HG21	1:C:526:MET:HE3	1.84	0.59
1:B:328:ASN:HD22	1:B:329:PRO:HD2	1.66	0.59
1:C:405:HIS:HD2	1:C:625:SER:OG	1.85	0.59
1:A:544:ILE:HB	1:A:587:VAL:HG11	1.84	0.58
1:C:417:THR:HB	1:C:418:PRO:HD2	1.85	0.58
1:C:671:VAL:HG11	1:C:676:LEU:HD21	1.84	0.58
1:A:265:LEU:HD13	1:A:265:LEU:N	2.17	0.58
1:A:541:GLN:HE21	1:A:542:HIS:H	1.50	0.58
1:A:615:PHE:N	1:A:615:PHE:CD2	2.70	0.58
1:B:496:THR:CG2	1:B:527:TYR:HB3	2.31	0.58
1:B:501:THR:HG22	1:B:502:LEU:N	2.18	0.58
1:A:241:THR:OG1	1:A:355:ALA:HB3	2.04	0.58
1:A:457:ASP:O	1:A:587:VAL:HG23	2.03	0.58
1:A:513:GLN:HG3	1:A:514:GLN:H	1.68	0.58
1:B:229:ASN:HB3	1:B:232:LEU:HB2	1.86	0.58
1:C:450:GLY:HA3	1:C:546:PRO:HB3	1.85	0.58
1:C:589:ILE:HG12	1:C:589:ILE:O	2.03	0.58
1:A:513:GLN:HG3	1:A:514:GLN:N	2.18	0.58
1:B:427:ILE:HG22	1:B:428:GLN:H	1.67	0.58
1:B:337:LYS:HD2	1:B:337:LYS:O	2.04	0.58
1:C:384:ASN:HD21	1:C:404:ARG:HB3	1.69	0.58
1:A:189:THR:HG22	1:A:191:LYS:N	2.18	0.57
1:C:511:ASP:OD1	1:C:515:ILE:HB	2.04	0.57
1:B:582:VAL:O	1:B:586:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:THR:HG22	1:C:483:THR:H	1.69	0.57
1:C:515:ILE:HG23	1:C:560:LEU:HD22	1.86	0.57
1:A:162:VAL:HG13	1:A:166:GLN:HB3	1.86	0.57
1:B:476:SER:HB3	1:B:488:GLU:HG3	1.87	0.57
1:C:483:THR:O	1:C:484:ILE:HG13	2.05	0.57
1:A:455:TRP:CZ2	1:A:528:VAL:HG13	2.39	0.57
1:B:491:THR:O	1:B:494:LYS:HG3	2.04	0.57
1:C:375:PRO:HA	1:C:376:ARG:NH1	2.20	0.57
1:C:464:THR:HG22	1:C:465:LYS:N	2.19	0.57
1:B:396:GLN:HG3	1:B:397:PRO:HD2	1.87	0.56
1:A:630:THR:HG22	1:A:634:LEU:HD12	1.86	0.56
1:A:384:ASN:HB2	1:A:404:ARG:HB2	1.87	0.56
1:A:386:TRP:H	1:A:624:ASN:HD21	1.53	0.56
1:C:654:SER:HB2	1:C:681:SER:CB	2.35	0.56
1:A:531:ALA:HA	1:A:541:GLN:HB3	1.86	0.56
1:A:612:VAL:HG12	1:A:613:GLY:N	2.21	0.56
1:B:255:SER:OG	1:B:257:VAL:HG12	2.05	0.56
1:B:529:VAL:CG1	1:B:530:THR:N	2.69	0.56
1:B:241:THR:CG2	1:B:355:ALA:HB3	2.35	0.56
1:A:328:ASN:HD22	1:A:329:PRO:CD	2.18	0.56
1:B:388:SER:OG	1:B:608:ASN:HB2	2.05	0.56
1:C:455:TRP:CH2	1:C:528:VAL:HG13	2.40	0.56
1:C:556:PRO:CB	1:C:560:LEU:HD12	2.35	0.56
1:A:401:GLN:O	1:A:593:PRO:HD2	2.05	0.56
1:B:515:ILE:HG21	1:B:560:LEU:HD13	1.87	0.56
1:B:573:LEU:HD12	1:B:574:VAL:H	1.71	0.56
1:A:629:MET:O	1:A:633:ARG:HG2	2.06	0.56
1:B:241:THR:HG23	1:B:307:PHE:CD1	2.41	0.56
1:C:241:THR:HG23	1:C:307:PHE:CD1	2.40	0.56
1:A:171:GLN:NE2	1:A:171:GLN:N	2.53	0.56
1:A:287:PHE:CE2	1:A:291:GLN:HB2	2.41	0.55
1:A:436:LYS:HA	1:A:436:LYS:HE2	1.88	0.55
1:B:452:PRO:HG2	1:B:455:TRP:HB2	1.88	0.55
1:C:654:SER:CB	1:C:681:SER:HB2	2.32	0.55
1:A:653:ASP:HB2	1:A:681:SER:O	2.06	0.55
1:C:193:VAL:CG1	1:C:194:GLU:H	2.17	0.55
1:C:244:GLY:HA3	1:C:352:PHE:HA	1.88	0.55
1:A:518:GLU:HG2	1:A:556:PRO:HB3	1.89	0.55
1:A:544:ILE:HG22	1:A:589:ILE:HA	1.88	0.55
1:A:605:PHE:CD2	1:A:623:TYR:HB3	2.41	0.55
1:B:373:LEU:HB3	1:B:630:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:VAL:CG1	1:B:560:LEU:HD11	2.36	0.55
1:C:513:GLN:CD	1:C:513:GLN:H	2.14	0.55
1:A:267:VAL:CG2	1:A:317:LYS:HB3	2.37	0.55
1:A:435:ASN:HD21	1:A:466:ALA:CB	2.16	0.55
1:C:236:ALA:HB2	1:C:354:PHE:CZ	2.41	0.55
1:A:409:ASP:OD2	1:A:411:THR:HB	2.07	0.55
1:A:425:ILE:HD11	1:A:566:LEU:HD21	1.89	0.55
1:B:545:SER:HB3	1:B:548:LYS:HG2	1.89	0.55
1:A:459:THR:HG21	1:A:541:GLN:H	1.72	0.54
1:C:282:TYR:CG	1:C:283:PRO:HD2	2.42	0.54
1:C:541:GLN:HG2	1:C:548:LYS:NZ	2.22	0.54
1:B:173:GLN:O	1:B:175:ALA:N	2.41	0.54
1:B:302:ILE:HG21	1:C:356:LEU:HD11	1.90	0.54
1:C:162:VAL:HG13	1:C:166:GLN:HB3	1.89	0.54
1:A:225:ASN:HD22	1:A:227:SER:CB	2.20	0.54
1:B:471:PHE:CD2	1:B:614:TYR:HB3	2.43	0.54
1:A:265:LEU:HD13	1:A:265:LEU:H	1.71	0.54
1:B:436:LYS:HG3	1:B:468:ASN:ND2	2.22	0.54
1:A:302:ILE:N	1:A:302:ILE:HD12	2.23	0.54
1:B:242:TRP:O	1:B:308:HIS:HB2	2.07	0.54
1:B:387:TRP:H	1:B:387:TRP:CD1	2.24	0.54
1:B:496:THR:HA	1:B:529:VAL:CG2	2.38	0.54
1:A:573:LEU:HD11	1:A:575:ASP:O	2.08	0.53
1:B:439:HIS:NE2	1:B:533:PHE:HB3	2.23	0.53
1:C:610:ILE:O	1:C:619:THR:HB	2.08	0.53
1:B:657:GLN:NE2	1:B:703:LYS:H	2.02	0.53
1:A:198:MET:HA	1:A:348:PRO:HG2	1.89	0.53
1:A:266:LEU:HD12	1:A:299:ILE:HG23	1.90	0.53
1:A:385:ARG:HH11	1:A:385:ARG:HB2	1.74	0.53
1:A:528:VAL:C	1:A:529:VAL:HG22	2.32	0.53
1:B:309:SER:O	1:B:311:ASP:N	2.41	0.53
1:A:201:PHE:HB3	1:A:345:GLU:HB3	1.89	0.53
1:C:384:ASN:ND2	1:C:404:ARG:HB3	2.23	0.53
1:C:460:ILE:HG22	1:C:494:LYS:O	2.08	0.53
1:A:274:ILE:H	1:A:279:MET:HE2	1.74	0.53
1:A:210:SER:OG	1:A:212:VAL:HG22	2.09	0.53
1:A:406:PHE:CD2	1:A:412:THR:HB	2.44	0.53
1:C:207:ILE:HB	1:C:342:ILE:HB	1.91	0.53
1:A:459:THR:HG22	1:A:460:ILE:HG12	1.90	0.53
1:A:498:ILE:HG13	1:A:527:TYR:CE2	2.44	0.53
1:B:403:ASN:ND2	1:B:416:SER:OG	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:ASP:HB3	1:C:577:GLN:HG2	1.91	0.53
1:A:220:TYR:HB3	1:A:320:ILE:HB	1.89	0.53
1:B:364:ILE:O	1:B:367:GLY:N	2.40	0.53
1:C:463:GLU:CB	1:C:539:LYS:HG2	2.39	0.53
1:B:386:TRP:CH2	1:B:568:PRO:HB2	2.43	0.53
1:B:651:ILE:HD12	1:B:651:ILE:N	2.23	0.53
1:A:597:THR:HA	1:A:603:PRO:HD3	1.91	0.52
1:A:646:LEU:HB2	1:A:663:ILE:O	2.09	0.52
1:A:498:ILE:HD12	1:A:498:ILE:N	2.24	0.52
1:B:364:ILE:O	1:B:365:LYS:C	2.52	0.52
1:B:240:SER:C	1:B:310:MET:HG2	2.35	0.52
1:B:399:VAL:HG13	1:B:605:PHE:CZ	2.44	0.52
1:B:421:VAL:HB	1:B:422:PRO:HD2	1.90	0.52
1:C:408:PHE:HB2	1:C:665:HIS:O	2.10	0.52
1:C:451:ILE:HD13	1:C:544:ILE:HD13	1.92	0.52
1:A:532:ASP:OD1	1:A:548:LYS:HE3	2.08	0.52
1:B:418:PRO:HG2	1:B:419:TYR:CE1	2.45	0.52
1:C:242:TRP:O	1:C:308:HIS:HB2	2.10	0.52
1:C:434:ASN:HD21	1:C:466:ALA:CB	2.22	0.52
1:A:501:THR:CG2	1:A:502:LEU:N	2.72	0.52
1:B:532:ASP:OD1	1:B:548:LYS:HD2	2.09	0.52
1:C:452:PRO:HG2	1:C:455:TRP:HB2	1.92	0.52
1:A:403:ASN:ND2	1:A:416:SER:OG	2.43	0.52
1:A:435:ASN:ND2	1:A:466:ALA:HB1	2.20	0.52
1:A:688:PHE:CE2	1:A:690:GLY:HA2	2.45	0.52
1:C:308:HIS:HA	1:C:312:GLU:OE1	2.09	0.52
1:B:515:ILE:C	1:B:517:THR:N	2.67	0.52
1:B:654:SER:CB	1:B:683:PRO:HG2	2.40	0.52
1:A:262:LEU:HD21	1:A:342:ILE:CD1	2.40	0.52
1:A:305:THR:HG21	1:C:304:LYS:HD3	1.92	0.52
1:A:533:PHE:CD1	1:A:538:VAL:HG22	2.45	0.52
1:A:197:TRP:HA	1:A:200:PHE:CE2	2.45	0.51
1:A:529:VAL:HG23	1:A:550:VAL:HG23	1.92	0.51
1:B:386:TRP:H	1:B:624:ASN:HD21	1.57	0.51
1:B:409:ASP:O	1:B:410:SER:HB2	2.09	0.51
1:C:501:THR:HB	1:C:566:LEU:HD23	1.92	0.51
1:C:328:ASN:HD22	1:C:330:TYR:H	1.57	0.51
1:C:423:ILE:HB	1:C:566:LEU:HB2	1.91	0.51
1:C:513:GLN:HB2	1:C:558:LYS:HG2	1.92	0.51
1:A:627:ILE:O	1:A:628:LEU:C	2.53	0.51
1:C:483:THR:C	1:C:484:ILE:HG13	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TYR:CG	1:A:354:PHE:HB3	2.45	0.51
1:A:399:VAL:HG12	1:A:400:PHE:N	2.26	0.51
1:A:682:PHE:O	1:A:684:LEU:N	2.43	0.51
1:B:209:TRP:CH2	1:B:262:LEU:HD13	2.46	0.51
1:C:239:TYR:CG	1:C:354:PHE:HB3	2.46	0.51
1:C:594:GLU:HG3	1:C:596:PHE:CE1	2.46	0.51
1:C:612:VAL:HG22	1:C:618:ALA:O	2.11	0.51
1:B:627:ILE:O	1:B:628:LEU:C	2.54	0.50
1:A:279:MET:HB2	1:A:321:MET:HE1	1.93	0.50
1:A:664:ASN:HD21	1:A:666:ASP:HB2	1.77	0.50
1:B:241:THR:CG2	1:B:355:ALA:CB	2.89	0.50
1:B:515:ILE:C	1:B:517:THR:H	2.19	0.50
1:C:405:HIS:O	1:C:412:THR:HG23	2.11	0.50
1:A:382:MET:HE3	1:A:628:LEU:HD23	1.92	0.50
1:B:209:TRP:CZ2	1:B:262:LEU:HD13	2.46	0.50
1:B:385:ARG:HD2	1:B:623:TYR:O	2.12	0.50
1:C:375:PRO:HG2	1:C:381:TRP:NE1	2.26	0.50
1:B:425:ILE:HD11	1:B:440:VAL:HG11	1.93	0.50
1:C:265:LEU:N	1:C:265:LEU:HD12	2.26	0.50
1:C:499:CYS:HB3	1:C:568:PRO:CA	2.37	0.50
1:A:265:LEU:N	1:A:265:LEU:CD1	2.75	0.50
1:B:560:LEU:HD12	1:B:561:THR:H	1.76	0.50
1:C:505:VAL:HG22	1:C:506:GLU:N	2.26	0.50
1:B:252:VAL:H	1:B:291:GLN:NE2	2.10	0.50
1:C:682:PHE:O	1:C:684:LEU:N	2.41	0.50
1:A:518:GLU:O	1:A:521:LYS:HB2	2.12	0.49
1:B:455:TRP:CZ2	1:B:528:VAL:CG1	2.95	0.49
1:A:406:PHE:CE2	1:A:412:THR:HB	2.47	0.49
1:B:501:THR:HG22	1:B:502:LEU:H	1.75	0.49
1:C:672:GLY:C	1:C:673:LEU:HD13	2.36	0.49
1:A:417:THR:HB	1:A:418:PRO:HD2	1.94	0.49
1:A:545:SER:C	1:A:547:GLN:H	2.21	0.49
1:A:386:TRP:CH2	1:A:568:PRO:HB2	2.47	0.49
1:B:500:GLY:HA2	1:B:525:THR:HG22	1.93	0.49
1:C:528:VAL:HG22	1:C:551:VAL:HG12	1.95	0.49
1:A:477:TYR:CD2	1:A:484:ILE:HD11	2.46	0.49
1:B:272:GLU:OE1	1:B:273:PRO:HD2	2.12	0.49
1:B:337:LYS:HE3	1:B:703:LYS:HZ3	1.78	0.49
1:B:582:VAL:HG23	1:B:585:ARG:HB2	1.95	0.49
1:C:655:SER:OG	1:C:656:SER:N	2.46	0.49
1:A:330:TYR:N	1:A:330:TYR:CD1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:PRO:CD	1:B:515:ILE:HD12	2.43	0.48
1:C:654:SER:OG	1:C:683:PRO:HD2	2.13	0.48
1:A:280:LEU:C	1:A:282:TYR:H	2.20	0.48
1:A:337:LYS:HB2	1:A:337:LYS:NZ	2.28	0.48
1:B:173:GLN:HB3	1:B:174:PRO:CD	2.43	0.48
1:A:261:LYS:H	1:A:324:ASN:HB2	1.77	0.48
1:A:464:THR:HG22	1:A:465:LYS:O	2.14	0.48
1:A:509:GLU:CD	1:A:509:GLU:H	2.22	0.48
1:A:528:VAL:O	1:A:529:VAL:HG13	2.13	0.48
1:B:181:LEU:HD23	1:B:181:LEU:HA	1.72	0.48
1:B:240:SER:HB3	1:B:358:LYS:HB2	1.94	0.48
1:C:514:GLN:HB3	1:C:517:THR:OG1	2.14	0.48
1:A:171:GLN:N	1:A:171:GLN:HE21	2.12	0.48
1:B:220:TYR:CZ	1:B:222:GLN:HB2	2.48	0.48
1:B:411:THR:HG22	1:B:412:THR:N	2.29	0.48
1:C:646:LEU:HD21	1:C:694:ALA:HA	1.94	0.48
1:A:655:SER:OG	1:A:656:SER:N	2.45	0.48
1:B:436:LYS:HE3	1:B:468:ASN:ND2	2.29	0.48
1:B:437:TRP:HB2	1:B:533:PHE:CZ	2.49	0.48
1:A:163:THR:HG23	1:A:166:GLN:HE21	1.73	0.48
1:B:401:GLN:O	1:B:593:PRO:HD2	2.14	0.48
1:B:544:ILE:HB	1:B:587:VAL:CG1	2.44	0.48
1:C:328:ASN:ND2	1:C:328:ASN:C	2.71	0.48
1:C:451:ILE:HD13	1:C:544:ILE:CD1	2.43	0.48
1:A:241:THR:HG23	1:A:356:LEU:N	2.28	0.48
1:A:484:ILE:HG21	1:A:576:GLU:HB2	1.95	0.48
1:A:680:LEU:N	1:A:680:LEU:CD2	2.77	0.48
1:B:304:LYS:HA	1:C:306:LEU:HB2	1.95	0.48
1:A:544:ILE:HB	1:A:587:VAL:CG1	2.43	0.47
1:B:177:ALA:N	1:B:178:PRO:HD2	2.29	0.47
1:B:412:THR:HG22	1:B:414:GLY:N	2.14	0.47
1:C:421:VAL:HB	1:C:422:PRO:HD2	1.95	0.47
1:C:513:GLN:H	1:C:513:GLN:NE2	2.11	0.47
1:B:460:ILE:HG13	1:B:540:PRO:HG3	1.97	0.47
1:B:664:ASN:HD22	1:B:665:HIS:H	1.61	0.47
1:C:439:HIS:NE2	1:C:533:PHE:HB3	2.29	0.47
1:C:529:VAL:CG2	1:C:530:THR:H	2.27	0.47
1:B:678:ASN:C	1:B:680:LEU:H	2.22	0.47
1:C:239:TYR:CD2	1:C:357:LEU:HD23	2.50	0.47
1:C:375:PRO:HA	1:C:376:ARG:HH11	1.78	0.47
1:C:460:ILE:HG13	1:C:540:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:GLU:HG2	1:A:565:THR:HG23	1.97	0.47
1:B:471:PHE:CG	1:B:614:TYR:HB3	2.49	0.47
1:C:458:THR:HB	1:C:497:TYR:HE1	1.79	0.47
1:B:528:VAL:C	1:B:529:VAL:HG23	2.39	0.47
1:A:207:ILE:HG13	1:A:342:ILE:HB	1.96	0.47
1:A:328:ASN:HD22	1:A:329:PRO:N	2.12	0.47
1:A:456:PRO:HG3	1:A:528:VAL:HG12	1.96	0.47
1:A:498:ILE:HD12	1:A:498:ILE:H	1.80	0.47
1:B:528:VAL:O	1:B:529:VAL:CG2	2.62	0.47
1:C:220:TYR:HB3	1:C:320:ILE:HB	1.96	0.47
1:C:512:GLU:HB3	1:C:513:GLN:NE2	2.29	0.47
1:C:545:SER:C	1:C:547:GLN:H	2.22	0.47
1:C:553:PHE:N	1:C:553:PHE:CD2	2.82	0.47
1:A:533:PHE:HD1	1:A:538:VAL:HG22	1.80	0.47
1:C:241:THR:CG2	1:C:355:ALA:HB3	2.44	0.47
1:C:464:THR:HG22	1:C:465:LYS:H	1.79	0.47
1:A:514:GLN:HB3	1:A:558:LYS:HE3	1.96	0.47
1:B:173:GLN:O	1:B:174:PRO:C	2.55	0.47
1:A:163:THR:HG23	1:A:166:GLN:HE22	1.75	0.46
1:A:329:PRO:C	1:A:330:TYR:CD1	2.93	0.46
1:A:560:LEU:HD12	1:A:560:LEU:O	2.15	0.46
1:A:595:ALA:HB2	1:A:668:PHE:CD1	2.50	0.46
1:B:378:SER:CB	1:B:684:LEU:HB2	2.39	0.46
1:C:416:SER:HB3	1:C:454:GLY:N	2.18	0.46
1:A:245:GLY:O	1:A:352:PHE:HB2	2.14	0.46
1:B:386:TRP:HH2	1:B:568:PRO:HB2	1.79	0.46
1:C:528:VAL:CG1	1:C:529:VAL:N	2.78	0.46
1:A:267:VAL:O	1:A:267:VAL:HG23	2.15	0.46
1:A:389:THR:O	1:A:390:ILE:C	2.58	0.46
1:B:658:TRP:NE1	1:B:701:LYS:HB3	2.31	0.46
1:C:261:LYS:HE2	1:C:288:ASP:OD2	2.15	0.46
1:C:413:THR:O	1:C:589:ILE:HG21	2.15	0.46
1:B:528:VAL:CG1	1:B:529:VAL:N	2.77	0.46
1:C:401:GLN:HG2	1:C:402:SER:H	1.80	0.46
1:C:401:GLN:HG2	1:C:402:SER:N	2.30	0.46
1:A:568:PRO:C	1:A:569:LEU:HD12	2.40	0.46
1:B:383:GLY:HA3	1:B:624:ASN:ND2	2.31	0.46
1:C:402:SER:HB2	1:C:593:PRO:HD2	1.97	0.46
1:C:615:PHE:O	1:C:616:ASP:C	2.59	0.46
1:A:452:PRO:HG2	1:A:455:TRP:HB2	1.97	0.46
1:A:612:VAL:CG1	1:A:613:GLY:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:LEU:HD23	1:B:566:LEU:H	1.77	0.46
1:C:653:ASP:HA	1:C:684:LEU:HD23	1.98	0.46
1:A:477:TYR:CE2	1:A:484:ILE:HD11	2.51	0.46
1:C:571:TYR:O	1:C:612:VAL:HA	2.16	0.46
1:A:573:LEU:HD12	1:A:574:VAL:N	2.28	0.46
1:B:278:SER:OG	1:C:361:GLY:N	2.49	0.46
1:C:228:ILE:HG22	1:C:346:THR:HG21	1.98	0.46
1:A:364:ILE:HD12	1:A:364:ILE:N	2.31	0.45
1:C:553:PHE:N	1:C:553:PHE:HD2	2.13	0.45
1:A:173:GLN:HB3	1:A:174:PRO:HD3	1.98	0.45
1:A:384:ASN:O	1:A:404:ARG:HD2	2.15	0.45
1:A:431:VAL:CG1	1:A:432:GLY:H	2.18	0.45
1:A:510:ASN:C	1:A:512:GLU:H	2.25	0.45
1:A:528:VAL:CG1	1:A:529:VAL:N	2.79	0.45
1:A:653:ASP:HA	1:A:684:LEU:HD23	1.98	0.45
1:A:405:HIS:HD2	1:A:625:SER:OG	1.99	0.45
1:B:239:TYR:CG	1:B:354:PHE:HB3	2.52	0.45
1:A:387:TRP:CD1	1:A:387:TRP:H	2.35	0.45
1:B:396:GLN:O	1:B:603:PRO:HG2	2.16	0.45
1:B:653:ASP:C	1:B:655:SER:H	2.24	0.45
1:C:589:ILE:O	1:C:589:ILE:CG1	2.63	0.45
1:A:375:PRO:HG3	1:A:629:MET:HG2	1.98	0.45
1:A:608:ASN:O	1:A:609:LYS:HG3	2.15	0.45
1:B:695:ARG:HH11	1:C:638:ASN:HD22	1.65	0.45
1:A:209:TRP:CZ2	1:A:262:LEU:HD13	2.51	0.45
1:A:240:SER:HB3	1:A:358:LYS:HB2	1.98	0.45
1:A:615:PHE:HD2	1:A:615:PHE:H	1.61	0.45
1:A:305:THR:HB	1:C:304:LYS:HB2	1.98	0.45
1:B:496:THR:HG23	1:B:529:VAL:CG2	2.39	0.45
1:A:209:TRP:CH2	1:A:262:LEU:HD13	2.52	0.45
1:A:267:VAL:HG12	1:B:359:PRO:HG2	1.99	0.45
1:A:386:TRP:HD1	1:A:388:SER:HB2	1.81	0.45
1:A:646:LEU:HD13	1:A:662:GLY:HA3	1.97	0.45
1:C:173:GLN:HB3	1:C:174:PRO:HD3	1.99	0.45
1:C:615:PHE:N	1:C:615:PHE:CD1	2.84	0.45
1:A:398:ARG:HG3	1:A:596:PHE:CE2	2.52	0.45
1:A:578:PRO:HG2	1:A:581:SER:HB2	1.99	0.45
1:A:659:PHE:HA	1:A:700:SER:HA	1.98	0.45
1:B:573:LEU:HD12	1:B:574:VAL:N	2.31	0.45
1:B:615:PHE:HD1	1:B:615:PHE:H	1.65	0.45
1:B:681:SER:C	1:B:683:PRO:HD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:ILE:HG12	1:C:527:TYR:CE2	2.52	0.45
1:C:545:SER:HB2	1:C:546:PRO:HD2	1.98	0.45
1:B:247:ASP:OD1	1:B:298:THR:HB	2.17	0.44
1:B:526:MET:HB3	1:B:551:VAL:CG1	2.47	0.44
1:C:239:TYR:CD1	1:C:354:PHE:HB3	2.52	0.44
1:A:328:ASN:C	1:A:328:ASN:ND2	2.75	0.44
1:A:589:ILE:HG23	1:A:590:ALA:N	2.32	0.44
1:B:458:THR:HB	1:B:497:TYR:HE1	1.81	0.44
1:C:272:GLU:OE1	1:C:273:PRO:HD2	2.17	0.44
1:C:293:GLU:HG3	1:C:294:PRO:CD	2.46	0.44
1:B:287:PHE:CD2	1:B:287:PHE:N	2.84	0.44
1:B:406:PHE:CZ	1:B:418:PRO:HD3	2.52	0.44
1:B:469:GLY:C	1:B:470:ASN:ND2	2.74	0.44
1:C:273:PRO:HB2	1:C:279:MET:HE1	1.98	0.44
1:C:390:ILE:HD13	1:C:606:TYR:HB3	1.99	0.44
1:B:615:PHE:CD1	1:B:615:PHE:N	2.85	0.44
1:C:195:GLN:HB3	1:C:198:MET:HG2	1.99	0.44
1:A:436:LYS:HG3	1:A:468:ASN:HB2	2.00	0.44
1:C:279:MET:CB	1:C:321:MET:HE1	2.47	0.44
1:A:616:ASP:C	1:A:618:ALA:H	2.24	0.44
1:B:359:PRO:HA	1:B:360:PRO:HD2	1.92	0.44
1:B:415:TRP:HA	1:B:448:VAL:HG23	1.98	0.44
1:B:553:PHE:CZ	1:B:562:MET:HE1	2.35	0.44
1:A:541:GLN:HG3	1:A:543:LYS:H	1.82	0.44
1:B:664:ASN:ND2	1:B:665:HIS:N	2.65	0.44
1:C:529:VAL:CG2	1:C:530:THR:N	2.75	0.44
1:A:405:HIS:HE1	1:A:666:ASP:O	2.01	0.44
1:B:245:GLY:C	1:B:246:ILE:HG13	2.43	0.44
1:B:458:THR:HB	1:B:497:TYR:CE1	2.53	0.44
1:B:657:GLN:HE21	1:B:703:LYS:N	2.07	0.44
1:A:399:VAL:CG1	1:A:400:PHE:N	2.80	0.44
1:A:537:ILE:HD12	1:A:537:ILE:O	2.17	0.44
1:C:225:ASN:O	1:C:226:PRO:C	2.61	0.44
1:C:496:THR:OG1	1:C:527:TYR:HB3	2.18	0.44
1:C:544:ILE:HB	1:C:587:VAL:CG1	2.48	0.44
1:A:642:PRO:CB	1:A:643:PRO:HD2	2.47	0.43
1:C:196:GLU:H	1:C:196:GLU:HG2	1.32	0.43
1:C:642:PRO:HB2	1:C:644:ASP:OD1	2.18	0.43
1:A:214:SER:O	1:A:215:GLN:C	2.61	0.43
1:A:365:LYS:HB2	1:C:270:GLY:HA2	1.99	0.43
1:A:505:VAL:HG12	1:A:506:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LEU:HG	1:B:561:THR:N	2.33	0.43
1:C:307:PHE:CD1	1:C:307:PHE:C	2.95	0.43
1:B:176:PRO:C	1:B:178:PRO:CD	2.86	0.43
1:B:222:GLN:HG2	1:B:228:ILE:HG22	2.00	0.43
1:C:513:GLN:HG3	1:C:558:LYS:HB3	2.00	0.43
1:C:646:LEU:N	1:C:646:LEU:CD2	2.81	0.43
1:A:358:LYS:HG3	1:C:271:VAL:HG11	2.00	0.43
1:C:279:MET:HB2	1:C:321:MET:HE1	2.01	0.43
1:A:408:PHE:HB2	1:A:665:HIS:O	2.18	0.43
1:B:244:GLY:HA3	1:B:352:PHE:HA	1.99	0.43
1:B:528:VAL:O	1:B:529:VAL:HG23	2.18	0.43
1:B:612:VAL:HB	1:B:613:GLY:H	1.70	0.43
1:A:225:ASN:ND2	1:A:227:SER:HB3	2.33	0.43
1:B:390:ILE:HG12	1:B:606:TYR:HB3	2.00	0.43
1:B:581:SER:HB3	1:B:623:TYR:CE2	2.53	0.43
1:C:493:PHE:CD2	1:C:552:TYR:CE2	3.07	0.43
1:A:241:THR:CG2	1:A:356:LEU:H	2.32	0.43
1:A:436:LYS:CD	1:A:468:ASN:HD22	2.32	0.43
1:A:475:GLU:HA	1:A:478:ARG:HG2	2.01	0.43
1:A:501:THR:HG22	1:A:502:LEU:H	1.80	0.43
1:A:513:GLN:HE21	1:A:558:LYS:HD3	1.82	0.43
1:B:427:ILE:CG2	1:B:428:GLN:N	2.79	0.43
1:B:539:LYS:HA	1:B:540:PRO:HD3	1.86	0.43
1:B:673:LEU:HD12	1:B:676:LEU:HD23	2.01	0.43
1:A:438:PHE:CD1	1:A:438:PHE:N	2.86	0.43
1:B:225:ASN:O	1:B:228:ILE:HG12	2.18	0.43
1:B:496:THR:HG23	1:B:528:VAL:O	2.19	0.43
1:C:650:ARG:HB2	1:C:687:THR:HG23	2.01	0.43
1:C:694:ALA:C	1:C:696:VAL:H	2.27	0.43
1:A:378:SER:HA	1:A:381:TRP:CD1	2.54	0.43
1:A:472:SER:OG	1:A:490:SER:HB2	2.19	0.43
1:A:545:SER:C	1:A:547:GLN:N	2.77	0.43
1:A:601:ASN:HA	1:A:671:VAL:O	2.18	0.43
1:B:204:HIS:HB3	1:B:344:VAL:O	2.19	0.43
1:B:232:LEU:HD23	1:B:232:LEU:HA	1.77	0.43
1:B:438:PHE:CZ	1:B:555:GLY:HA3	2.54	0.43
1:C:386:TRP:HA	1:C:386:TRP:CE3	2.53	0.43
1:A:225:ASN:HD22	1:A:227:SER:HB3	1.82	0.43
1:A:248:VAL:HG21	1:A:299:ILE:HD11	2.00	0.43
1:A:259:GLY:O	1:A:326:LEU:HD12	2.19	0.43
1:A:304:LYS:O	1:B:306:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:NH1	1:A:623:TYR:O	2.51	0.43
1:B:271:VAL:CG1	1:C:362:SER:HB2	2.49	0.43
1:C:191:LYS:NZ	1:C:196:GLU:OE2	2.51	0.43
1:C:381:TRP:HH2	1:C:651:ILE:HD12	1.83	0.43
1:C:573:LEU:HD12	1:C:574:VAL:N	2.25	0.43
1:B:386:TRP:H	1:B:624:ASN:ND2	2.16	0.42
1:B:496:THR:H	1:B:572:THR:HB	1.83	0.42
1:B:527:TYR:N	1:B:527:TYR:CD1	2.86	0.42
1:A:227:SER:HA	1:A:233:ASP:HB2	2.01	0.42
1:A:650:ARG:HD2	1:A:658:TRP:CE3	2.55	0.42
1:B:400:PHE:O	1:B:401:GLN:HB2	2.19	0.42
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.79	0.42
1:C:399:VAL:CG2	1:C:603:PRO:HB2	2.50	0.42
1:A:383:GLY:HA3	1:A:624:ASN:ND2	2.34	0.42
1:A:638:ASN:C	1:A:638:ASN:ND2	2.75	0.42
1:B:329:PRO:HG2	1:B:330:TYR:N	2.34	0.42
1:B:516:LYS:O	1:B:520:GLU:HG3	2.19	0.42
1:C:366:HIS:O	1:C:367:GLY:O	2.38	0.42
1:B:642:PRO:C	1:B:644:ASP:H	2.28	0.42
1:C:226:PRO:HB3	1:C:352:PHE:HZ	1.83	0.42
1:C:324:ASN:HD22	1:C:324:ASN:HA	1.50	0.42
1:C:405:HIS:CD2	1:C:625:SER:OG	2.70	0.42
1:A:328:ASN:ND2	1:A:330:TYR:HD1	2.18	0.42
1:A:589:ILE:O	1:A:589:ILE:HG12	2.20	0.42
1:B:615:PHE:O	1:B:616:ASP:O	2.37	0.42
1:B:653:ASP:HB3	1:B:680:LEU:HD22	2.01	0.42
1:A:429:GLY:O	1:A:559:ASP:HA	2.20	0.42
1:A:544:ILE:HD11	1:A:549:LEU:HD21	2.02	0.42
1:C:436:LYS:HB3	1:C:552:TYR:CE1	2.55	0.42
1:A:356:LEU:H	1:A:356:LEU:HG	1.64	0.42
1:A:403:ASN:C	1:A:405:HIS:H	2.27	0.42
1:B:553:PHE:N	1:B:553:PHE:CD2	2.88	0.42
1:C:181:LEU:HD23	1:C:181:LEU:HA	1.87	0.42
1:C:403:ASN:ND2	1:C:416:SER:OG	2.53	0.42
1:A:280:LEU:HD13	1:A:323:TYR:CD1	2.54	0.42
1:B:632:GLN:O	1:B:633:ARG:C	2.63	0.42
1:C:383:GLY:O	1:C:628:LEU:HB2	2.20	0.42
1:C:406:PHE:CE2	1:C:412:THR:OG1	2.73	0.42
1:A:263:ALA:HA	1:A:285:VAL:O	2.20	0.41
1:B:385:ARG:NH2	1:B:457:ASP:OD2	2.52	0.41
1:C:193:VAL:CG1	1:C:194:GLU:N	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PHE:CD2	1:A:614:TYR:HB2	2.54	0.41
1:B:616:ASP:C	1:B:618:ALA:N	2.72	0.41
1:C:250:PHE:CE2	1:C:320:ILE:HG13	2.55	0.41
1:C:268:PRO:O	1:C:271:VAL:HG23	2.20	0.41
1:B:601:ASN:HD22	1:B:672:GLY:HA2	1.85	0.41
1:C:596:PHE:CD1	1:C:596:PHE:N	2.88	0.41
1:A:257:VAL:HG11	1:A:330:TYR:CE1	2.55	0.41
1:A:267:VAL:HG22	1:A:317:LYS:HB3	2.02	0.41
1:B:313:THR:HG22	1:B:369:ILE:HD11	2.02	0.41
1:B:425:ILE:HD12	1:B:425:ILE:HA	1.80	0.41
1:B:515:ILE:O	1:B:517:THR:N	2.53	0.41
1:B:605:PHE:CD2	1:B:623:TYR:HB3	2.56	0.41
1:A:328:ASN:HD22	1:A:329:PRO:HD2	1.84	0.41
1:A:579:VAL:HG21	1:A:610:ILE:HD12	2.03	0.41
1:B:197:TRP:HB3	1:B:231:TYR:CG	2.56	0.41
1:B:436:LYS:HE3	1:B:468:ASN:HD22	1.85	0.41
1:B:477:TYR:OH	1:B:489:ASN:HB2	2.21	0.41
1:B:560:LEU:CD1	1:B:561:THR:H	2.33	0.41
1:B:612:VAL:HG22	1:B:618:ALA:C	2.46	0.41
1:C:427:ILE:CD1	1:C:551:VAL:HG21	2.51	0.41
1:A:436:LYS:HD2	1:A:468:ASN:HD22	1.86	0.41
1:A:608:ASN:HB3	1:A:609:LYS:H	1.54	0.41
1:B:309:SER:O	1:B:310:MET:C	2.63	0.41
1:C:682:PHE:C	1:C:684:LEU:N	2.78	0.41
1:B:542:HIS:O	1:B:588:ARG:HD3	2.21	0.41
1:B:560:LEU:CG	1:B:561:THR:N	2.84	0.41
1:A:278:SER:O	1:A:281:GLN:HG3	2.20	0.41
1:A:427:ILE:CG1	1:A:562:MET:HB3	2.50	0.41
1:A:608:ASN:HD22	1:A:608:ASN:HA	1.47	0.41
1:B:176:PRO:O	1:B:178:PRO:CD	2.69	0.41
1:B:231:TYR:O	1:B:232:LEU:C	2.64	0.41
1:B:311:ASP:HB3	1:B:364:ILE:HG21	2.03	0.41
1:B:458:THR:HG22	1:B:459:THR:N	2.36	0.41
1:C:443:THR:HG22	1:C:444:ASP:N	2.35	0.41
1:C:516:LYS:HG2	1:C:520:GLU:OE2	2.20	0.41
1:C:533:PHE:CD1	1:C:538:VAL:HG22	2.56	0.41
1:A:407:ASP:OD1	1:A:666:ASP:HA	2.21	0.41
1:A:641:LEU:HA	1:A:642:PRO:HD2	1.89	0.41
1:A:693:LEU:HA	1:A:693:LEU:HD12	1.78	0.41
1:B:499:CYS:HB3	1:B:566:LEU:HB2	2.03	0.41
1:A:235:ILE:HG22	1:A:354:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASN:HD22	1:A:328:ASN:C	2.29	0.40
1:A:616:ASP:C	1:A:618:ALA:N	2.79	0.40
1:B:403:ASN:HD22	1:B:403:ASN:HA	1.76	0.40
1:C:378:SER:HA	1:C:381:TRP:CG	2.56	0.40
1:C:601:ASN:OD1	1:C:698:LEU:HG	2.21	0.40
1:A:641:LEU:O	1:A:642:PRO:C	2.62	0.40
1:B:196:GLU:C	1:B:198:MET:H	2.29	0.40
1:C:195:GLN:HG3	1:C:197:TRP:CZ2	2.56	0.40
1:C:626:GLN:HG3	1:C:631:SER:OG	2.21	0.40
1:A:560:LEU:C	1:A:560:LEU:CD1	2.93	0.40
1:B:385:ARG:H	1:B:624:ASN:ND2	2.17	0.40
1:B:485:LYS:HA	1:B:486:PRO:HD2	1.95	0.40
1:B:502:LEU:C	1:B:502:LEU:HD23	2.45	0.40
1:B:688:PHE:CZ	1:B:690:GLY:HA2	2.57	0.40
1:C:274:ILE:HD12	1:C:274:ILE:HA	1.91	0.40
1:C:474:GLY:HA3	1:C:488:GLU:HB3	2.03	0.40
1:C:556:PRO:HB2	1:C:560:LEU:HD12	2.02	0.40
1:C:682:PHE:C	1:C:684:LEU:H	2.28	0.40
1:B:307:PHE:CD1	1:B:307:PHE:C	3.00	0.40
1:B:610:ILE:O	1:B:610:ILE:HG23	2.22	0.40
1:C:688:PHE:CZ	1:C:690:GLY:HA2	2.57	0.40
1:A:416:SER:HB3	1:A:454:GLY:H	1.87	0.40
1:B:515:ILE:O	1:B:518:GLU:N	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:THR:OG1	1:C:616:ASP:O[2_555]	2.06	0.14

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	542/558 (97%)	451 (83%)	75 (14%)	16 (3%)	3	23
1	B	539/558 (97%)	466 (86%)	61 (11%)	12 (2%)	5	29
1	C	542/558 (97%)	446 (82%)	78 (14%)	18 (3%)	3	21
All	All	1623/1674 (97%)	1363 (84%)	214 (13%)	46 (3%)	4	25

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	ASN
1	B	535	ASP
1	B	616	ASP
1	C	589	ILE
1	C	616	ASP
1	A	337	LYS
1	A	509	GLU
1	A	514	GLN
1	A	587	VAL
1	A	590	ALA
1	B	310	MET
1	B	335	GLU
1	B	444	ASP
1	B	613	GLY
1	C	367	GLY
1	C	403	ASN
1	C	511	ASP
1	C	590	ALA
1	A	365	LYS
1	A	478	ARG
1	A	643	PRO
1	B	509	GLU
1	B	679	ASP
1	C	548	LYS
1	A	456	PRO
1	A	481	SER
1	A	615	PHE
1	A	616	ASP
1	B	177	ALA
1	C	466	ALA
1	C	529	VAL
1	C	614	TYR
1	A	655	SER
1	B	461	PRO

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Mol	Chain	Res	Type
1	C	482	THR
1	C	535	ASP
1	A	642	PRO
1	B	456	PRO
1	B	510	ASN
1	C	553	PHE
1	C	682	PHE
1	A	682	PHE
1	C	555	GLY
1	C	599	GLY
1	C	702	VAL
1	C	441	ILE

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	481/490 (98%)	436 (91%)	45 (9%)	8	33
1	B	478/490 (98%)	436 (91%)	42 (9%)	9	35
1	C	481/490 (98%)	448 (93%)	33 (7%)	14	45
All	All	1440/1470 (98%)	1320 (92%)	120 (8%)	10	38

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	171	GLN
1	A	189	THR
1	A	195	GLN
1	A	196	GLU
1	A	213	GLU
1	A	235	ILE
1	A	241	THR
1	A	265	LEU
1	A	274	ILE

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Mol	Chain	Res	Type
1	A	277	VAL
1	A	286	LEU
1	A	310	MET
1	A	325	GLU
1	A	330	TYR
1	A	331	GLU
1	A	337	LYS
1	A	338	THR
1	A	360	PRO
1	A	385	ARG
1	A	389	THR
1	A	403	ASN
1	A	408	PHE
1	A	411	THR
1	A	416	SER
1	A	435	ASN
1	A	509	GLU
1	A	518	GLU
1	A	529	VAL
1	A	537	ILE
1	A	561	THR
1	A	566	LEU
1	A	591	THR
1	A	608	ASN
1	A	615	PHE
1	A	640	ASN
1	A	645	SER
1	A	650	ARG
1	A	652	THR
1	A	656	SER
1	A	675	ASP
1	A	678	ASN
1	A	680	LEU
1	A	686	SER
1	A	693	LEU
1	B	172	GLN
1	B	181	LEU
1	B	192	SER
1	B	198	MET
1	B	202	SER
1	B	222	GLN
1	B	243	SER

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Mol	Chain	Res	Type
1	B	249	ARG
1	B	262	LEU
1	B	278	SER
1	B	285	VAL
1	B	286	LEU
1	B	292	THR
1	B	298	THR
1	B	303	ARG
1	B	312	GLU
1	B	327	ILE
1	B	328	ASN
1	B	337	LYS
1	B	341	SER
1	B	353	THR
1	B	376	ARG
1	B	389	THR
1	B	396	GLN
1	B	403	ASN
1	B	416	SER
1	B	424	GLU
1	B	488	GLU
1	B	511	ASP
1	B	512	GLU
1	B	547	GLN
1	B	553	PHE
1	B	566	LEU
1	B	576	GLU
1	B	588	ARG
1	B	614	TYR
1	B	619	THR
1	B	636	GLU
1	B	654	SER
1	B	669	SER
1	B	679	ASP
1	B	686	SER
1	C	163	THR
1	C	164	GLU
1	C	176	PRO
1	C	179	THR
1	C	183	THR
1	C	196	GLU
1	C	262	LEU

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Mol	Chain	Res	Type
1	C	266	LEU
1	C	271	VAL
1	C	274	ILE
1	C	300	PRO
1	C	324	ASN
1	C	328	ASN
1	C	339	THR
1	C	341	SER
1	C	360	PRO
1	C	364	ILE
1	C	376	ARG
1	C	398	ARG
1	C	403	ASN
1	C	463	GLU
1	C	482	THR
1	C	483	THR
1	C	530	THR
1	C	535	ASP
1	C	550	VAL
1	C	553	PHE
1	C	646	LEU
1	C	648	VAL
1	C	652	THR
1	C	673	LEU
1	C	681	SER
1	C	687	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	171	GLN
1	A	204	HIS
1	A	225	ASN
1	A	291	GLN
1	A	328	ASN
1	A	336	ASN
1	A	403	ASN
1	A	405	HIS
1	A	435	ASN
1	A	468	ASN
1	A	489	ASN

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Mol	Chain	Res	Type
1	A	513	GLN
1	A	541	GLN
1	A	577	GLN
1	A	608	ASN
1	A	624	ASN
1	A	632	GLN
1	A	657	GLN
1	B	166	GLN
1	B	281	GLN
1	B	291	GLN
1	B	324	ASN
1	B	328	ASN
1	B	332	ASN
1	B	336	ASN
1	B	403	ASN
1	B	468	ASN
1	B	470	ASN
1	B	489	ASN
1	B	514	GLN
1	B	541	GLN
1	B	542	HIS
1	B	547	GLN
1	B	601	ASN
1	B	624	ASN
1	B	638	ASN
1	B	657	GLN
1	B	664	ASN
1	C	171	GLN
1	C	172	GLN
1	C	208	ASN
1	C	215	GLN
1	C	222	GLN
1	C	225	ASN
1	C	281	GLN
1	C	324	ASN
1	C	328	ASN
1	C	377	ASN
1	C	384	ASN
1	C	403	ASN
1	C	405	HIS
1	C	428	GLN
1	C	513	GLN

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Mol	Chain	Res	Type
1	C	542	HIS
1	C	547	GLN
1	C	577	GLN
1	C	598	GLN
1	C	608	ASN
1	C	626	GLN
1	C	657	GLN
1	C	665	HIS
1	C	692	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	544/558 (97%)	-0.30	10 (1%) 67 48	16, 48, 112, 144	0
1	B	541/558 (96%)	-0.40	3 (0%) 85 73	16, 46, 111, 134	0
1	C	544/558 (97%)	-0.36	4 (0%) 84 69	15, 50, 110, 139	0
All	All	1629/1674 (97%)	-0.35	17 (1%) 79 63	15, 48, 112, 144	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	392	GLY	3.8
1	A	511	ASP	3.8
1	B	479	ALA	3.7
1	B	653	ASP	3.2
1	A	523	SER	3.1
1	A	482	THR	3.0
1	C	674	SER	2.9
1	A	259	GLY	2.8
1	A	607	VAL	2.8
1	A	613	GLY	2.4
1	A	328	ASN	2.3
1	A	616	ASP	2.2
1	C	434	ASN	2.2
1	C	476	SER	2.1
1	A	481	SER	2.1
1	A	501	THR	2.1
1	C	672	GLY	2.1

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.