



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:23 AM GMT

PDB ID : 3EH2
Title : Crystal structure of the human COPII-coat protein Sec24c
Authors : Goldberg, J.; Mancias, J.D.
Deposited on : 2008-09-11
Resolution : 2.35 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

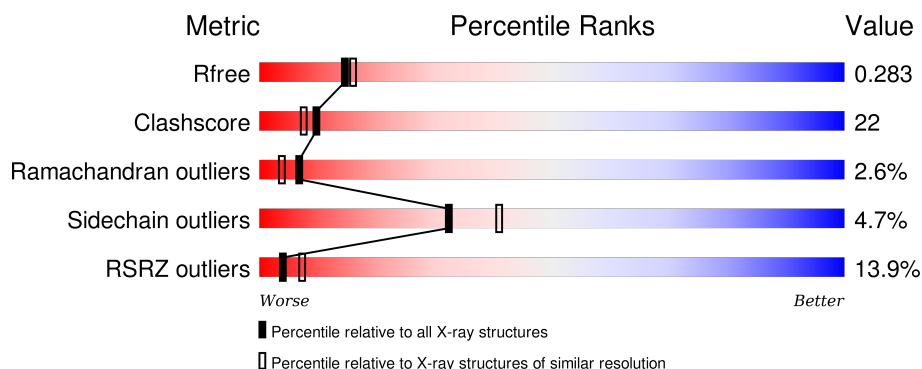
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	766	<div> <div>4%</div> <div>68%</div> <div>28%</div> <div>..</div> </div>
1	B	766	<div> <div>8%</div> <div>63%</div> <div>29%</div> <div>..</div> </div>
1	C	766	<div> <div>28%</div> <div>54%</div> <div>39%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17790 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 Protein transport protein Sec24C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	0	0	0
			5946	3772	1016	1114	44			
1	B	739	Total	C	N	O	S	9	0	0
			5799	3683	986	1086	44			
1	C	739	Total	C	N	O	S	49	0	0
			5802	3680	992	1086	44			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

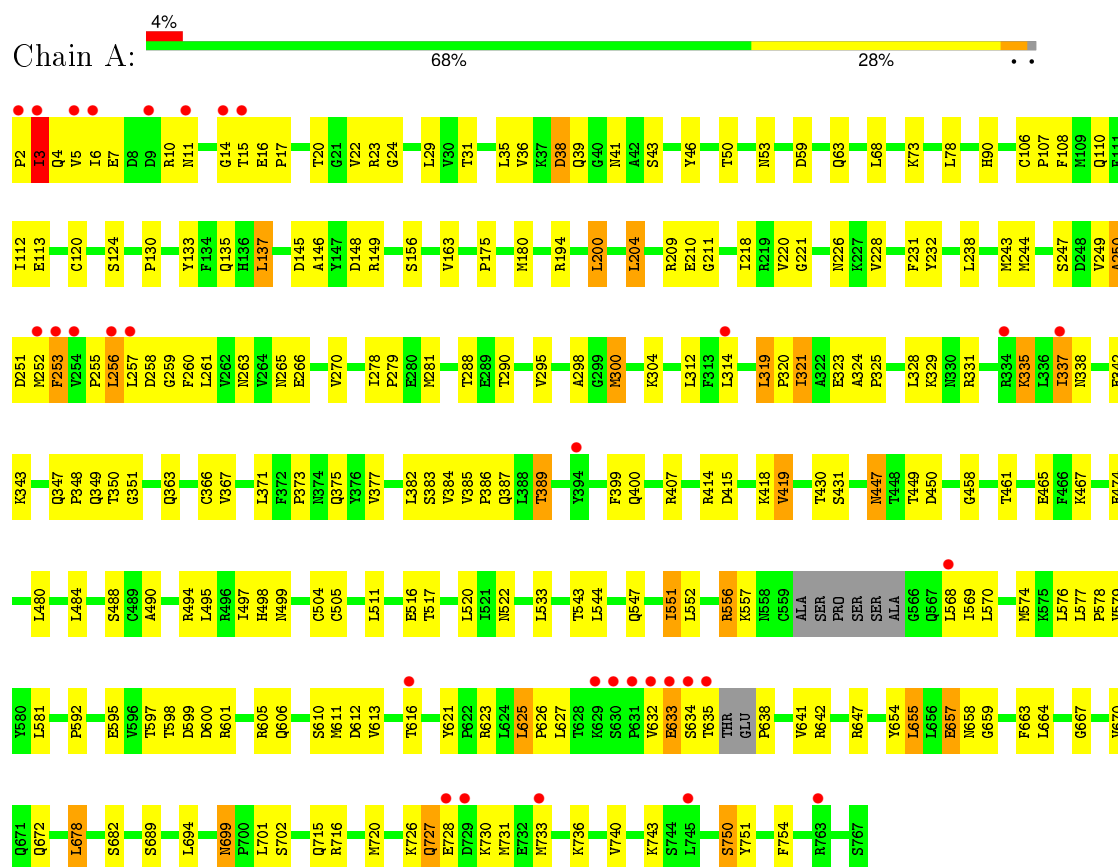
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		
3	B	75	Total	O	0	0
			75	75		
3	C	36	Total	O	0	0
			36	36		

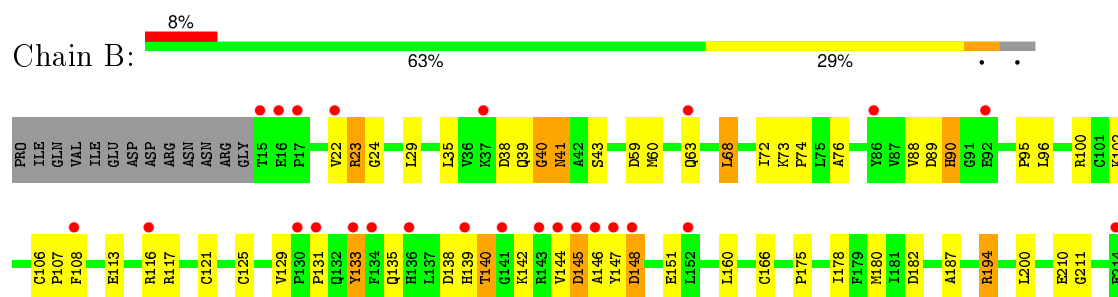
3 Residue-property plots

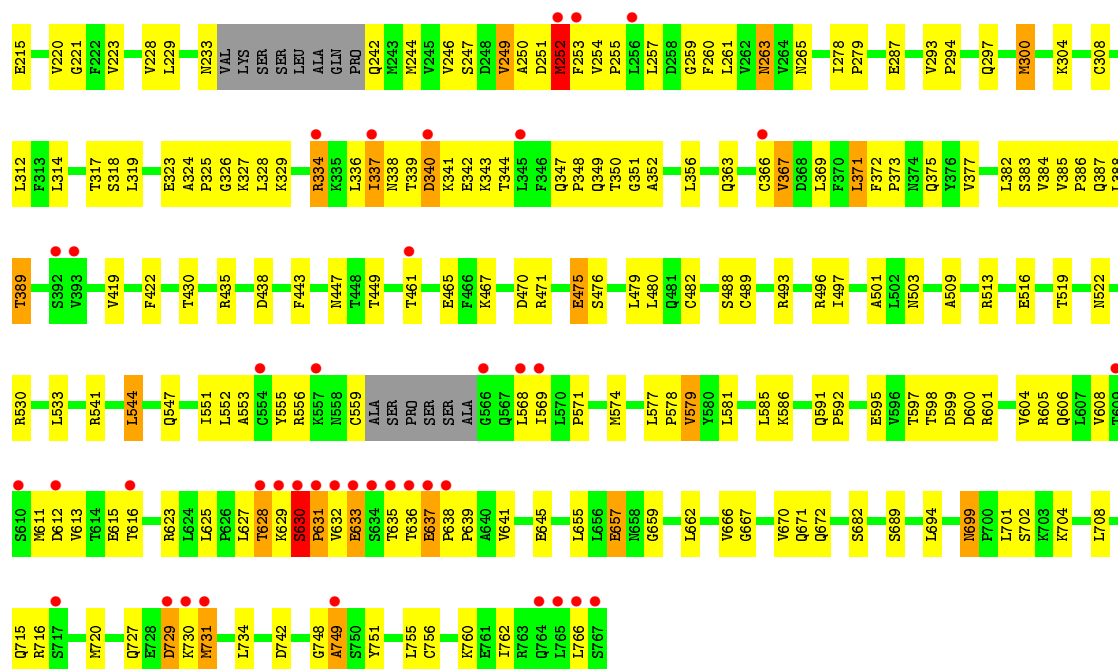
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Protein transport protein Sec24C

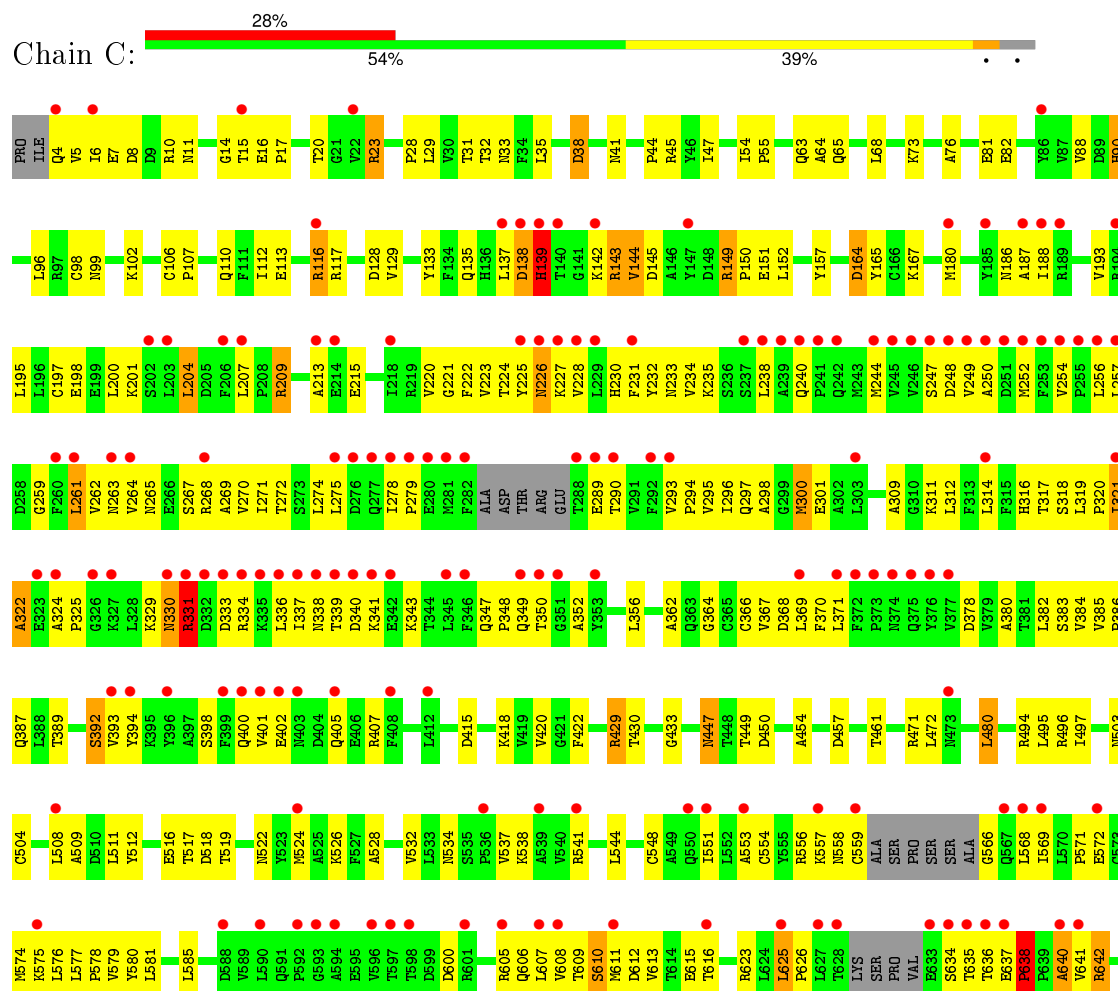


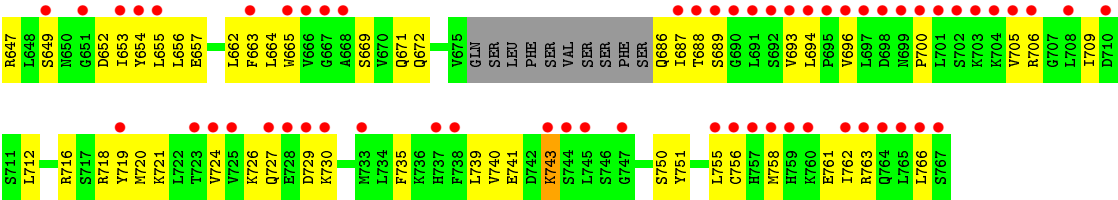
- Molecule 1: Protein transport protein Sec24C





• Molecule 1: Protein transport protein Sec24C





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.69Å 182.98Å 201.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.78 – 2.35 41.78 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.78-2.35) 96.3 (41.78-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.284 0.240 , 0.283	Depositor DCC
R_{free} test set	5281 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 107861 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17790	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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	0.42	0/6061	0.68	1/8215 (0.0%)
1	B	0.35	0/5912	0.64	2/8015 (0.0%)
1	C	0.34	0/5911	0.62	2/8010 (0.0%)
All	All	0.37	0/17884	0.65	5/24240 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	THR	N-CA-C	8.30	133.41	111.00
1	C	729	ASP	N-CA-C	5.68	126.35	111.00
1	A	727	GLN	N-CA-C	5.55	125.98	111.00
1	C	480	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	308	CYS	N-CA-C	-5.10	97.24	111.00

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	5946	0	5958	249	0
1	B	5799	0	5805	236	0
1	C	5802	0	5809	305	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	129	0	0	17	0
3	B	75	0	0	14	0
3	C	36	0	0	20	0
All	All	17790	0	17572	781	0

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 22.

All (781) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ASN:O	1:C:290:THR:HA	1.42	1.19
1:B:632:VAL:HB	1:B:636:THR:HB	1.28	1.07
1:B:180:MET:HE1	1:B:312:LEU:HD13	1.37	1.06
1:A:228:VAL:HG23	1:A:247:SER:HA	1.37	1.04
1:B:249:VAL:HG12	1:B:250:ALA:H	1.22	1.00
1:C:571:PRO:HG2	1:C:574:MET:HB2	1.44	0.99
1:B:329:LYS:H	1:B:349:GLN:HE22	1.02	0.99
1:C:524:MET:HB2	1:C:544:LEU:HD21	1.44	0.97
1:B:367:VAL:H	1:B:389:THR:HG21	1.26	0.97
1:B:629:LYS:O	1:B:630:SER:HB2	1.66	0.95
1:A:657:GLU:OE2	1:A:716:ARG:HD2	1.66	0.95
1:A:367:VAL:H	1:A:389:THR:HG21	1.30	0.95
1:C:636:THR:HG22	1:C:638:PRO:HD3	1.46	0.95
1:A:447:ASN:HD21	1:A:450:ASP:H	0.96	0.95
1:A:180:MET:HE1	1:A:312:LEU:HD13	1.48	0.94
1:A:194:ARG:HE	1:B:672:GLN:HE21	1.14	0.91
1:B:533:LEU:HD11	1:B:605:ARG:HE	1.35	0.90
1:C:14:GLY:HA3	3:C:819:HOH:O	1.72	0.89
1:B:90:HIS:HD2	1:B:96:LEU:H	1.22	0.87
1:C:200:LEU:HB3	3:C:830:HOH:O	1.75	0.86
1:C:139:HIS:HB3	1:C:142:LYS:HB3	1.58	0.85
1:B:630:SER:H	1:B:631:PRO:HD3	1.42	0.84
1:A:447:ASN:ND2	1:A:450:ASP:H	1.74	0.84
1:C:112:ILE:HG23	1:C:113:GLU:HG3	1.60	0.83
1:C:686:GLN:HG3	1:C:687:ILE:HG13	1.60	0.83
1:C:568:LEU:H	1:C:568:LEU:HD23	1.43	0.82
1:C:321:ILE:HD13	1:C:321:ILE:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:ASN:HD21	1:C:450:ASP:H	1.27	0.81
1:C:743:LYS:HG2	1:C:750:SER:HB2	1.60	0.81
1:B:387:GLN:HG3	1:B:606:GLN:HE22	1.47	0.80
1:A:16:GLU:HB3	1:A:17:PRO:HD2	1.62	0.80
1:B:254:VAL:HA	3:B:871:HOH:O	1.81	0.80
1:B:592:PRO:HB3	1:B:601:ARG:HD2	1.62	0.79
1:A:194:ARG:HE	1:B:672:GLN:NE2	1.80	0.79
1:C:566:GLY:N	1:C:763:ARG:HH22	1.80	0.79
1:B:385:VAL:O	1:B:389:THR:HB	1.82	0.79
1:A:533:LEU:HD11	1:A:605:ARG:HE	1.48	0.79
1:A:228:VAL:CG2	1:A:247:SER:HA	2.13	0.78
1:C:90:HIS:HD2	1:C:96:LEU:H	1.32	0.78
1:A:300:MET:HE3	1:A:304:LYS:HE3	1.66	0.78
1:C:387:GLN:HB2	1:C:606:GLN:HE22	1.47	0.78
1:A:490:ALA:HB3	3:A:903:HOH:O	1.83	0.77
1:A:415:ASP:HA	1:A:418:LYS:HD3	1.66	0.77
1:C:641:VAL:HG11	1:C:647:ARG:HE	1.49	0.77
1:B:260:PHE:HA	3:B:858:HOH:O	1.83	0.77
1:A:329:LYS:H	1:A:349:GLN:HE22	1.30	0.77
1:A:210:GLU:CD	1:A:494:ARG:HH22	1.88	0.77
1:A:556:ARG:HD3	1:A:569:ILE:CD1	2.14	0.77
1:A:180:MET:CE	1:A:312:LEU:HD13	2.16	0.76
1:A:579:VAL:HG22	1:A:751:TYR:CE1	2.20	0.76
1:B:249:VAL:HG12	1:B:250:ALA:N	2.01	0.76
1:B:366:CYS:HA	1:B:389:THR:HG23	1.67	0.76
1:C:579:VAL:HG22	1:C:751:TYR:CE1	2.21	0.76
1:A:385:VAL:O	1:A:389:THR:HB	1.85	0.75
1:C:429:ARG:HB2	1:C:429:ARG:HH11	1.51	0.75
1:B:748:GLY:O	1:B:749:ALA:HB3	1.84	0.75
1:A:249:VAL:HG11	1:A:324:ALA:HB1	1.66	0.75
1:A:24:GLY:N	3:A:801:HOH:O	2.18	0.74
1:A:231:PHE:HZ	1:A:298:ALA:HB1	1.50	0.74
1:B:90:HIS:CD2	1:B:96:LEU:H	2.03	0.74
1:A:556:ARG:HD3	1:A:569:ILE:HD11	1.69	0.74
1:C:16:GLU:HB3	1:C:17:PRO:HD2	1.69	0.74
1:A:447:ASN:ND2	1:A:449:THR:H	1.86	0.74
1:A:579:VAL:HG22	1:A:751:TYR:CZ	2.23	0.73
1:A:4:GLN:NE2	3:A:805:HOH:O	2.15	0.73
1:A:659:GLY:HA2	1:A:716:ARG:HD3	1.70	0.73
1:A:672:GLN:HB3	1:B:194:ARG:HD3	1.69	0.73
1:B:41:ASN:HD22	1:B:41:ASN:N	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD23	1:A:320:PRO:HD2	1.68	0.73
1:C:233:ASN:HB2	1:C:257:LEU:HD21	1.70	0.73
1:B:233:ASN:CG	1:B:259:GLY:HA3	2.09	0.73
1:B:633:GLU:HG3	1:B:704:LYS:HE2	1.69	0.73
1:C:116:ARG:HD2	1:C:117:ARG:HG3	1.71	0.72
1:C:541:ARG:HD3	1:C:585:LEU:HD22	1.71	0.72
1:B:623:ARG:HD3	1:B:625:LEU:HD21	1.71	0.72
1:B:22:VAL:HG12	3:B:837:HOH:O	1.90	0.72
1:A:373:PRO:HB3	1:A:377:VAL:HG21	1.71	0.72
1:C:164:ASP:HB3	3:C:804:HOH:O	1.88	0.71
1:C:300:MET:HE1	1:C:301:GLU:HA	1.71	0.71
1:C:228:VAL:HG23	1:C:247:SER:HA	1.73	0.71
1:C:429:ARG:CB	1:C:429:ARG:HH11	2.04	0.70
1:C:401:VAL:O	1:C:405:GLN:HB2	1.90	0.70
1:C:689:SER:OG	1:C:730:LYS:HG3	1.91	0.70
1:C:226:ASN:O	1:C:289:GLU:O	2.08	0.70
1:A:180:MET:HE2	1:A:312:LEU:HB3	1.73	0.70
1:B:350:THR:HG22	1:B:352:ALA:H	1.57	0.70
1:B:533:LEU:HD11	1:B:605:ARG:NE	2.07	0.69
1:B:667:GLY:O	1:B:670:VAL:HG23	1.92	0.69
1:A:461:THR:HG22	1:A:610:SER:O	1.91	0.69
1:A:533:LEU:HD11	1:A:605:ARG:NE	2.08	0.69
1:A:488:SER:OG	3:A:903:HOH:O	2.11	0.69
1:C:343:LYS:HB3	1:C:347:GLN:HE21	1.58	0.69
1:C:324:ALA:HB1	1:C:325:PRO:HD2	1.74	0.69
1:B:40:GLY:C	1:B:41:ASN:HD22	1.96	0.69
1:C:367:VAL:HG22	1:C:389:THR:HG21	1.75	0.68
1:A:556:ARG:HH11	1:A:556:ARG:HB2	1.59	0.68
1:C:611:MET:HB2	1:C:615:GLU:HB2	1.76	0.68
1:C:297:GLN:HG2	1:C:356:LEU:HD13	1.75	0.68
1:B:367:VAL:H	1:B:389:THR:CG2	2.03	0.68
1:C:689:SER:CB	1:C:730:LYS:HG3	2.24	0.68
1:B:135:GLN:HB3	1:B:142:LYS:HE2	1.73	0.68
1:A:672:GLN:NE2	1:B:194:ARG:HD2	2.08	0.68
1:B:144:VAL:HG21	3:B:835:HOH:O	1.93	0.68
1:A:10:ARG:HH21	1:A:14:GLY:HA3	1.59	0.68
1:C:149:ARG:HG3	1:C:149:ARG:HH11	1.58	0.68
1:A:319:LEU:HD21	1:A:328:LEU:HB2	1.75	0.68
1:A:252:MET:O	1:A:253:PHE:HB3	1.94	0.67
1:C:625:LEU:O	1:C:625:LEU:HD22	1.94	0.67
1:A:337:ILE:O	1:A:342:GLU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:HD21	1:A:450:ASP:N	1.81	0.67
1:B:623:ARG:HH22	1:B:715:GLN:HE22	1.41	0.67
1:C:641:VAL:CG1	1:C:647:ARG:HE	2.07	0.67
1:A:547:GLN:O	1:A:551:ILE:HG23	1.95	0.67
1:A:577:LEU:HB3	1:A:578:PRO:HD3	1.76	0.67
1:B:339:THR:HG22	1:B:341:LYS:H	1.60	0.66
1:B:608:VAL:HA	1:B:611:MET:HG2	1.77	0.66
1:C:386:PRO:HA	1:C:389:THR:HG22	1.77	0.66
1:C:139:HIS:HD2	1:C:142:LYS:HD2	1.61	0.66
1:C:418:LYS:HG3	1:C:420:VAL:HG13	1.77	0.66
1:C:6:ILE:HG13	1:C:576:LEU:HD11	1.77	0.65
1:C:554:CYS:HA	1:C:557:LYS:HE2	1.77	0.65
1:B:73:LYS:HB3	1:B:76:ALA:HB2	1.78	0.65
1:C:15:THR:O	1:C:15:THR:HG22	1.97	0.65
1:A:249:VAL:O	1:A:250:ALA:HB3	1.96	0.65
1:A:375:GLN:O	1:A:377:VAL:HG23	1.97	0.65
1:A:149:ARG:NH1	1:C:102:LYS:HD3	2.12	0.65
1:B:329:LYS:H	1:B:349:GLN:NE2	1.86	0.65
1:A:367:VAL:H	1:A:389:THR:CG2	2.07	0.65
1:C:387:GLN:HB2	1:C:606:GLN:NE2	2.12	0.65
1:A:22:VAL:HG12	3:A:801:HOH:O	1.95	0.65
1:A:678:LEU:HD23	1:A:701:LEU:CD1	2.27	0.65
1:A:556:ARG:NH1	1:A:569:ILE:HG12	2.12	0.64
1:C:293:VAL:HB	1:C:294:PRO:HD3	1.79	0.64
1:C:133:TYR:O	1:C:143:ARG:NH2	2.31	0.64
1:A:2:PRO:HD2	1:A:642:ARG:HH12	1.62	0.64
1:B:233:ASN:OD1	1:B:259:GLY:HA3	1.97	0.64
1:C:248:ASP:O	1:C:252:MET:HE2	1.97	0.64
1:A:522:ASN:HD22	1:A:616:THR:HG21	1.62	0.64
1:C:331:ARG:HD3	1:C:349:GLN:HG2	1.80	0.64
1:C:532:VAL:HG13	1:C:537:VAL:HG22	1.80	0.64
1:C:430:THR:HG22	1:C:480:LEU:HD23	1.80	0.64
1:C:68:LEU:N	1:C:68:LEU:HD22	2.13	0.64
1:C:180:MET:HE1	1:C:312:LEU:HD13	1.80	0.64
1:C:383:SER:HB2	1:C:393:VAL:HG21	1.77	0.64
1:B:369:LEU:HG	1:B:371:LEU:HD13	1.79	0.63
1:C:512:TYR:HD2	3:C:823:HOH:O	1.81	0.63
1:A:543:THR:O	1:A:547:GLN:HG3	1.98	0.63
1:C:143:ARG:HH11	1:C:143:ARG:HG2	1.63	0.63
1:B:337:ILE:HG22	1:B:338:ASN:N	2.12	0.63
1:B:611:MET:HB2	1:B:615:GLU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:LYS:HG2	1:B:731:MET:HG3	1.80	0.63
1:B:350:THR:HG22	1:B:351:GLY:N	2.14	0.63
1:A:447:ASN:HD22	1:A:449:THR:H	1.45	0.63
1:A:300:MET:CE	1:A:304:LYS:HE3	2.27	0.63
1:A:592:PRO:HB3	1:A:601:ARG:HD3	1.79	0.63
1:B:568:LEU:HD12	1:B:568:LEU:O	1.98	0.63
1:B:748:GLY:O	1:B:749:ALA:CB	2.44	0.63
1:C:139:HIS:CD2	1:C:142:LYS:HD2	2.34	0.63
1:C:696:VAL:HG13	1:C:706:ARG:NH1	2.13	0.63
1:C:494:ARG:CZ	3:C:801:HOH:O	2.46	0.63
1:B:631:PRO:HB2	3:B:833:HOH:O	1.98	0.62
1:B:348:PRO:HB3	1:B:384:VAL:HG21	1.81	0.62
1:A:597:THR:HG22	1:A:599:ASP:H	1.64	0.62
1:A:743:LYS:NZ	3:A:888:HOH:O	2.32	0.62
1:C:197:CYS:O	1:C:201:LYS:HG3	1.98	0.62
1:B:387:GLN:CG	1:B:606:GLN:HE22	2.10	0.62
1:C:566:GLY:N	1:C:763:ARG:HH12	1.98	0.62
1:B:377:VAL:HG12	1:B:382:LEU:HD11	1.81	0.62
1:B:597:THR:HG22	1:B:599:ASP:H	1.65	0.62
1:B:447:ASN:ND2	1:B:449:THR:HG23	2.14	0.62
1:A:447:ASN:C	1:A:447:ASN:HD22	2.02	0.62
1:A:556:ARG:HA	1:A:569:ILE:HD11	1.81	0.62
1:B:367:VAL:N	1:B:389:THR:HG21	2.08	0.62
1:C:296:ILE:HD13	1:C:385:VAL:HG11	1.81	0.62
1:A:337:ILE:HG22	1:A:338:ASN:N	2.15	0.62
1:A:3:ILE:H	1:A:576:LEU:HD21	1.65	0.61
1:A:232:TYR:CE1	1:A:243:MET:HE2	2.35	0.61
1:B:556:ARG:NE	1:B:569:ILE:HD11	2.15	0.61
1:B:300:MET:CE	1:B:304:LYS:HE3	2.30	0.61
1:B:252:MET:O	1:B:253:PHE:HB3	2.01	0.61
1:A:414:ARG:O	1:A:418:LYS:HG3	1.99	0.61
1:B:541:ARG:HG3	1:B:585:LEU:HD22	1.82	0.61
1:C:577:LEU:HB3	1:C:578:PRO:HD3	1.82	0.61
1:A:15:THR:HB	3:A:874:HOH:O	1.99	0.61
1:C:15:THR:HA	3:C:831:HOH:O	2.00	0.61
1:A:699:ASN:ND2	1:A:702:SER:H	1.98	0.61
1:A:295:VAL:HG11	1:A:314:LEU:HD11	1.82	0.61
1:B:39:GLN:O	1:B:39:GLN:HG2	2.01	0.61
1:B:630:SER:H	1:B:631:PRO:CD	2.13	0.61
1:B:68:LEU:HD22	1:B:68:LEU:N	2.16	0.61
1:C:294:PRO:HG3	1:C:325:PRO:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:SER:OG	1:A:726:LYS:HD3	2.00	0.60
1:C:233:ASN:HD22	1:C:257:LEU:HD11	1.66	0.60
1:C:329:LYS:H	1:C:349:GLN:HE22	1.49	0.60
1:C:226:ASN:O	1:C:290:THR:CA	2.35	0.60
1:A:210:GLU:CD	1:A:494:ARG:NH2	2.55	0.60
1:A:226:ASN:O	1:A:290:THR:HA	2.02	0.60
1:B:655:LEU:HD12	1:B:708:LEU:HD23	1.84	0.60
1:C:188:ILE:HD13	1:C:193:VAL:HB	1.82	0.60
1:A:39:GLN:O	1:A:39:GLN:HG2	2.02	0.60
1:C:509:ALA:HA	3:C:823:HOH:O	2.00	0.60
1:C:137:LEU:O	1:C:138:ASP:CB	2.50	0.59
1:A:659:GLY:HA2	1:A:716:ARG:CD	2.33	0.59
1:C:568:LEU:CD2	1:C:568:LEU:H	2.13	0.59
1:B:571:PRO:HG2	1:B:574:MET:HB2	1.84	0.59
1:C:278:ILE:HB	1:C:279:PRO:HD3	1.84	0.59
1:B:90:HIS:HE1	1:B:151:GLU:OE2	1.85	0.59
1:C:579:VAL:HG22	1:C:751:TYR:CZ	2.38	0.59
1:B:699:ASN:ND2	1:B:702:SER:H	2.01	0.59
1:C:528:ALA:O	1:C:532:VAL:HG23	2.02	0.59
1:C:265:ASN:HD22	1:C:265:ASN:N	2.00	0.59
1:C:548:CYS:SG	1:C:581:LEU:HD22	2.42	0.59
1:A:657:GLU:HG2	1:A:659:GLY:H	1.68	0.58
1:B:210:GLU:HG3	1:B:489:CYS:SG	2.42	0.58
1:A:90:HIS:CE1	1:A:137:LEU:HD11	2.38	0.58
1:C:10:ARG:HE	1:C:28:PRO:HA	1.67	0.58
1:C:23:ARG:HD2	1:C:503:ASN:OD1	2.03	0.58
1:C:220:VAL:O	1:C:261:LEU:HA	2.04	0.58
1:C:7:GLU:OE2	1:C:31:THR:HG21	2.03	0.58
1:B:293:VAL:HB	1:B:294:PRO:HD3	1.85	0.58
1:C:407:ARG:HD2	1:C:721:LYS:HB2	1.86	0.58
1:B:625:LEU:N	1:B:625:LEU:HD22	2.19	0.58
1:C:343:LYS:CB	1:C:347:GLN:HE21	2.15	0.58
1:A:348:PRO:HB3	1:A:384:VAL:HG21	1.84	0.58
1:C:143:ARG:NH1	1:C:152:LEU:HD11	2.18	0.58
1:B:579:VAL:HG13	1:B:751:TYR:CD1	2.39	0.58
1:A:497:ILE:N	1:A:497:ILE:HD12	2.19	0.58
1:B:242:GLN:NE2	3:B:869:HOH:O	2.33	0.58
1:B:579:VAL:HG22	3:B:810:HOH:O	2.03	0.57
1:C:516:GLU:HG2	1:C:519:THR:OG1	2.03	0.57
1:A:667:GLY:O	1:A:670:VAL:HG23	2.04	0.57
1:B:100:ARG:CZ	1:B:125:CYS:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:HH21	1:A:14:GLY:CA	2.16	0.57
1:B:278:ILE:HB	1:B:279:PRO:HD3	1.85	0.57
1:C:716:ARG:HG3	1:C:720:MET:CE	2.35	0.57
1:B:555:TYR:CD2	1:B:571:PRO:HD3	2.40	0.57
1:A:350:THR:HG22	1:A:351:GLY:N	2.19	0.57
1:C:623:ARG:HG2	1:C:625:LEU:HD12	1.87	0.57
1:A:244:MET:CE	1:A:255:PRO:HG2	2.34	0.57
1:B:178:ILE:HB	1:B:312:LEU:HD23	1.86	0.57
1:B:629:LYS:O	1:B:630:SER:CB	2.47	0.57
1:A:366:CYS:HA	1:A:389:THR:HG23	1.87	0.57
1:A:300:MET:CE	1:A:363:GLN:HG3	2.35	0.57
1:C:224:THR:HG23	1:C:232:TYR:HE2	1.70	0.57
1:C:641:VAL:HG12	1:C:642:ARG:H	1.70	0.57
1:B:373:PRO:HB3	1:B:377:VAL:CG2	2.35	0.57
1:A:4:GLN:HG3	1:A:5:VAL:N	2.20	0.57
1:C:238:LEU:C	1:C:240:GLN:H	2.08	0.57
1:A:642:ARG:HD2	3:A:884:HOH:O	2.04	0.56
1:A:108:PHE:CE2	1:A:499:ASN:HB3	2.39	0.56
1:B:547:GLN:O	1:B:551:ILE:HG23	2.04	0.56
1:B:496:ARG:C	1:B:497:ILE:HD12	2.26	0.56
1:B:699:ASN:HD21	1:B:702:SER:H	1.53	0.56
1:B:636:THR:HG23	3:B:855:HOH:O	2.05	0.56
1:A:2:PRO:C	1:A:3:ILE:HG12	2.25	0.56
1:C:461:THR:HG22	1:C:610:SER:O	2.04	0.56
1:C:63:GLN:NE2	1:C:508:LEU:HD11	2.20	0.56
1:B:447:ASN:HD22	1:B:449:THR:HG23	1.71	0.56
1:C:541:ARG:HB2	3:C:822:HOH:O	2.05	0.56
1:C:447:ASN:ND2	1:C:450:ASP:H	1.99	0.56
1:C:516:GLU:HG3	1:C:519:THR:H	1.71	0.56
1:A:2:PRO:O	1:A:3:ILE:HG12	2.07	0.55
1:B:716:ARG:HD3	3:B:864:HOH:O	2.06	0.55
1:C:55:PRO:HD3	1:C:511:LEU:HD23	1.89	0.55
1:C:309:ALA:HB1	1:C:364:GLY:O	2.05	0.55
1:A:4:GLN:HG2	3:A:884:HOH:O	2.05	0.55
1:A:657:GLU:HG2	1:A:658:ASN:N	2.17	0.55
1:A:249:VAL:O	1:A:250:ALA:CB	2.54	0.55
1:A:10:ARG:CD	1:A:29:LEU:HD23	2.37	0.55
1:A:556:ARG:HD3	1:A:569:ILE:HD13	1.88	0.55
1:C:343:LYS:HD2	1:C:534:ASN:HA	1.88	0.55
1:B:249:VAL:O	1:B:250:ALA:HB3	2.06	0.55
1:A:319:LEU:CD2	1:A:328:LEU:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLN:HG2	1:C:145:ASP:CG	2.28	0.55
1:C:532:VAL:HG12	1:C:532:VAL:O	2.07	0.55
1:A:232:TYR:HE1	1:A:243:MET:HE2	1.71	0.55
1:A:733:MET:O	1:A:736:LYS:HB2	2.07	0.55
1:A:16:GLU:HB3	1:A:17:PRO:CD	2.35	0.55
1:C:201:LYS:HE3	1:C:272:THR:HG23	1.89	0.55
1:B:556:ARG:HG3	1:B:569:ILE:HD11	1.89	0.55
1:C:54:ILE:O	1:C:504:CYS:HA	2.06	0.54
1:C:415:ASP:O	1:C:418:LYS:HG2	2.06	0.54
1:C:333:ASP:HA	1:C:334:ARG:NH2	2.21	0.54
1:A:641:VAL:HG11	1:A:647:ARG:HB3	1.89	0.54
1:C:321:ILE:H	1:C:321:ILE:CD1	2.18	0.54
1:A:300:MET:HE3	1:A:363:GLN:HG3	1.90	0.54
1:C:296:ILE:HB	1:C:356:LEU:HD21	1.89	0.54
1:C:693:VAL:HG12	1:C:694:LEU:N	2.23	0.54
1:B:138:ASP:C	1:B:140:THR:H	2.10	0.54
1:A:672:GLN:HE21	1:B:194:ARG:HD2	1.73	0.54
1:C:88:VAL:CG2	1:C:150:PRO:HG2	2.38	0.54
1:C:143:ARG:HG2	1:C:145:ASP:OD1	2.08	0.54
1:C:319:LEU:HD12	1:C:320:PRO:HD2	1.88	0.54
1:C:705:VAL:O	1:C:709:ILE:HG13	2.08	0.54
1:B:645:GLU:HG2	1:B:742:ASP:OD2	2.08	0.54
1:C:553:ALA:HB1	1:C:766:LEU:HD21	1.90	0.54
1:C:90:HIS:CD2	1:C:96:LEU:H	2.21	0.53
1:B:597:THR:HG22	1:B:598:THR:N	2.22	0.53
1:C:225:TYR:O	1:C:226:ASN:HB3	2.09	0.53
1:A:699:ASN:HD22	1:A:701:LEU:H	1.57	0.53
1:A:243:MET:CE	1:A:281:MET:SD	2.97	0.53
1:C:234:VAL:O	1:C:234:VAL:HG12	2.09	0.53
1:A:399:PHE:O	1:A:400:GLN:HG3	2.09	0.53
1:A:383:SER:C	1:A:386:PRO:HD2	2.29	0.53
1:A:377:VAL:O	1:A:377:VAL:HG12	2.07	0.53
1:C:655:LEU:HD23	1:C:656:LEU:N	2.23	0.53
1:B:147:TYR:O	1:B:148:ASP:HB2	2.09	0.53
1:B:113:GLU:O	1:B:116:ARG:HG2	2.08	0.53
1:C:653:ILE:HG23	1:C:665:TRP:O	2.08	0.53
1:C:655:LEU:HD21	1:C:662:LEU:HD22	1.91	0.53
1:C:608:VAL:HA	1:C:611:MET:HG2	1.91	0.53
1:C:234:VAL:HG11	1:C:271:ILE:HG12	1.90	0.53
1:A:569:ILE:O	1:A:569:ILE:HG13	2.08	0.53
1:A:146:ALA:O	1:C:102:LYS:HE3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ARG:HH11	1:C:152:LEU:HD11	1.73	0.53
1:B:597:THR:HB	1:B:600:ASP:OD1	2.09	0.53
1:C:55:PRO:HD3	1:C:511:LEU:CD2	2.39	0.53
1:B:522:ASN:HB2	1:B:616:THR:HG21	1.89	0.53
1:B:180:MET:HB2	1:B:314:LEU:HD23	1.90	0.53
1:A:743:LYS:HD2	1:A:750:SER:CB	2.38	0.53
1:A:249:VAL:HG11	1:A:324:ALA:CB	2.35	0.52
1:B:612:ASP:HB3	1:B:615:GLU:H	1.74	0.52
1:C:420:VAL:HG12	1:C:457:ASP:HB3	1.89	0.52
1:B:623:ARG:CD	1:B:625:LEU:HD21	2.38	0.52
1:B:366:CYS:HA	1:B:389:THR:CG2	2.39	0.52
1:B:24:GLY:N	3:B:837:HOH:O	2.42	0.52
1:C:369:LEU:HG	1:C:371:LEU:HD22	1.91	0.52
1:C:566:GLY:N	1:C:763:ARG:NH2	2.53	0.52
1:B:730:LYS:HG2	1:B:731:MET:H	1.74	0.52
1:C:626:PRO:HB3	1:C:654:TYR:CE2	2.44	0.52
1:C:164:ASP:N	1:C:164:ASP:OD2	2.35	0.52
1:C:68:LEU:HD22	1:C:68:LEU:H	1.73	0.52
1:C:348:PRO:HB3	1:C:384:VAL:HG21	1.91	0.52
1:B:530:ARG:O	1:B:533:LEU:HD13	2.10	0.52
1:C:687:ILE:HG22	1:C:688:THR:N	2.23	0.52
1:C:568:LEU:N	1:C:568:LEU:HD23	2.21	0.52
1:C:180:MET:HA	1:C:223:VAL:O	2.10	0.52
1:C:401:VAL:HG13	1:C:402:GLU:OE2	2.10	0.52
1:A:53:ASN:OD1	1:A:505:CYS:HB3	2.09	0.52
1:A:68:LEU:HD22	1:A:68:LEU:N	2.23	0.52
1:B:516:GLU:HG2	1:B:519:THR:OG1	2.09	0.52
1:B:59:ASP:O	1:B:63:GLN:HG2	2.09	0.52
1:A:516:GLU:HG2	3:A:920:HOH:O	2.08	0.52
1:B:623:ARG:HH22	1:B:715:GLN:NE2	2.07	0.52
1:A:263:ASN:HD21	1:A:265:ASN:HB2	1.75	0.52
1:B:435:ARG:HD3	3:B:836:HOH:O	2.09	0.52
1:A:249:VAL:HG13	3:A:917:HOH:O	2.09	0.51
1:A:10:ARG:HG2	1:A:29:LEU:H	1.75	0.51
1:C:418:LYS:HE2	1:C:457:ASP:HB2	1.92	0.51
1:C:551:ILE:HD11	1:C:577:LEU:HD21	1.91	0.51
1:B:553:ALA:HB2	1:B:762:ILE:HG23	1.91	0.51
1:C:64:ALA:O	1:C:65:GLN:HB2	2.10	0.51
1:B:228:VAL:HG13	1:B:246:VAL:O	2.11	0.51
1:A:263:ASN:ND2	1:A:265:ASN:H	2.09	0.51
1:B:623:ARG:HH12	1:B:715:GLN:NE2	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:LEU:N	1:C:625:LEU:HD13	2.24	0.51
1:C:295:VAL:HG11	1:C:314:LEU:HD11	1.92	0.51
1:B:180:MET:HB2	1:B:314:LEU:CD2	2.40	0.51
1:A:3:ILE:HG21	1:A:621:TYR:CZ	2.46	0.51
1:C:385:VAL:N	1:C:386:PRO:HD2	2.24	0.51
1:B:627:LEU:HD11	1:B:655:LEU:HG	1.92	0.51
1:A:3:ILE:HD13	1:A:3:ILE:N	2.25	0.51
1:C:559:CYS:SG	3:C:823:HOH:O	2.60	0.51
1:B:60:MET:O	1:B:63:GLN:HB2	2.09	0.51
1:B:249:VAL:C	1:B:251:ASP:H	2.14	0.51
1:B:113:GLU:OE1	1:B:117:ARG:HD2	2.11	0.51
1:C:297:GLN:O	1:C:301:GLU:HB2	2.11	0.51
1:B:509:ALA:O	1:B:513:ARG:HG3	2.10	0.51
1:B:215:GLU:HG3	1:B:265:ASN:ND2	2.26	0.51
1:B:373:PRO:HB3	1:B:377:VAL:HG21	1.91	0.51
1:C:557:LYS:HG3	1:C:558:ASN:ND2	2.26	0.51
1:A:20:THR:HB	1:A:41:ASN:HB2	1.92	0.51
1:C:112:ILE:HG23	1:C:113:GLU:N	2.25	0.51
1:B:144:VAL:HG11	3:B:835:HOH:O	2.11	0.51
1:A:612:ASP:CG	1:A:613:VAL:H	2.14	0.51
1:B:324:ALA:HB1	1:B:325:PRO:HD2	1.92	0.51
1:B:657:GLU:OE2	1:B:716:ARG:NH1	2.44	0.51
1:A:50:THR:HB	1:A:520:LEU:CD2	2.41	0.51
1:B:497:ILE:HD12	1:B:497:ILE:N	2.26	0.50
1:A:511:LEU:HD23	1:A:511:LEU:C	2.32	0.50
1:A:367:VAL:N	1:A:389:THR:HG21	2.12	0.50
1:B:228:VAL:HG12	1:B:229:LEU:N	2.25	0.50
1:A:672:GLN:HG3	1:A:682:SER:O	2.11	0.50
1:B:41:ASN:ND2	1:B:41:ASN:N	2.58	0.50
1:C:188:ILE:HD13	1:C:193:VAL:CB	2.41	0.50
1:C:447:ASN:HD22	1:C:447:ASN:C	2.15	0.50
1:B:233:ASN:ND2	1:B:259:GLY:HA3	2.25	0.50
1:C:143:ARG:HH11	1:C:152:LEU:CD1	2.24	0.50
1:A:263:ASN:HD22	1:A:266:GLU:H	1.59	0.50
1:A:220:VAL:O	1:A:261:LEU:HA	2.11	0.50
1:C:289:GLU:HG2	1:C:322:ALA:HA	1.92	0.50
1:B:377:VAL:HG12	1:B:377:VAL:O	2.11	0.50
1:C:20:THR:HB	1:C:41:ASN:HB2	1.92	0.50
1:C:204:LEU:O	1:C:264:VAL:HG11	2.10	0.50
1:A:243:MET:HE1	1:A:281:MET:SD	2.52	0.50
1:B:623:ARG:HG2	1:B:625:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:O	1:B:74:PRO:HD3	2.11	0.50
1:B:671:GLN:HB2	3:B:801:HOH:O	2.11	0.50
1:B:304:LYS:HA	1:B:363:GLN:NE2	2.27	0.50
1:C:312:LEU:HB2	1:C:367:VAL:HG12	1.93	0.49
1:C:234:VAL:HG11	1:C:271:ILE:CG1	2.42	0.49
1:A:180:MET:CE	1:A:312:LEU:HB3	2.41	0.49
1:A:522:ASN:HD22	1:A:616:THR:CG2	2.24	0.49
1:B:334:ARG:HH11	1:B:334:ARG:HG2	1.76	0.49
1:A:3:ILE:O	1:A:7:GLU:HG3	2.13	0.49
1:A:430:THR:HG22	1:A:480:LEU:HD22	1.94	0.49
1:A:331:ARG:HD3	1:A:349:GLN:HG2	1.95	0.49
1:A:250:ALA:HA	1:A:325:PRO:CG	2.42	0.49
1:C:662:LEU:HD13	1:C:709:ILE:HG23	1.94	0.49
1:A:625:LEU:HG	1:A:638:PRO:HG2	1.94	0.49
1:C:311:LYS:HA	1:C:366:CYS:O	2.12	0.49
1:B:29:LEU:H	1:B:29:LEU:HD22	1.77	0.49
1:C:663:PHE:CD2	1:C:735:PHE:HD1	2.31	0.49
1:B:544:LEU:HD13	1:B:581:LEU:CD1	2.42	0.49
1:C:289:GLU:CG	1:C:322:ALA:HA	2.42	0.49
1:B:586:LYS:HD3	1:B:748:GLY:C	2.33	0.49
1:B:263:ASN:ND2	1:B:265:ASN:H	2.10	0.49
1:B:329:LYS:N	1:B:349:GLN:HE22	1.88	0.49
1:A:641:VAL:HG12	1:A:642:ARG:N	2.27	0.49
1:C:398:SER:O	1:C:400:GLN:HG3	2.13	0.49
1:C:226:ASN:HA	1:C:290:THR:HG22	1.95	0.49
1:C:447:ASN:ND2	1:C:449:THR:H	2.11	0.49
1:C:739:LEU:O	1:C:741:GLU:N	2.46	0.49
1:A:4:GLN:HG3	1:A:5:VAL:H	1.78	0.49
1:C:180:MET:HG2	1:C:223:VAL:HB	1.95	0.49
1:A:516:GLU:OE2	3:A:820:HOH:O	2.20	0.49
1:C:16:GLU:HB3	1:C:17:PRO:CD	2.42	0.48
1:A:257:LEU:O	1:A:259:GLY:N	2.39	0.48
1:A:597:THR:HB	1:A:600:ASP:OD1	2.13	0.48
1:A:387:GLN:HB2	1:A:606:GLN:OE1	2.13	0.48
1:A:321:ILE:H	1:A:321:ILE:HD13	1.77	0.48
1:A:657:GLU:HG3	1:A:720:MET:SD	2.53	0.48
1:C:180:MET:HE2	1:C:312:LEU:HD22	1.95	0.48
1:B:300:MET:HE3	1:B:304:LYS:HE3	1.95	0.48
1:C:415:ASP:HA	1:C:418:LYS:HD2	1.94	0.48
1:C:557:LYS:HE3	1:C:558:ASN:ND2	2.28	0.48
1:C:330:ASN:O	1:C:331:ARG:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:THR:CG2	1:B:598:THR:N	2.76	0.48
1:B:447:ASN:ND2	1:B:449:THR:H	2.12	0.48
1:A:632:VAL:HG13	1:A:632:VAL:O	2.13	0.48
1:B:255:PRO:HB2	1:B:257:LEU:CD1	2.43	0.48
1:C:44:PRO:HA	1:C:47:ILE:O	2.13	0.48
1:C:522:ASN:O	1:C:526:LYS:HG3	2.13	0.48
1:B:577:LEU:HB3	1:B:578:PRO:HD3	1.94	0.48
1:C:270:VAL:HG23	3:C:807:HOH:O	2.13	0.48
1:A:533:LEU:HD12	1:A:533:LEU:N	2.28	0.48
1:C:656:LEU:HD23	1:C:657:GLU:N	2.29	0.48
1:C:311:LYS:HG3	1:C:422:PHE:HE1	1.78	0.48
1:C:195:LEU:O	1:C:198:GLU:HB2	2.13	0.48
1:C:612:ASP:HB3	1:C:615:GLU:HG3	1.96	0.48
1:A:522:ASN:HB2	1:A:616:THR:HG21	1.96	0.48
1:C:274:LEU:O	1:C:278:ILE:HG13	2.13	0.48
1:A:200:LEU:HG	1:A:204:LEU:HD11	1.96	0.48
1:C:180:MET:HE1	1:C:312:LEU:HB3	1.96	0.48
1:A:633:GLU:HG3	1:A:634:SER:N	2.29	0.48
1:A:295:VAL:CG1	1:A:314:LEU:HD11	2.42	0.48
1:A:678:LEU:HD23	1:A:701:LEU:HD13	1.96	0.48
1:A:612:ASP:CG	1:A:613:VAL:N	2.67	0.48
1:A:415:ASP:HA	1:A:418:LYS:CD	2.40	0.48
1:C:293:VAL:HB	1:C:325:PRO:O	2.14	0.48
1:C:149:ARG:HG3	1:C:149:ARG:NH1	2.25	0.48
1:B:552:LEU:HB2	1:B:762:ILE:HD11	1.96	0.47
1:C:268:ARG:HG3	1:C:268:ARG:HH11	1.78	0.47
1:A:743:LYS:HD2	1:A:750:SER:HB2	1.95	0.47
1:A:461:THR:HG21	1:A:611:MET:O	2.14	0.47
1:C:557:LYS:HE3	1:C:558:ASN:HD21	1.80	0.47
1:A:595:GLU:HB2	3:A:898:HOH:O	2.14	0.47
1:C:612:ASP:OD1	1:C:613:VAL:N	2.48	0.47
1:B:297:GLN:HG2	1:B:356:LEU:HD13	1.96	0.47
1:A:655:LEU:HD23	1:A:663:PHE:O	2.15	0.47
1:A:59:ASP:O	1:A:63:GLN:HG3	2.15	0.47
1:C:209:ARG:HG2	1:C:209:ARG:HH11	1.79	0.47
1:C:117:ARG:HA	1:C:129:VAL:HG23	1.95	0.47
1:C:386:PRO:HA	1:C:389:THR:CG2	2.43	0.47
1:A:465:GLU:OE2	1:A:467:LYS:HE3	2.15	0.47
1:B:246:VAL:HG21	3:B:871:HOH:O	2.14	0.47
1:B:337:ILE:O	1:B:342:GLU:HB2	2.15	0.47
1:B:323:GLU:OE1	1:B:327:LYS:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:LEU:HG	1:C:371:LEU:CD2	2.44	0.47
1:C:378:ASP:O	1:C:382:LEU:HG	2.15	0.47
1:C:269:ALA:HB3	3:C:807:HOH:O	2.15	0.47
1:A:249:VAL:CG1	1:A:324:ALA:HB1	2.40	0.47
1:A:250:ALA:HA	1:A:325:PRO:HG2	1.96	0.47
1:A:156:SER:HA	1:A:497:ILE:O	2.15	0.47
1:A:120:CYS:O	1:A:124:SER:HA	2.15	0.47
1:C:554:CYS:HA	1:C:557:LYS:HG2	1.96	0.47
1:A:597:THR:HG22	1:A:598:THR:N	2.30	0.47
1:B:375:GLN:O	1:B:377:VAL:HG23	2.15	0.47
1:A:517:THR:OG1	1:A:574:MET:HA	2.15	0.47
1:A:238:LEU:O	1:A:270:VAL:HG22	2.15	0.46
1:C:249:VAL:HG12	1:C:250:ALA:N	2.29	0.46
1:C:98:CYS:O	1:C:102:LYS:HA	2.15	0.46
1:B:657:GLU:HG3	1:B:720:MET:SD	2.55	0.46
1:B:23:ARG:HD2	1:B:503:ASN:OD1	2.16	0.46
1:A:647:ARG:HH11	1:A:647:ARG:HA	1.80	0.46
1:A:699:ASN:HD21	1:A:702:SER:H	1.62	0.46
1:C:265:ASN:ND2	1:C:265:ASN:N	2.63	0.46
1:B:263:ASN:HD22	1:B:265:ASN:H	1.64	0.46
1:A:657:GLU:OE2	1:A:716:ARG:NH1	2.38	0.46
1:C:625:LEU:HB3	1:C:640:ALA:HA	1.98	0.46
1:A:243:MET:HE3	1:A:281:MET:SD	2.55	0.46
1:C:572:GLU:HA	1:C:575:LYS:HE3	1.97	0.46
1:B:88:VAL:HG12	1:B:89:ASP:N	2.30	0.46
1:B:350:THR:CG2	1:B:351:GLY:N	2.78	0.46
1:C:625:LEU:H	1:C:625:LEU:HD13	1.80	0.46
1:A:551:ILE:HG13	1:A:552:LEU:N	2.31	0.46
1:C:187:ALA:HB2	1:C:317:THR:HG21	1.97	0.46
1:B:182:ASP:OD2	1:B:317:THR:HG23	2.14	0.46
1:C:204:LEU:HD22	3:C:830:HOH:O	2.15	0.46
1:C:275:LEU:HD11	3:C:830:HOH:O	2.15	0.46
1:C:233:ASN:CG	1:C:259:GLY:HA3	2.36	0.46
1:C:267:SER:O	1:C:271:ILE:HG13	2.15	0.46
1:B:595:GLU:OE2	1:B:734:LEU:HD21	2.16	0.46
1:A:385:VAL:HB	1:A:386:PRO:HD3	1.97	0.46
1:C:636:THR:HG22	1:C:637:GLU:N	2.30	0.46
1:C:418:LYS:HE2	1:C:457:ASP:CB	2.46	0.46
1:C:516:GLU:OE2	1:C:518:ASP:HB2	2.15	0.46
1:A:249:VAL:HG12	1:A:325:PRO:HD2	1.98	0.46
1:B:555:TYR:O	1:B:559:CYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PHE:O	1:A:261:LEU:HB2	2.15	0.46
1:A:632:VAL:HG13	1:A:635:THR:HB	1.98	0.46
1:C:45:ARG:HE	1:C:82:GLU:CD	2.19	0.46
1:A:544:LEU:C	1:A:544:LEU:HD13	2.36	0.46
1:C:112:ILE:CG2	1:C:113:GLU:HG3	2.40	0.46
1:A:2:PRO:HD2	1:A:642:ARG:NH1	2.29	0.46
1:C:383:SER:O	1:C:386:PRO:HG2	2.16	0.46
1:C:607:LEU:HD21	1:C:718:ARG:NH1	2.31	0.46
1:A:627:LEU:CD1	1:A:664:LEU:HD11	2.46	0.46
1:C:368:ASP:OD1	1:C:392:SER:N	2.43	0.46
1:A:556:ARG:CZ	1:A:569:ILE:HG12	2.45	0.46
1:C:541:ARG:CD	1:C:585:LEU:HD22	2.45	0.46
1:B:145:ASP:OD1	1:B:146:ALA:N	2.49	0.46
1:B:138:ASP:OD1	1:B:140:THR:N	2.49	0.45
1:C:10:ARG:CZ	3:C:819:HOH:O	2.64	0.45
1:C:331:ARG:HD3	1:C:349:GLN:CG	2.46	0.45
1:C:371:LEU:HD22	1:C:371:LEU:N	2.30	0.45
1:C:15:THR:CA	3:C:831:HOH:O	2.62	0.45
1:B:377:VAL:HG12	1:B:382:LEU:CD1	2.46	0.45
1:C:7:GLU:O	1:C:11:ASN:OD1	2.34	0.45
1:A:377:VAL:HG12	1:A:382:LEU:CD1	2.46	0.45
1:C:238:LEU:C	1:C:240:GLN:N	2.68	0.45
1:B:544:LEU:HD13	1:B:581:LEU:HD11	1.99	0.45
1:A:350:THR:HG22	1:A:351:GLY:H	1.80	0.45
1:C:649:SER:HB3	1:C:652:ASP:HB2	1.97	0.45
1:B:623:ARG:HG2	1:B:625:LEU:CD2	2.47	0.45
1:A:323:GLU:O	1:A:324:ALA:HB2	2.17	0.45
1:A:252:MET:O	1:A:253:PHE:CB	2.65	0.45
1:C:512:TYR:CD2	3:C:823:HOH:O	2.55	0.45
1:C:6:ILE:HG13	1:C:576:LEU:CD1	2.44	0.45
1:A:278:ILE:HB	1:A:279:PRO:HD3	1.99	0.45
1:C:222:PHE:O	1:C:223:VAL:HG23	2.17	0.45
1:A:90:HIS:CE1	1:A:133:TYR:CZ	3.05	0.45
1:C:244:MET:SD	1:C:257:LEU:HD22	2.57	0.45
1:C:694:LEU:HD23	1:C:706:ARG:HG2	1.98	0.45
1:C:224:THR:OG1	1:C:230:HIS:HB2	2.17	0.45
1:A:557:LYS:HE3	3:A:839:HOH:O	2.16	0.45
1:C:743:LYS:CG	1:C:750:SER:HB2	2.37	0.45
1:C:401:VAL:HG22	1:C:401:VAL:O	2.16	0.45
1:C:213:ALA:C	1:C:215:GLU:H	2.19	0.45
1:A:10:ARG:CG	1:A:29:LEU:HD23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ARG:HG2	1:C:143:ARG:NH1	2.28	0.44
1:C:430:THR:HG22	1:C:480:LEU:CD2	2.47	0.44
1:A:20:THR:OG1	1:A:38:ASP:O	2.26	0.44
1:B:89:ASP:OD2	1:B:160:LEU:HD12	2.16	0.44
1:B:465:GLU:OE2	1:B:467:LYS:HE3	2.17	0.44
1:C:90:HIS:HE1	1:C:151:GLU:OE2	2.00	0.44
1:A:7:GLU:OE2	1:A:31:THR:HG21	2.18	0.44
1:C:623:ARG:HH11	1:C:712:LEU:HD22	1.82	0.44
1:C:626:PRO:HA	1:C:654:TYR:HA	1.98	0.44
1:A:727:GLN:HG3	1:A:727:GLN:O	2.16	0.44
1:B:337:ILE:N	1:B:337:ILE:HD12	2.32	0.44
1:B:180:MET:CE	1:B:314:LEU:HD21	2.47	0.44
1:C:642:ARG:HG3	1:C:741:GLU:OE2	2.17	0.44
1:B:666:VAL:HG13	1:B:670:VAL:HG21	1.99	0.44
1:B:117:ARG:CA	1:B:129:VAL:HG23	2.48	0.44
1:A:238:LEU:O	1:A:270:VAL:CG2	2.65	0.44
1:B:180:MET:HE1	1:B:312:LEU:CD1	2.27	0.44
1:A:533:LEU:HD11	1:A:605:ARG:CZ	2.48	0.44
1:C:541:ARG:HH11	1:C:541:ARG:HG2	1.82	0.44
1:B:319:LEU:N	1:B:377:VAL:HG13	2.32	0.44
1:C:249:VAL:HG12	1:C:250:ALA:H	1.82	0.44
1:B:632:VAL:HG12	1:B:635:THR:HG23	2.00	0.44
1:B:180:MET:HE2	1:B:314:LEU:HD21	2.00	0.44
1:A:180:MET:HE1	1:A:312:LEU:CD1	2.35	0.44
1:A:533:LEU:HD11	1:A:605:ARG:NH2	2.33	0.44
1:A:175:PRO:HG2	1:A:218:ILE:CD1	2.47	0.44
1:B:625:LEU:HD12	1:B:638:PRO:O	2.18	0.44
1:A:6:ILE:HG13	1:A:576:LEU:HD11	1.99	0.44
1:C:143:ARG:CG	1:C:145:ASP:OD1	2.66	0.44
1:C:10:ARG:HG2	1:C:29:LEU:HG	2.00	0.44
1:C:407:ARG:HA	1:C:719:TYR:CD2	2.53	0.44
1:C:20:THR:OG1	1:C:38:ASP:O	2.25	0.44
1:C:231:PHE:CZ	1:C:254:VAL:HG13	2.53	0.44
1:B:470:ASP:CG	1:B:471:ARG:H	2.21	0.44
1:C:386:PRO:CA	1:C:389:THR:HG22	2.47	0.44
1:B:135:GLN:CB	1:B:142:LYS:HE2	2.46	0.44
1:B:293:VAL:HB	1:B:325:PRO:O	2.18	0.44
1:B:293:VAL:HG21	1:B:326:GLY:HA3	2.00	0.44
1:A:220:VAL:HG12	1:A:221:GLY:N	2.33	0.44
1:C:758:MET:O	1:C:762:ILE:HG13	2.18	0.44
1:C:387:GLN:CB	1:C:606:GLN:HE22	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:THR:O	1:C:454:ALA:HB3	2.18	0.43
1:B:175:PRO:HG3	1:B:422:PHE:CE2	2.53	0.43
1:B:383:SER:O	1:B:386:PRO:HG2	2.18	0.43
1:C:576:LEU:HD23	1:C:580:TYR:OH	2.18	0.43
1:A:2:PRO:HB2	1:A:3:ILE:CD1	2.48	0.43
1:A:3:ILE:HG21	1:A:621:TYR:CE1	2.54	0.43
1:A:461:THR:HG23	3:A:857:HOH:O	2.18	0.43
1:C:605:ARG:O	1:C:609:THR:HG22	2.18	0.43
1:A:180:MET:HB2	1:A:314:LEU:HD13	2.01	0.43
1:C:233:ASN:ND2	1:C:259:GLY:HA3	2.33	0.43
1:C:81:GLU:CD	1:C:81:GLU:H	2.22	0.43
1:A:568:LEU:HD23	1:A:568:LEU:H	1.82	0.43
1:C:496:ARG:C	1:C:497:ILE:HD12	2.39	0.43
1:B:612:ASP:CB	1:B:615:GLU:HG3	2.48	0.43
1:C:113:GLU:OE1	1:C:116:ARG:NE	2.51	0.43
1:C:336:LEU:O	1:C:339:THR:HB	2.18	0.43
1:B:475:GLU:HG3	1:B:476:SER:N	2.34	0.43
1:B:131:PRO:C	1:B:133:TYR:H	2.21	0.43
1:B:106:CYS:HB2	1:B:107:PRO:CD	2.49	0.43
1:A:231:PHE:CZ	1:A:298:ALA:HB1	2.39	0.43
1:B:293:VAL:HG13	1:B:356:LEU:HD22	2.00	0.43
1:C:336:LEU:HG	1:C:341:LYS:HB2	1.99	0.43
1:A:46:TYR:OH	1:A:78:LEU:HD11	2.19	0.43
1:A:419:VAL:HG13	3:A:853:HOH:O	2.18	0.43
1:A:447:ASN:C	1:A:447:ASN:ND2	2.70	0.43
1:B:591:GLN:NE2	1:B:748:GLY:HA2	2.33	0.43
1:A:2:PRO:O	1:A:4:GLN:HG2	2.18	0.43
1:B:604:VAL:O	1:B:608:VAL:HG23	2.19	0.43
1:A:533:LEU:CD1	1:A:533:LEU:N	2.82	0.43
1:C:367:VAL:H	1:C:389:THR:HG21	1.84	0.43
1:A:657:GLU:HG3	1:A:720:MET:CE	2.49	0.43
1:A:716:ARG:HG3	1:A:720:MET:CE	2.48	0.43
1:B:556:ARG:CD	1:B:569:ILE:HD11	2.48	0.43
1:A:112:ILE:HG13	1:A:113:GLU:HG3	2.00	0.43
1:C:6:ILE:HG22	1:C:29:LEU:HD11	2.01	0.43
1:A:533:LEU:HD11	1:A:605:ARG:HH21	1.83	0.43
1:B:135:GLN:HB3	1:B:142:LYS:CE	2.43	0.43
1:C:334:ARG:HA	1:C:337:ILE:HD12	2.01	0.43
1:A:623:ARG:HG2	1:A:625:LEU:HD13	2.00	0.43
1:A:36:VAL:HG11	1:A:43:SER:HB2	2.00	0.43
1:C:471:ARG:NH1	1:C:471:ARG:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:PRO:HA	1:B:639:PRO:HD2	1.96	0.42
1:C:268:ARG:HG3	1:C:268:ARG:NH1	2.34	0.42
1:C:566:GLY:N	1:C:763:ARG:NH1	2.66	0.42
1:C:494:ARG:NE	3:C:801:HOH:O	2.51	0.42
1:C:274:LEU:HD11	1:C:278:ILE:HD11	2.00	0.42
1:A:244:MET:HE3	1:A:257:LEU:HD22	2.01	0.42
1:A:430:THR:HG22	1:A:480:LEU:CD2	2.49	0.42
1:A:581:LEU:HD23	1:A:754:PHE:HZ	1.83	0.42
1:B:430:THR:HG22	1:B:480:LEU:CD2	2.49	0.42
1:B:249:VAL:C	1:B:251:ASP:N	2.72	0.42
1:C:117:ARG:HG2	1:C:128:ASP:HA	2.00	0.42
1:A:16:GLU:HG3	3:A:874:HOH:O	2.18	0.42
1:C:611:MET:HB2	1:C:615:GLU:CB	2.46	0.42
1:B:632:VAL:HG12	1:B:632:VAL:O	2.18	0.42
1:B:636:THR:O	1:B:637:GLU:O	2.37	0.42
1:B:385:VAL:N	1:B:386:PRO:HD2	2.34	0.42
1:C:297:GLN:NE2	3:C:834:HOH:O	2.53	0.42
1:B:334:ARG:HA	1:B:337:ILE:CD1	2.49	0.42
1:C:716:ARG:HG3	1:C:720:MET:HE2	2.00	0.42
1:A:544:LEU:CD1	1:A:581:LEU:HD11	2.50	0.42
1:C:756:CYS:C	1:C:758:MET:H	2.21	0.42
1:A:366:CYS:HA	1:A:389:THR:CG2	2.49	0.42
1:C:151:GLU:HA	1:C:157:TYR:CE2	2.54	0.42
1:B:372:PHE:N	1:B:373:PRO:HD3	2.34	0.42
1:C:350:THR:HG22	1:C:352:ALA:H	1.85	0.42
1:B:319:LEU:HD11	1:B:328:LEU:HB2	2.02	0.42
1:C:137:LEU:O	1:C:144:VAL:HB	2.19	0.42
1:B:716:ARG:HA	1:B:716:ARG:HD3	1.83	0.42
1:B:613:VAL:HA	1:B:616:THR:HG22	2.00	0.42
1:C:380:ALA:O	1:C:384:VAL:HG23	2.19	0.42
1:A:106:CYS:HB2	1:A:107:PRO:CD	2.49	0.42
1:C:538:LYS:HD3	1:C:538:LYS:O	2.19	0.42
1:C:642:ARG:NH1	1:C:741:GLU:OE1	2.52	0.42
1:B:260:PHE:O	1:B:261:LEU:HB2	2.19	0.42
1:B:597:THR:HG22	1:B:599:ASP:N	2.30	0.42
1:C:207:LEU:O	1:C:209:ARG:NE	2.51	0.42
1:B:187:ALA:HB2	1:B:317:THR:HG21	2.02	0.42
1:C:106:CYS:HB2	1:C:107:PRO:CD	2.49	0.42
1:B:672:GLN:HG3	1:B:682:SER:O	2.19	0.42
1:A:4:GLN:HG3	1:A:5:VAL:HG13	2.02	0.42
1:B:657:GLU:CD	1:B:716:ARG:NH1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:PRO:HB2	1:B:257:LEU:HD11	2.02	0.42
1:A:135:GLN:HG3	1:C:99:ASN:HB2	2.02	0.42
1:B:479:LEU:HD23	1:B:501:ALA:HA	2.01	0.42
1:A:613:VAL:HA	1:A:616:THR:HG22	2.01	0.42
1:C:137:LEU:O	1:C:138:ASP:HB3	2.20	0.42
1:C:758:MET:HA	1:C:761:GLU:HB3	2.01	0.42
1:B:90:HIS:CD2	1:B:95:PRO:HA	2.54	0.42
1:B:373:PRO:HB3	1:B:377:VAL:HG23	2.01	0.42
1:A:130:PRO:HB2	1:A:133:TYR:HB2	2.02	0.42
1:B:522:ASN:HD22	1:B:616:THR:HG21	1.85	0.42
1:B:166:CYS:SG	1:B:493:ARG:HG2	2.60	0.42
1:C:32:THR:C	1:C:33:ASN:HD22	2.23	0.42
1:A:149:ARG:HG3	3:C:818:HOH:O	2.20	0.41
1:B:482:CYS:O	1:B:497:ILE:HA	2.20	0.41
1:C:295:VAL:O	1:C:298:ALA:HB3	2.19	0.41
1:A:343:LYS:O	1:A:347:GLN:HG3	2.20	0.41
1:B:343:LYS:HG3	1:B:344:THR:N	2.34	0.41
1:A:35:LEU:HD21	3:C:806:HOH:O	2.18	0.41
1:C:252:MET:CE	1:C:294:PRO:HB3	2.49	0.41
1:B:210:GLU:OE2	1:B:488:SER:HB2	2.20	0.41
1:A:474:GLU:HA	1:A:504:CYS:HB2	2.01	0.41
1:A:335:LYS:O	1:A:335:LYS:HG3	2.21	0.41
1:C:433:GLY:HA3	1:C:472:LEU:CD2	2.50	0.41
1:B:228:VAL:HG13	1:B:247:SER:HA	2.02	0.41
1:B:339:THR:HG22	1:B:340:ASP:N	2.36	0.41
1:C:220:VAL:HG12	1:C:221:GLY:N	2.35	0.41
1:B:636:THR:O	1:B:637:GLU:C	2.58	0.41
1:A:180:MET:CE	1:A:314:LEU:HD21	2.50	0.41
1:B:336:LEU:O	1:B:342:GLU:HB2	2.21	0.41
1:A:90:HIS:CE1	1:A:137:LEU:CD1	3.03	0.41
1:C:213:ALA:C	1:C:215:GLU:N	2.74	0.41
1:C:316:HIS:NE2	1:C:318:SER:O	2.53	0.41
1:C:73:LYS:HD2	1:C:76:ALA:HB2	2.02	0.41
1:B:180:MET:HA	1:B:223:VAL:O	2.21	0.41
1:A:626:PRO:HA	1:A:654:TYR:CD2	2.55	0.41
1:B:102:LYS:HB3	1:B:102:LYS:HE2	1.93	0.41
1:B:755:LEU:HA	1:B:755:LEU:HD23	1.86	0.41
1:A:73:LYS:HE2	1:A:458:GLY:O	2.21	0.41
1:C:165:TYR:CE1	1:C:495:LEU:HD11	2.55	0.41
1:A:15:THR:O	1:A:15:THR:HG22	2.21	0.41
1:A:2:PRO:O	1:A:4:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ASN:HD22	1:B:265:ASN:N	2.19	0.41
1:B:756:CYS:SG	1:B:760:LYS:HE3	2.61	0.41
1:C:5:VAL:O	1:C:5:VAL:HG12	2.20	0.41
1:C:517:THR:OG1	1:C:574:MET:HA	2.21	0.41
1:C:387:GLN:OE1	1:C:606:GLN:NE2	2.54	0.41
1:C:81:GLU:CD	1:C:81:GLU:N	2.74	0.41
1:C:497:ILE:CD1	1:C:497:ILE:N	2.84	0.41
1:C:112:ILE:CG2	1:C:113:GLU:N	2.83	0.41
1:C:17:PRO:HA	1:C:35:LEU:O	2.21	0.41
1:A:4:GLN:CG	1:A:5:VAL:N	2.84	0.41
1:B:244:MET:CE	1:B:255:PRO:HD2	2.51	0.41
1:B:151:GLU:OE1	1:B:151:GLU:N	2.53	0.41
1:C:264:VAL:HG12	1:C:268:ARG:NH2	2.36	0.41
1:B:591:GLN:HE21	1:B:748:GLY:HA2	1.84	0.41
1:B:552:LEU:HB2	1:B:762:ILE:CD1	2.51	0.41
1:B:553:ALA:HB1	1:B:766:LEU:HG	2.02	0.41
1:A:632:VAL:CG1	1:A:635:THR:HB	2.51	0.41
1:C:556:ARG:HG3	1:C:569:ILE:HD11	2.03	0.41
1:B:220:VAL:HG12	1:B:221:GLY:N	2.36	0.41
1:B:388:LEU:HA	1:B:443:PHE:O	2.21	0.41
1:A:484:LEU:O	1:A:495:LEU:HA	2.21	0.41
1:C:370:PHE:CE1	1:C:394:TYR:CD2	3.09	0.41
1:A:148:ASP:OD1	1:C:429:ARG:NH2	2.54	0.41
1:A:249:VAL:CG1	1:A:325:PRO:HD2	2.51	0.41
1:C:259:GLY:O	1:C:262:VAL:HG13	2.21	0.41
1:A:256:LEU:O	1:A:257:LEU:HB3	2.20	0.41
1:C:209:ARG:HG2	1:C:209:ARG:NH1	2.36	0.41
1:B:533:LEU:CD1	1:B:605:ARG:HE	2.20	0.40
1:C:686:GLN:HG2	1:C:726:LYS:NZ	2.35	0.40
1:A:249:VAL:HG12	1:A:325:PRO:CD	2.51	0.40
1:A:2:PRO:C	1:A:3:ILE:CG1	2.89	0.40
1:C:180:MET:CE	1:C:312:LEU:HB3	2.50	0.40
1:A:623:ARG:HH12	1:A:715:GLN:NE2	2.19	0.40
1:C:167:LYS:NZ	1:C:362:ALA:O	2.46	0.40
1:B:637:GLU:HA	1:B:638:PRO:HD2	1.91	0.40
1:C:576:LEU:HB3	1:C:580:TYR:CE2	2.56	0.40
1:A:319:LEU:HD23	1:A:320:PRO:CD	2.46	0.40
1:B:337:ILE:O	1:B:342:GLU:CD	2.60	0.40
1:B:657:GLU:HG2	1:B:659:GLY:H	1.86	0.40
1:C:289:GLU:HG2	1:C:322:ALA:CB	2.52	0.40
1:B:533:LEU:HD12	1:B:533:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HD22	1:B:68:LEU:H	1.84	0.40
1:B:555:TYR:CZ	1:B:571:PRO:HB3	2.56	0.40
1:B:293:VAL:N	1:B:294:PRO:CD	2.84	0.40
1:C:497:ILE:HD12	1:C:497:ILE:N	2.36	0.40
1:B:249:VAL:CG1	1:B:250:ALA:H	2.07	0.40
1:A:533:LEU:HD21	1:A:605:ARG:NH2	2.35	0.40
1:C:8:ASP:O	1:C:11:ASN:HB2	2.22	0.40
1:B:343:LYS:CD	1:B:347:GLN:HE22	2.34	0.40
1:A:626:PRO:HB3	1:A:654:TYR:CE2	2.56	0.40
1:B:108:PHE:O	1:B:121:CYS:HB3	2.22	0.40
1:A:678:LEU:HD13	1:A:678:LEU:O	2.22	0.40
1:B:326:GLY:O	1:B:327:LYS:C	2.60	0.40
1:C:511:LEU:HD13	1:C:511:LEU:C	2.42	0.40
1:A:634:SER:O	1:A:635:THR:C	2.60	0.40
1:A:46:TYR:CG	1:A:498:HIS:CE1	3.10	0.40
1:C:664:LEU:HD23	1:C:724:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

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	752/766 (98%)	705 (94%)	34 (4%)	13 (2%)	11	9
1	B	733/766 (96%)	673 (92%)	40 (6%)	20 (3%)	6	3
1	C	729/766 (95%)	626 (86%)	79 (11%)	24 (3%)	5	2
All	All	2214/2298 (96%)	2004 (90%)	153 (7%)	57 (3%)	7	4

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ARG

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Mol	Chain	Res	Type
1	A	38	ASP
1	A	258	ASP
1	A	337	ILE
1	A	633	GLU
1	B	23	ARG
1	B	38	ASP
1	B	252	MET
1	B	337	ILE
1	B	630	SER
1	B	633	GLU
1	C	23	ARG
1	C	38	ASP
1	C	138	ASP
1	C	139	HIS
1	C	226	ASN
1	C	634	SER
1	C	671	GLN
1	C	740	VAL
1	A	211	GLY
1	A	250	ALA
1	A	253	PHE
1	A	256	LEU
1	A	731	MET
1	B	133	TYR
1	B	140	THR
1	B	148	ASP
1	B	729	ASP
1	B	731	MET
1	C	261	LEU
1	C	322	ALA
1	C	330	ASN
1	C	669	SER
1	C	727	GLN
1	A	3	ILE
1	B	727	GLN
1	B	749	ALA
1	C	227	LYS
1	C	235	LYS
1	C	331	ARG
1	C	638	PRO
1	C	640	ALA
1	A	730	LYS

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Mol	Chain	Res	Type
1	B	139	HIS
1	B	637	GLU
1	C	340	ASP
1	C	672	GLN
1	A	740	VAL
1	B	334	ARG
1	C	186	ASN
1	C	204	LEU
1	C	635	THR
1	C	700	PRO
1	B	211	GLY
1	B	249	VAL
1	B	40	GLY
1	B	631	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	667/673 (99%)	635 (95%)	32 (5%)	31	40
1	B	650/673 (97%)	617 (95%)	33 (5%)	29	36
1	C	649/673 (96%)	622 (96%)	27 (4%)	36	46
All	All	1966/2019 (97%)	1874 (95%)	92 (5%)	32	41

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	11	ASN
1	A	110	GLN
1	A	137	LEU
1	A	145	ASP
1	A	163	VAL
1	A	200	LEU
1	A	204	LEU

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Mol	Chain	Res	Type
1	A	209	ARG
1	A	251	ASP
1	A	288	THR
1	A	300	MET
1	A	319	LEU
1	A	321	ILE
1	A	335	LYS
1	A	371	LEU
1	A	389	THR
1	A	407	ARG
1	A	419	VAL
1	A	431	SER
1	A	447	ASN
1	A	551	ILE
1	A	556	ARG
1	A	570	LEU
1	A	625	LEU
1	A	655	LEU
1	A	657	GLU
1	A	678	LEU
1	A	694	LEU
1	A	699	ASN
1	A	728	GLU
1	A	750	SER
1	B	35	LEU
1	B	41	ASN
1	B	43	SER
1	B	68	LEU
1	B	90	HIS
1	B	145	ASP
1	B	194	ARG
1	B	200	LEU
1	B	252	MET
1	B	263	ASN
1	B	287	GLU
1	B	300	MET
1	B	318	SER
1	B	340	ASP
1	B	367	VAL
1	B	371	LEU
1	B	389	THR
1	B	419	VAL

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Mol	Chain	Res	Type
1	B	438	ASP
1	B	461	THR
1	B	475	GLU
1	B	544	LEU
1	B	579	VAL
1	B	628	THR
1	B	630	SER
1	B	641	VAL
1	B	657	GLU
1	B	662	LEU
1	B	689	SER
1	B	694	LEU
1	B	699	ASN
1	B	701	LEU
1	B	729	ASP
1	C	4	GLN
1	C	90	HIS
1	C	110	GLN
1	C	116	ARG
1	C	139	HIS
1	C	143	ARG
1	C	144	VAL
1	C	149	ARG
1	C	164	ASP
1	C	209	ARG
1	C	256	LEU
1	C	263	ASN
1	C	300	MET
1	C	321	ILE
1	C	331	ARG
1	C	338	ASN
1	C	392	SER
1	C	429	ARG
1	C	447	ASN
1	C	600	ASP
1	C	610	SER
1	C	616	THR
1	C	625	LEU
1	C	638	PRO
1	C	642	ARG
1	C	743	LYS
1	C	755	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	33	ASN
1	A	119	GLN
1	A	242	GLN
1	A	263	ASN
1	A	349	GLN
1	A	354	GLN
1	A	374	ASN
1	A	447	ASN
1	A	550	GLN
1	A	582	ASN
1	A	591	GLN
1	A	617	ASN
1	A	671	GLN
1	A	672	GLN
1	A	676	GLN
1	A	699	ASN
1	A	715	GLN
1	B	33	ASN
1	B	41	ASN
1	B	90	HIS
1	B	119	GLN
1	B	242	GLN
1	B	263	ASN
1	B	347	GLN
1	B	349	GLN
1	B	363	GLN
1	B	387	GLN
1	B	417	GLN
1	B	507	GLN
1	B	591	GLN
1	B	606	GLN
1	B	672	GLN
1	B	699	ASN
1	B	715	GLN
1	B	737	HIS
1	C	33	ASN
1	C	63	GLN
1	C	90	HIS
1	C	119	GLN
1	C	139	HIS

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Mol	Chain	Res	Type
1	C	230	HIS
1	C	242	GLN
1	C	263	ASN
1	C	265	ASN
1	C	330	ASN
1	C	338	ASN
1	C	347	GLN
1	C	349	GLN
1	C	363	GLN
1	C	375	GLN
1	C	387	GLN
1	C	405	GLN
1	C	417	GLN
1	C	447	ASN
1	C	492	GLN
1	C	558	ASN
1	C	606	GLN
1	C	715	GLN
1	C	727	GLN

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 carbohydrates 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	758/766 (98%)	0.24	31 (4%) 41 55	13, 29, 65, 105	0
1	B	738/766 (96%)	0.57	65 (8%) 12 20	20, 40, 79, 104	0
1	C	732/766 (95%)	1.46	213 (29%) 1 1	22, 64, 98, 111	0
All	All	2228/2298 (96%)	0.75	309 (13%) 4 7	13, 41, 91, 111	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	635	THR	11.5
1	A	632	VAL	11.3
1	C	256	LEU	10.6
1	C	250	ALA	10.1
1	C	253	PHE	9.8
1	B	147	TYR	9.5
1	C	705	VAL	9.4
1	B	633	GLU	8.0
1	C	729	ASP	7.9
1	C	701	LEU	7.9
1	B	635	THR	7.8
1	A	629	LYS	7.2
1	B	566	GLY	7.2
1	C	568	LEU	6.8
1	C	257	LEU	6.8
1	C	760	LYS	6.8
1	C	282	PHE	6.7
1	C	627	LEU	6.7
1	A	631	PRO	6.6
1	C	288	THR	6.5
1	C	697	LEU	6.5
1	C	634	SER	6.4
1	C	653	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	B	636	THR	6.2
1	B	16	GLU	6.2
1	B	568	LEU	6.1
1	C	255	PRO	6.0
1	A	633	GLU	6.0
1	B	634	SER	5.9
1	C	326	GLY	5.9
1	C	252	MET	5.9
1	C	335	LYS	5.7
1	A	568	LEU	5.7
1	C	246	VAL	5.7
1	B	15	THR	5.6
1	A	635	THR	5.5
1	C	339	THR	5.4
1	A	256	LEU	5.4
1	C	733	MET	5.4
1	C	139	HIS	5.4
1	A	15	THR	5.4
1	C	687	ILE	5.4
1	C	765	LEU	5.3
1	B	148	ASP	5.2
1	C	350	THR	5.2
1	C	241	PRO	5.1
1	C	704	LYS	5.1
1	B	632	VAL	5.0
1	C	245	VAL	4.9
1	C	375	GLN	4.9
1	C	651	GLY	4.9
1	B	765	LEU	4.9
1	C	766	LEU	4.9
1	C	694	LEU	4.9
1	C	206	PHE	4.9
1	C	227	LYS	4.8
1	C	138	ASP	4.8
1	C	403	ASN	4.8
1	B	146	ALA	4.8
1	C	700	PRO	4.6
1	C	331	ARG	4.6
1	C	248	ASP	4.6
1	C	240	GLN	4.5
1	C	702	SER	4.5
1	B	214	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	185	TYR	4.5
1	B	629	LYS	4.5
1	C	349	GLN	4.5
1	A	745	LEU	4.5
1	B	256	LEU	4.4
1	C	371	LEU	4.4
1	C	237	SER	4.4
1	C	137	LEU	4.4
1	C	276	ASP	4.3
1	B	630	SER	4.2
1	C	743	LYS	4.2
1	C	264	VAL	4.2
1	C	592	PRO	4.1
1	B	764	GLN	4.1
1	C	189	ARG	4.1
1	C	667	GLY	4.1
1	C	708	LEU	4.0
1	C	728	GLU	4.0
1	C	249	VAL	4.0
1	C	374	ASN	4.0
1	C	238	LEU	4.0
1	C	649	SER	4.0
1	C	666	VAL	3.9
1	C	214	GLU	3.9
1	C	147	TYR	3.9
1	B	729	ASP	3.9
1	C	278	ILE	3.9
1	C	228	VAL	3.9
1	C	598	THR	3.8
1	C	254	VAL	3.8
1	A	729	ASP	3.8
1	C	665	TRP	3.8
1	B	767	SER	3.8
1	C	290	THR	3.8
1	C	244	MET	3.7
1	C	340	ASP	3.7
1	C	628	THR	3.7
1	C	251	ASP	3.6
1	C	767	SER	3.6
1	C	737	HIS	3.6
1	C	336	LEU	3.6
1	C	229	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	17	PRO	3.6
1	C	551	ILE	3.6
1	C	762	ILE	3.6
1	C	536	PRO	3.6
1	C	342	GLU	3.6
1	C	345	LEU	3.6
1	C	689	SER	3.5
1	C	239	ALA	3.5
1	C	275	LEU	3.5
1	C	321	ILE	3.5
1	C	280	GLU	3.5
1	C	763	ARG	3.5
1	C	655	LEU	3.4
1	C	213	ALA	3.4
1	C	727	GLN	3.4
1	C	277	GLN	3.4
1	C	597	THR	3.3
1	C	703	LYS	3.3
1	C	180	MET	3.3
1	A	334	ARG	3.3
1	C	15	THR	3.3
1	C	758	MET	3.3
1	B	145	ASP	3.3
1	C	279	PRO	3.3
1	C	590	LEU	3.3
1	C	281	MET	3.2
1	A	2	PRO	3.2
1	C	6	ILE	3.2
1	B	334	ARG	3.2
1	A	733	MET	3.2
1	C	400	GLN	3.2
1	C	293	VAL	3.2
1	C	636	THR	3.2
1	B	731	MET	3.2
1	B	637	GLU	3.1
1	C	353	TYR	3.1
1	A	254	VAL	3.1
1	B	143	ARG	3.1
1	C	334	ARG	3.1
1	B	337	ILE	3.1
1	B	638	PRO	3.0
1	C	401	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	376	TYR	3.0
1	B	139	HIS	3.0
1	C	764	GLN	3.0
1	C	202	SER	3.0
1	B	569	ILE	3.0
1	C	289	GLU	3.0
1	B	557	LYS	3.0
1	A	5	VAL	3.0
1	C	338	ASN	3.0
1	C	625	LEU	3.0
1	C	745	LEU	3.0
1	B	766	LEU	2.9
1	C	116	ARG	2.9
1	C	601	ARG	2.9
1	A	634	SER	2.9
1	C	292	PHE	2.9
1	B	22	VAL	2.9
1	C	633	GLU	2.9
1	B	628	THR	2.8
1	A	6	ILE	2.8
1	C	231	PHE	2.8
1	C	399	PHE	2.8
1	C	747	GLY	2.8
1	B	252	MET	2.8
1	C	207	LEU	2.8
1	C	696	VAL	2.8
1	B	134	PHE	2.8
1	C	692	SER	2.7
1	C	369	LEU	2.7
1	B	133	TYR	2.7
1	C	557	LYS	2.7
1	C	756	CYS	2.7
1	A	630	SER	2.7
1	C	757	HIS	2.7
1	A	257	LEU	2.7
1	C	260	PHE	2.7
1	C	663	PHE	2.7
1	B	86	TYR	2.7
1	B	610	SER	2.6
1	C	140	THR	2.6
1	C	654	TYR	2.6
1	C	719	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	724	VAL	2.6
1	C	698	ASP	2.6
1	C	225	TYR	2.6
1	C	607	LEU	2.6
1	C	4	GLN	2.6
1	C	341	LYS	2.6
1	C	203	LEU	2.6
1	C	691	LEU	2.6
1	B	461	THR	2.6
1	C	346	PHE	2.5
1	C	405	GLN	2.5
1	A	252	MET	2.5
1	C	303	LEU	2.5
1	C	723	THR	2.5
1	C	327	LYS	2.5
1	C	550	GLN	2.5
1	B	136	HIS	2.5
1	C	641	VAL	2.5
1	C	730	LYS	2.5
1	C	187	ALA	2.4
1	C	690	GLY	2.4
1	B	392	SER	2.4
1	C	688	THR	2.4
1	B	554	CYS	2.4
1	B	108	PHE	2.4
1	C	668	ALA	2.4
1	C	268	ARG	2.4
1	B	631	PRO	2.4
1	C	377	VAL	2.4
1	B	749	ALA	2.4
1	C	575	LYS	2.4
1	C	755	LEU	2.4
1	C	394	TYR	2.4
1	C	738	PHE	2.4
1	C	247	SER	2.4
1	C	86	TYR	2.4
1	C	616	THR	2.4
1	C	22	VAL	2.3
1	B	616	THR	2.3
1	C	567	GLN	2.3
1	C	593	GLY	2.3
1	B	152	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	541	ARG	2.3
1	B	609	THR	2.3
1	C	695	PRO	2.3
1	C	710	ASP	2.3
1	C	637	GLU	2.3
1	B	340	ASP	2.3
1	C	332	ASP	2.3
1	C	351	GLY	2.3
1	C	323	GLU	2.3
1	B	366	CYS	2.3
1	C	324	ALA	2.3
1	C	553	ALA	2.3
1	C	372	PHE	2.3
1	C	242	GLN	2.2
1	C	594	ALA	2.2
1	C	693	VAL	2.2
1	C	333	ASP	2.2
1	C	396	TYR	2.2
1	B	253	PHE	2.2
1	C	263	ASN	2.2
1	C	330	ASN	2.2
1	B	345	LEU	2.2
1	C	314	LEU	2.2
1	C	611	MET	2.2
1	B	131	PRO	2.2
1	C	569	ILE	2.2
1	A	14	GLY	2.2
1	C	194	ARG	2.2
1	C	412	LEU	2.2
1	C	226	ASN	2.2
1	C	337	ILE	2.2
1	C	393	VAL	2.2
1	C	559	CYS	2.2
1	A	314	LEU	2.2
1	C	572	GLU	2.2
1	C	218	ILE	2.2
1	C	596	VAL	2.2
1	C	725	VAL	2.2
1	A	9	ASP	2.2
1	A	394	TYR	2.2
1	C	508	LEU	2.2
1	C	640	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	730	LYS	2.1
1	C	408	PHE	2.1
1	C	699	ASN	2.1
1	C	261	LEU	2.1
1	B	144	VAL	2.1
1	B	717	SER	2.1
1	C	706	ARG	2.1
1	C	539	ALA	2.1
1	C	373	PRO	2.1
1	C	402	GLU	2.1
1	C	759	HIS	2.1
1	A	616	THR	2.1
1	B	116	ARG	2.1
1	C	605	ARG	2.1
1	A	337	ILE	2.1
1	C	188	ILE	2.1
1	C	142	LYS	2.1
1	A	11	ASN	2.1
1	A	763	ARG	2.1
1	A	728	GLU	2.0
1	B	393	VAL	2.1
1	B	141	GLY	2.0
1	B	63	GLN	2.0
1	C	588	ASP	2.0
1	B	130	PRO	2.0
1	C	473	ASN	2.0
1	A	253	PHE	2.0
1	A	3	ILE	2.0
1	B	37	LYS	2.0
1	B	612	ASP	2.0
1	C	608	VAL	2.0
1	B	92	GLU	2.0
1	C	524	MET	2.0
1	C	744	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	A	800	1/1	0.99	0.12	-0.08	27,27,27,27	0
2	ZN	C	800	1/1	1.00	0.11	-1.08	26,26,26,26	0
2	ZN	B	800	1/1	0.99	0.07	-1.17	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.