



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:43 PM UTC

PDB ID : 3EH2 / pdb_00003eh2
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

<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

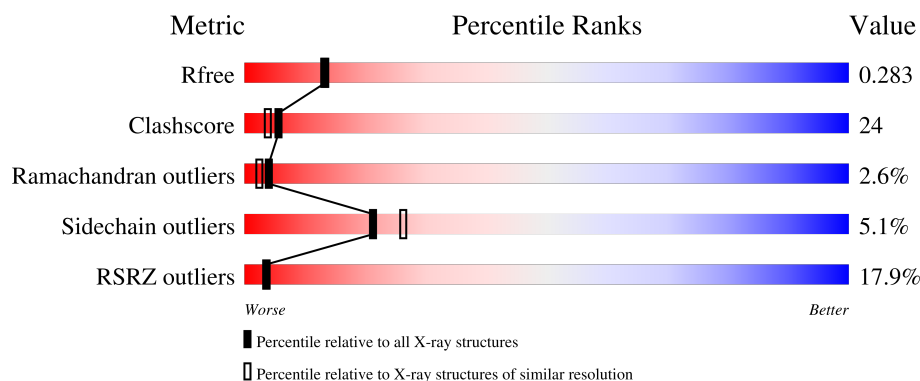
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	766	6% 64% 30% .
1	B	766	10% 60% 30% 6% .
1	C	766	36% 52% 38% 5% .

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 (CCD ID: ZN) (formula: Zn).

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

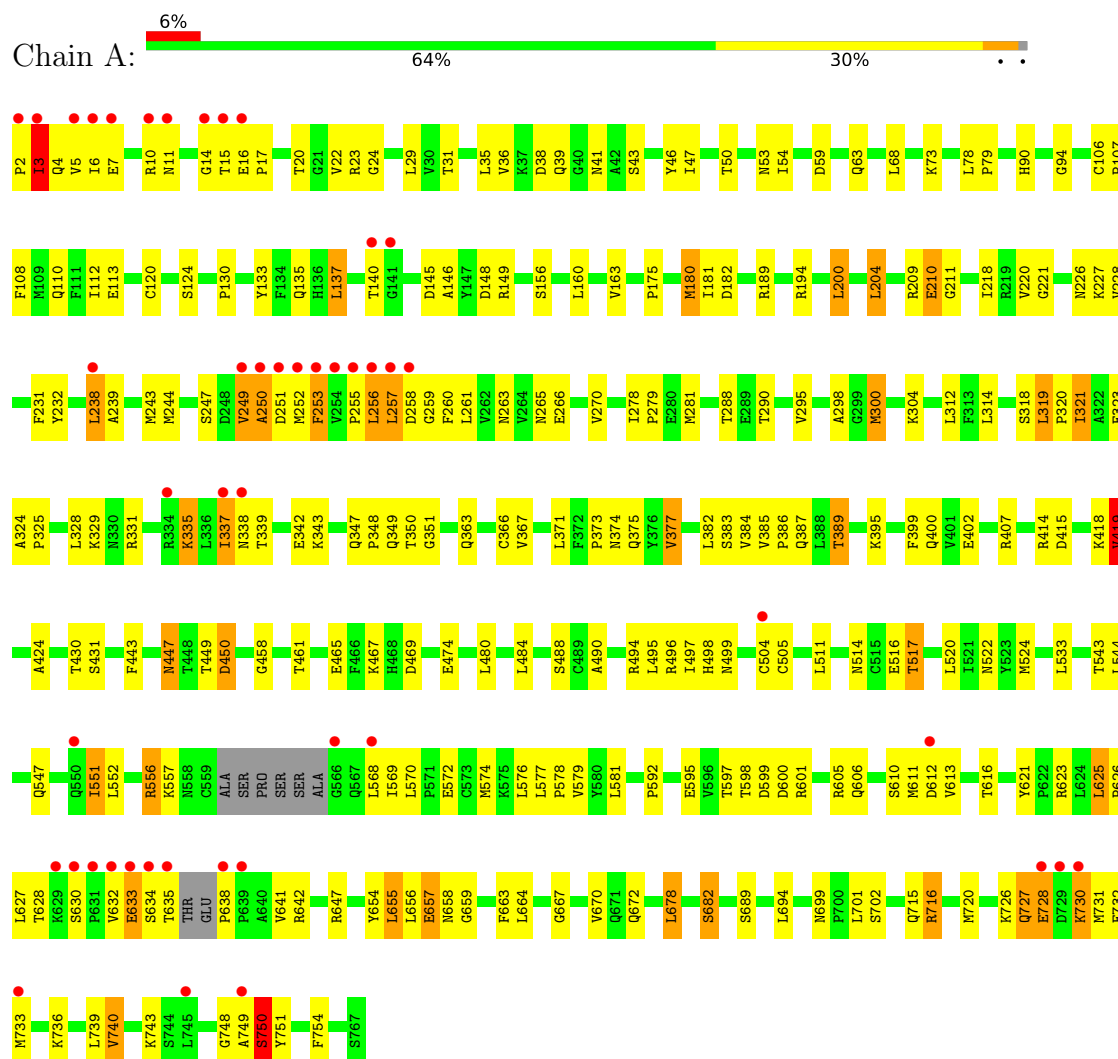
- Molecule 3 is water.

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		

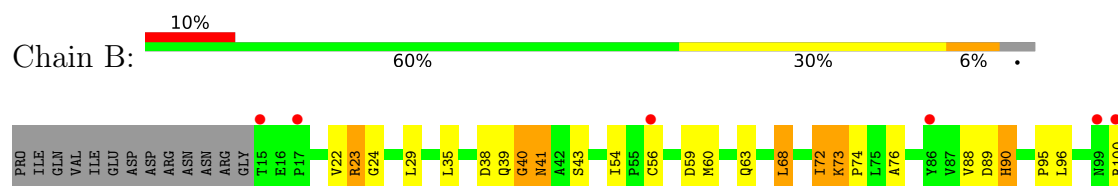
3 Residue-property plots [i](#)

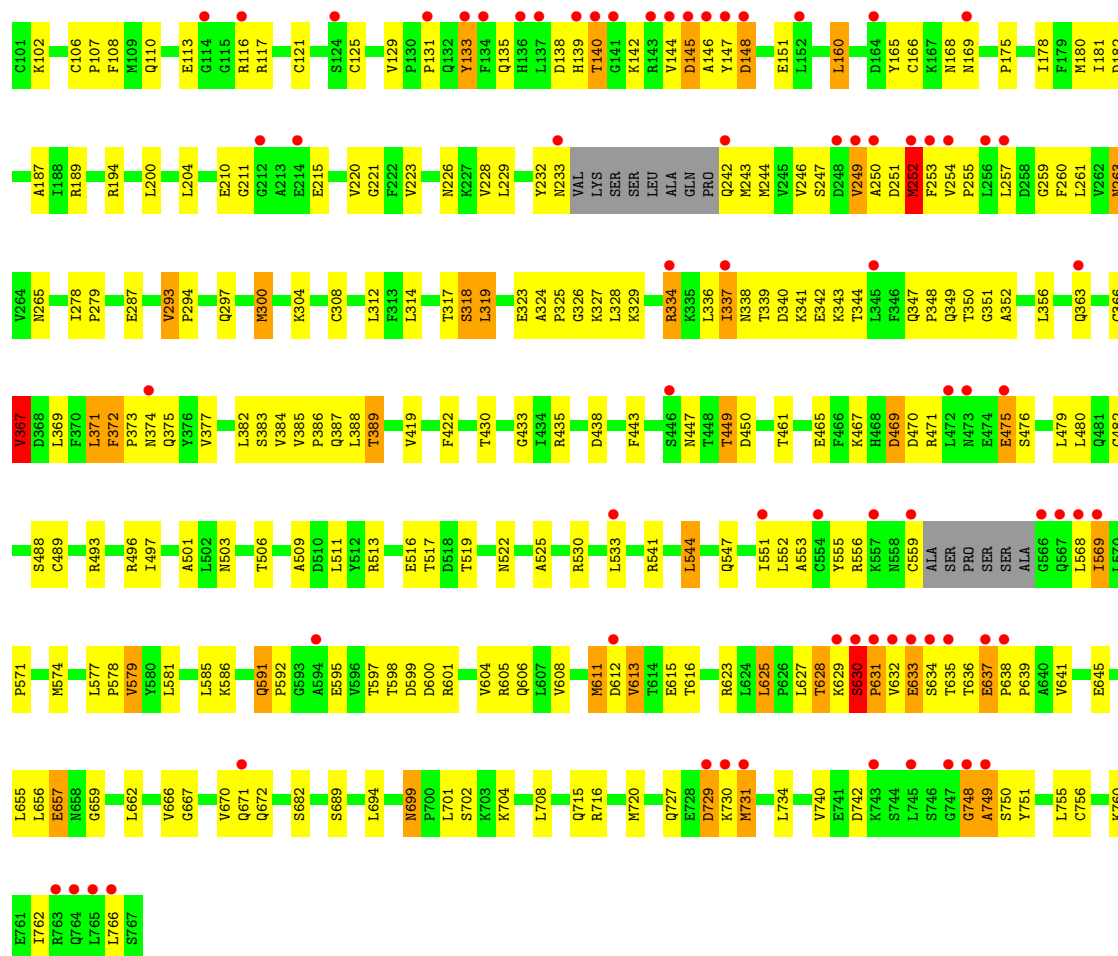
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein transport protein Sec24C

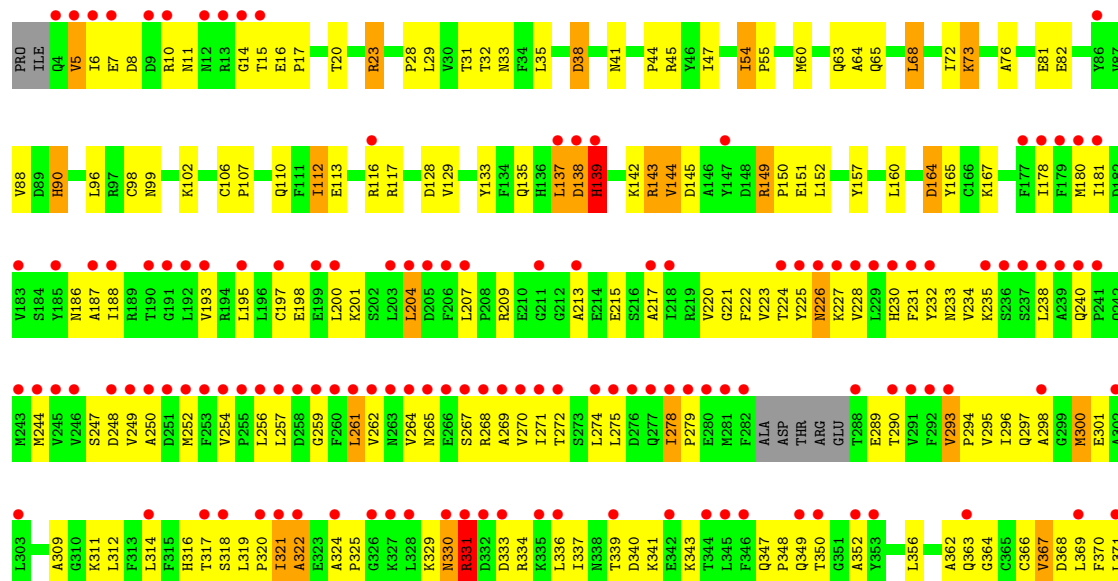


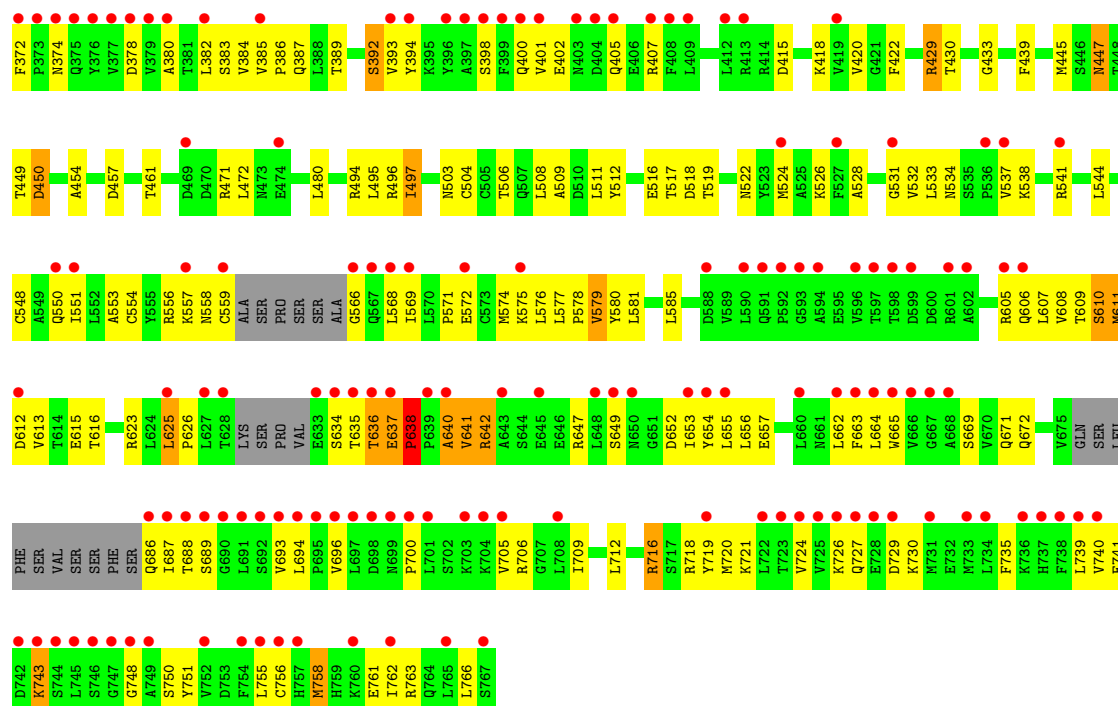
• Molecule 1: Protein transport protein Sec24C





• 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) 96.2 (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	5450 reflections (5.05%)	wwPDB-VP
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 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.49	2/6061 (0.0%)	1.01	40/8215 (0.5%)
1	B	0.42	0/5912	1.00	25/8015 (0.3%)
1	C	0.40	1/5911 (0.0%)	0.94	24/8010 (0.3%)
All	All	0.44	3/17884 (0.0%)	0.98	89/24240 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	MET	SD-CE	-6.12	1.64	1.79
1	C	139	HIS	N-CA	-5.74	1.38	1.46
1	A	750	SER	N-CA	-5.59	1.39	1.45

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	THR	N-CA-C	20.30	133.41	111.28
1	A	727	GLN	N-CA-C	11.12	125.98	111.75
1	B	611	MET	N-CA-C	9.28	122.78	110.53
1	C	636	THR	N-CA-C	9.19	117.57	108.75
1	A	54	ILE	N-CA-C	8.15	116.60	109.02
1	A	140	THR	N-CA-C	-7.86	98.83	110.46
1	A	181	ILE	N-CA-C	7.79	119.07	108.17
1	B	308	CYS	N-CA-C	-7.79	97.24	109.07
1	C	374	ASN	N-CA-C	-7.69	103.51	113.12
1	B	374	ASN	N-CA-C	-7.63	104.50	113.88
1	B	181	ILE	N-CA-C	7.50	118.67	108.17
1	C	729	ASP	N-CA-C	7.30	126.35	110.80
1	C	5	VAL	N-CA-C	-7.23	103.23	113.07
1	B	613	VAL	N-CA-C	-7.13	102.18	111.09
1	A	419	VAL	N-CA-C	-6.99	99.67	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	TYR	N-CA-C	-6.97	104.66	113.02
1	C	611	MET	N-CA-C	6.96	121.38	110.32
1	A	210	GLU	N-CA-C	6.96	115.43	108.75
1	B	372	PHE	CA-C-N	6.95	126.71	119.76
1	B	372	PHE	C-N-CA	6.95	126.71	119.76
1	B	750	SER	N-CA-C	-6.91	99.43	110.14
1	C	217	ALA	N-CA-C	-6.81	105.25	113.97
1	A	728	GLU	N-CA-C	6.78	121.81	112.04
1	A	239	ALA	N-CA-C	-6.78	105.05	113.38
1	B	318	SER	N-CA-C	6.49	118.71	108.79
1	B	748	GLY	N-CA-C	6.39	120.41	112.73
1	A	682	SER	N-CA-C	6.39	120.81	112.89
1	B	56	CYS	N-CA-C	6.39	118.24	111.28
1	B	517	THR	N-CA-C	6.38	117.90	111.07
1	B	160	LEU	N-CA-C	-6.37	100.85	110.28
1	A	318	SER	N-CA-C	6.34	118.81	109.24
1	A	189	ARG	N-CA-C	6.23	119.05	111.82
1	A	249	VAL	N-CA-C	-6.21	103.28	110.05
1	B	450	ASP	N-CA-C	6.13	118.28	108.41
1	A	739	LEU	N-CA-C	-6.02	103.06	110.65
1	A	628	THR	CA-C-N	5.97	132.94	121.54
1	A	628	THR	C-N-CA	5.97	132.94	121.54
1	A	740	VAL	N-CA-C	5.94	121.69	109.34
1	C	758	MET	N-CA-C	-5.92	106.68	114.31
1	A	517	THR	N-CA-C	5.91	117.40	111.07
1	B	72	ILE	N-CA-C	5.80	116.30	108.17
1	A	748	GLY	N-CA-C	-5.78	104.85	112.82
1	A	227	LYS	N-CA-C	-5.74	105.60	113.30
1	C	748	GLY	N-CA-C	-5.68	101.08	111.25
1	C	181	ILE	N-CA-C	5.64	116.42	108.36
1	C	372	PHE	CA-C-N	5.63	126.88	119.84
1	C	372	PHE	C-N-CA	5.63	126.88	119.84
1	A	257	LEU	N-CA-C	-5.63	103.68	111.28
1	A	749	ALA	N-CA-C	-5.61	101.87	109.95
1	A	572	GLU	N-CA-C	5.55	117.33	111.28
1	C	636	THR	CB-CA-C	-5.54	108.39	116.53
1	C	160	LEU	N-CA-C	-5.49	101.03	109.76
1	B	367	VAL	N-CA-C	5.47	115.77	108.11
1	A	628	THR	O-C-N	5.45	129.30	122.65
1	B	740	VAL	N-CA-C	5.43	120.64	109.34
1	A	748	GLY	CA-C-N	-5.42	113.24	123.27
1	A	748	GLY	C-N-CA	-5.42	113.24	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	450	ASP	N-CA-C	5.42	117.07	108.67
1	A	750	SER	N-CA-C	-5.39	101.09	109.72
1	B	469	ASP	N-CA-C	-5.39	106.57	114.39
1	B	525	ALA	N-CA-C	-5.39	105.07	111.69
1	C	137	LEU	N-CA-C	-5.34	99.43	110.80
1	C	72	ILE	N-CA-C	5.32	115.61	108.17
1	A	160	LEU	N-CA-C	-5.30	102.01	109.96
1	A	424	ALA	N-CA-C	5.27	118.31	110.14
1	B	226	ASN	N-CA-C	-5.25	99.61	110.80
1	A	469	ASP	N-CA-C	-5.24	107.44	113.88
1	C	54	ILE	N-CA-C	5.21	114.69	108.96
1	B	189	ARG	N-CA-C	5.18	117.60	111.33
1	A	630	SER	CA-C-N	5.18	126.31	119.84
1	A	630	SER	C-N-CA	5.18	126.31	119.84
1	A	377	VAL	N-CA-C	-5.17	108.23	113.20
1	A	450	ASP	N-CA-C	5.17	117.18	108.96
1	B	54	ILE	N-CA-C	5.16	114.64	108.96
1	C	367	VAL	N-CA-C	5.15	115.32	108.11
1	C	278	ILE	CB-CA-C	-5.15	108.81	113.70
1	A	238	LEU	N-CA-C	-5.13	101.39	109.50
1	A	374	ASN	N-CA-C	-5.09	107.62	113.88
1	A	514	ASN	N-CA-C	5.09	119.05	111.87
1	C	293	VAL	CB-CA-C	-5.05	108.90	113.70
1	A	79	PRO	N-CA-C	-5.05	105.62	110.47
1	C	73	LYS	CA-C-N	5.04	126.14	119.84
1	C	73	LYS	C-N-CA	5.04	126.14	119.84
1	A	47	ILE	N-CA-C	5.04	115.00	108.35
1	B	293	VAL	CB-CA-C	-5.04	108.91	113.70
1	C	637	GLU	CA-C-N	5.04	125.57	120.38
1	C	637	GLU	C-N-CA	5.04	125.57	120.38
1	A	94	GLY	CA-C-N	5.01	124.78	119.76
1	A	94	GLY	C-N-CA	5.01	124.78	119.76

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	260	0
1	B	5799	0	5805	255	0
1	C	5802	0	5809	317	0
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	17	0
3	C	36	0	0	20	0
All	All	17790	0	17572	823	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 24.

All (823) 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: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:A:300:MET:HE3	1:A:363:GLN:HG3	1.39	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:243:MET:HE1	1:A:281:MET:SD	2.08	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:B:180:MET:HE3	1:B:314:LEU:HD21	1.51	0.90
1:C:14:GLY:HA3	3:C:819:HOH:O	1.72	0.89
1:C:716:ARG:HG3	1:C:720:MET:HE2	1.55	0.89
1:A:300:MET:HE1	1:A:304:LYS:HE3	1.54	0.88
1:B:90:HIS:HD2	1:B:96:LEU:H	1.22	0.87
1:A:180:MET:HE3	1:A:314:LEU:HD21	1.58	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:300:MET:HE3	1:C:363:GLN:HG3	1.59	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:321:ILE:HD13	1:C:321:ILE:H	1.44	0.82
1:C:568:LEU:HD23	1:C:568:LEU:H	1.43	0.82
1:C:447:ASN:HD21	1:C:450:ASP:H	1.27	0.81
1:A:210:GLU:CD	1:A:494:ARG:HH22	1.88	0.81
1:C:180:MET:HE1	1:C:312:LEU:HD13	1.59	0.81
1:C:743:LYS:HG2	1:C:750:SER:HB2	1.60	0.81
1:A:180:MET:HE1	1:A:312:LEU:HD13	1.61	0.81
1:A:180:MET:HE2	1:A:312:LEU:HB3	1.61	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:A:533:LEU:HD11	1:A:605:ARG:HE	1.48	0.79
1:B:385:VAL:O	1:B:389:THR:HB	1.82	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:B:233:ASN:CG	1:B:259:GLY:HA3	2.09	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:B:180:MET:HE2	1:B:312:LEU:HB3	1.63	0.77
1:C:641:VAL:HG11	1:C:647:ARG:HE	1.49	0.77
1:A:329:LYS:H	1:A:349:GLN:HE22	1.30	0.77
1:B:260:PHE:HA	3:B:858:HOH:O	1.83	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:HH11	1:C:429:ARG:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:716:ARG:HG3	1:A:720:MET:HE2	1.70	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:4:GLN:NE2	3:A:805:HOH:O	2.15	0.73
1:A:579:VAL:HG22	1:A:751:TYR:CZ	2.23	0.73
1:A:319:LEU:HD23	1:A:320:PRO:HD2	1.68	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
1:B:40:GLY:C	1:B:41:ASN:HD22	1.96	0.73
1:C:233:ASN:HB2	1:C:257:LEU:HD21	1.70	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:228:VAL:HG23	1:C:247:SER:HA	1.73	0.71
1:C:429:ARG:HH11	1:C:429:ARG:CB	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: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:488:SER:OG	3:A:903:HOH:O	2.11	0.69
1:A:533:LEU:HD11	1:A:605:ARG:NE	2.08	0.69
1:C:324:ALA:HB1	1:C:325:PRO:HD2	1.74	0.69
1:C:343:LYS:HB3	1:C:347:GLN:HE21	1.58	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:135:GLN:HB3	1:B:142:LYS:HE2	1.73	0.68
1:B:367:VAL:H	1:B:389:THR:CG2	2.03	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:689:SER:CB	1:C:730:LYS:HG3	2.24	0.68
1:A:10:ARG:HH21	1:A:14:GLY:HA3	1.59	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: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:C:625:LEU:HD22	1:C:625:LEU:O	1.94	0.67
1:A:337:ILE:O	1:A:342:GLU:HB2	1.94	0.67
1:A:447:ASN:HD21	1:A:450:ASP:N	1.81	0.67
1:A:447:ASN:C	1:A:447:ASN:HD22	2.02	0.67
1:B:623:ARG:HH22	1:B:715:GLN:HE22	1.41	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:C:641:VAL:CG1	1:C:647:ARG:HE	2.07	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:A:252:MET:O	1:A:253:PHE:HB3	1.94	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:A:210:GLU:CD	1:A:494:ARG:NH2	2.55	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:A:22:VAL:HG12	3:A:801:HOH:O	1.95	0.65
1:A:367:VAL:H	1:A:389:THR:CG2	2.07	0.65
1:B:329:LYS:H	1:B:349:GLN:NE2	1.86	0.65
1:C:387:GLN:HB2	1:C:606:GLN:NE2	2.12	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:133:TYR:O	1:C:143:ARG:NH2	2.31	0.64
1:C:293:VAL:HB	1:C:294:PRO:HD3	1.79	0.64
1:A:2:PRO:HD2	1:A:642:ARG:HH12	1.62	0.64
1:A:522:ASN:HD22	1:A:616:THR:HG21	1.62	0.64
1:B:233:ASN:OD1	1:B:259:GLY:HA3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LEU:N	1:C:68:LEU:HD22	2.13	0.64
1:C:430:THR:HG22	1:C:480:LEU:HD23	1.80	0.64
1:C:383:SER:HB2	1:C:393:VAL:HG21	1.77	0.64
1:B:300:MET:HE1	1:B:304:LYS:HE3	1.79	0.63
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:HG2	1:C:143:ARG:HH11	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
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:300:MET:CE	1:A:304:LYS:HE3	2.27	0.63
1:A:447:ASN:HD22	1:A:449:THR:H	1.45	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:494:ARG:CZ	3:C:801:HOH:O	2.46	0.63
1:C:696:VAL:HG13	1:C:706:ARG:NH1	2.13	0.63
1:A:597:THR:HG22	1:A:599:ASP:H	1.64	0.62
1:B:348:PRO:HB3	1:B:384:VAL:HG21	1.81	0.62
1:B:631:PRO:HB2	3:B:833:HOH:O	1.98	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:A:232:TYR:CE1	1:A:243:MET:HE2	2.35	0.62
1:B:377:VAL:HG12	1:B:382:LEU:HD11	1.81	0.62
1:B:387:GLN:CG	1:B:606:GLN:HE22	2.10	0.62
1:B:597:THR:HG22	1:B:599:ASP:H	1.65	0.62
1:C:566:GLY:N	1:C:763:ARG:HH12	1.98	0.62
1:B:447:ASN:ND2	1:B:449:THR:HG23	2.14	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:3:ILE:H	1:A:576:LEU:HD21	1.65	0.61
1:B:556:ARG:NE	1:B:569:ILE:HD11	2.15	0.61
1:B:252:MET:O	1:B:253:PHE:HB3	2.01	0.61
1:B:496:ARG:C	1:B:497:ILE:HD12	2.26	0.61
1:A:2:PRO:C	1:A:3:ILE:HG12	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:699:ASN:ND2	1:A:702:SER:H	1.98	0.61
1:C:15:THR:HA	3:C:831:HOH:O	2.00	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:A:337:ILE:HG22	1:A:338:ASN:N	2.15	0.61
1:B:68:LEU:N	1:B:68:LEU:HD22	2.16	0.61
1:B:630:SER:H	1:B:631:PRO:CD	2.13	0.61
1:C:294:PRO:HG3	1:C:325:PRO:HG2	1.82	0.60
1:A:689:SER:OG	1:A:726:LYS:HD3	2.00	0.60
1:C:238:LEU:C	1:C:240:GLN:H	2.08	0.60
1:B:180:MET:CE	1:B:312:LEU:HD13	2.31	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:B:300:MET:CE	1:B:304:LYS:HE3	2.30	0.60
1:C:226:ASN:O	1:C:290:THR:CA	2.35	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:A:39:GLN:O	1:A:39:GLN:HG2	2.02	0.60
1:C:188:ILE:HD13	1:C:193:VAL:HB	1.82	0.60
1:C:509:ALA:HA	3:C:823:HOH:O	2.00	0.60
1:A:300:MET:O	1:A:300:MET:HE2	2.01	0.60
1:C:137:LEU:O	1:C:138:ASP:CB	2.50	0.59
1:C:135:GLN:HG2	1:C:145:ASP:CG	2.28	0.59
1:A:659:GLY:HA2	1:A:716:ARG:CD	2.33	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:C:568:LEU:H	1:C:568:LEU:CD2	2.13	0.59
1:B:90:HIS:HE1	1:B:151:GLU:OE2	1.85	0.59
1:B:699:ASN:ND2	1:B:702:SER:H	2.01	0.59
1:C:579:VAL:HG22	1:C:751:TYR:CZ	2.38	0.59
1:C:265:ASN:N	1:C:265:ASN:HD22	2.00	0.59
1:C:528:ALA:O	1:C:532:VAL:HG23	2.02	0.59
1:C:548:CYS:SG	1:C:581:LEU:HD22	2.42	0.59
1:B:138:ASP:C	1:B:140:THR:H	2.10	0.59
1:C:300:MET:C	1:C:300:MET:HE2	2.27	0.59
1:A:657:GLU:HG2	1:A:659:GLY:H	1.68	0.58
1:A:90:HIS:CE1	1:A:137:LEU:HD11	2.38	0.58
1:B:210:GLU:HG3	1:B:489:CYS:SG	2.42	0.58
1:C:10:ARG:HE	1:C:28:PRO:HA	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ARG:HD2	1:C:503:ASN:OD1	2.03	0.58
1:B:293:VAL:HB	1:B:294:PRO:HD3	1.85	0.58
1:C:7:GLU:OE2	1:C:31:THR:HG21	2.03	0.58
1:C:220:VAL:O	1:C:261:LEU:HA	2.04	0.58
1:C:407:ARG:HD2	1:C:721:LYS:HB2	1.86	0.58
1:A:348:PRO:HB3	1:A:384:VAL:HG21	1.84	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:383:SER:C	1:A:386:PRO:HD2	2.29	0.58
1:A:497:ILE:N	1:A:497:ILE:HD12	2.19	0.58
1:B:579:VAL:HG13	1:B:751:TYR:CD1	2.39	0.58
1:C:143:ARG:NH1	1:C:152:LEU:HD11	2.18	0.58
1:B:242:GLN:NE2	3:B:869:HOH:O	2.33	0.58
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
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: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:A:350:THR:HG22	1:A:351:GLY:N	2.19	0.57
1:B:555:TYR:CD2	1:B:571:PRO:HD3	2.40	0.57
1:A:244:MET:CE	1:A:255:PRO:HG2	2.34	0.57
1:C:623:ARG:HG2	1:C:625:LEU:HD12	1.87	0.57
1:B:178:ILE:HB	1:B:312:LEU:HD23	1.86	0.57
1:B:180:MET:HE1	1:B:312:LEU:HD13	1.85	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:C:224:THR:HG23	1:C:232:TYR:HE2	1.70	0.57
1:A:244:MET:HE1	1:A:255:PRO:HG2	1.85	0.57
1:A:657:GLU:HG3	1:A:720:MET:HE1	1.86	0.57
1:B:373:PRO:HB3	1:B:377:VAL:CG2	2.35	0.57
1:C:641:VAL:HG12	1:C:642:ARG:H	1.70	0.57
1:A:4:GLN:HG3	1:A:5:VAL:N	2.20	0.57
1:A:108:PHE:CE2	1:A:499:ASN:HB3	2.39	0.56
1:A:642:ARG:HD2	3:A:884:HOH:O	2.04	0.56
1:B:547:GLN:O	1:B:551:ILE:HG23	2.04	0.56
1:A:180:MET:HE3	1:A:314:LEU:CD2	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ASN:HD22	1:B:449:THR:HG23	1.71	0.56
1:C:252:MET:HE3	1:C:294:PRO:HB3	1.86	0.56
1:C:541:ARG:HB2	3:C:822:HOH:O	2.05	0.56
1:B:249:VAL:C	1:B:251:ASP:H	2.14	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:612:ASP:CG	1:A:613:VAL:H	2.14	0.55
1:A:511:LEU:HD23	1:A:511:LEU:C	2.32	0.55
1:A:4:GLN:HG2	3:A:884:HOH:O	2.05	0.55
1:A:10:ARG:CD	1:A:29:LEU:HD23	2.37	0.55
1:A:249:VAL:O	1:A:250:ALA:CB	2.54	0.55
1:A:657:GLU:HG2	1:A:658:ASN:N	2.17	0.55
1:C:447:ASN:C	1:C:447:ASN:HD22	2.15	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:C:300:MET:HE2	1:C:300:MET:O	2.07	0.55
1:A:319:LEU:CD2	1:A:328:LEU:HB2	2.37	0.55
1:A:733:MET:O	1:A:736:LYS:HB2	2.07	0.55
1:B:249:VAL:O	1:B:250:ALA:HB3	2.06	0.55
1:C:532:VAL:HG12	1:C:532:VAL:O	2.07	0.55
1:A:16:GLU:HB3	1:A:17:PRO:CD	2.35	0.55
1:B:556:ARG:HG3	1:B:569:ILE:HD11	1.89	0.55
1:C:201:LYS:HE3	1:C:272:THR:HG23	1.89	0.55
1:C:54:ILE:O	1:C:504:CYS:HA	2.06	0.54
1:C:716:ARG:HG3	1:C:720:MET:CE	2.35	0.54
1:C:333:ASP:HA	1:C:334:ARG:NH2	2.21	0.54
1:C:415:ASP:O	1:C:418:LYS:HG2	2.06	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: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: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:A:520:LEU:HB3	1:A:524:MET:HE3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:597:THR:HG22	1:B:598:THR:N	2.22	0.53
1:C:90:HIS:CD2	1:C:96:LEU:H	2.21	0.53
1:B:232:TYR:CE1	1:B:243:MET:HE3	2.44	0.53
1:A:399:PHE:O	1:A:400:GLN:HG3	2.09	0.53
1:A:699:ASN:HD22	1:A:701:LEU:H	1.57	0.53
1:C:225:TYR:O	1:C:226:ASN:HB3	2.09	0.53
1:C:234:VAL:HG12	1:C:234:VAL:O	2.09	0.53
1:A:377:VAL:HG12	1:A:377:VAL:O	2.07	0.53
1:B:113:GLU:O	1:B:116:ARG:HG2	2.08	0.53
1:B:147:TYR:O	1:B:148:ASP:HB2	2.09	0.53
1:C:330:ASN:O	1:C:331:ARG:C	2.51	0.53
1:C:653:ILE:HG23	1:C:665:TRP:O	2.08	0.53
1:C:655:LEU:HD23	1:C:656:LEU:N	2.23	0.53
1:C:655:LEU:HD21	1:C:662:LEU:HD22	1.91	0.53
1:B:586:LYS:HD3	1:B:748:GLY:C	2.33	0.53
1:C:234:VAL:HG11	1:C:271:ILE:HG12	1.90	0.53
1:C:608:VAL:HA	1:C:611:MET:HG2	1.91	0.53
1:A:146:ALA:O	1:C:102:LYS:HE3	2.08	0.53
1:A:569:ILE:HG13	1:A:569:ILE:O	2.08	0.53
1:B:522:ASN:HB2	1:B:616:THR:HG21	1.89	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:C:143:ARG:HH11	1:C:152:LEU:HD11	1.73	0.53
1:A:743:LYS:HD2	1:A:750:SER:CB	2.38	0.53
1:B:180:MET:HB2	1:B:314:LEU:HD23	1.90	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:24:GLY:N	3:B:837:HOH:O	2.42	0.52
1:B:366:CYS:HA	1:B:389:THR:CG2	2.39	0.52
1:B:623:ARG:CD	1:B:625:LEU:HD21	2.38	0.52
1:C:369:LEU:HG	1:C:371:LEU:HD22	1.91	0.52
1:A:612:ASP:CG	1:A:613:VAL:N	2.67	0.52
1:B:730:LYS:HG2	1:B:731:MET:H	1.74	0.52
1:C:566:GLY:N	1:C:763:ARG:NH2	2.53	0.52
1:C:626:PRO:HB3	1:C:654:TYR:CE2	2.44	0.52
1:C:68:LEU:HD22	1:C:68:LEU:H	1.73	0.52
1:C:164:ASP:OD2	1:C:164:ASP:N	2.35	0.52
1:C:348:PRO:HB3	1:C:384:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:ARG:O	1:B:533:LEU:HD13	2.10	0.52
1:C:180:MET:HA	1:C:223:VAL:O	2.10	0.52
1:C:568:LEU:HD23	1:C:568:LEU:N	2.21	0.52
1:C:687:ILE:HG22	1:C:688:THR:N	2.23	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:C:401:VAL:HG13	1:C:402:GLU:OE2	2.10	0.52
1:A:516:GLU:HG2	3:A:920:HOH:O	2.08	0.52
1:B:59:ASP:O	1:B:63:GLN:HG2	2.09	0.52
1:B:244:MET:HE3	1:B:255:PRO:HD2	1.92	0.52
1:B:516:GLU:HG2	1:B:519:THR:OG1	2.09	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:B:623:ARG:HH22	1:B:715:GLN:NE2	2.07	0.52
1:A:10:ARG:HG2	1:A:29:LEU:H	1.75	0.51
1:A:249:VAL:HG13	3:A:917:HOH:O	2.09	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: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:A:263:ASN:ND2	1:A:265:ASN:H	2.09	0.51
1:B:228:VAL:HG13	1:B:246:VAL:O	2.11	0.51
1:B:623:ARG:HH12	1:B:715:GLN:NE2	2.07	0.51
1:C:295:VAL:HG11	1:C:314:LEU:HD11	1.92	0.51
1:C:625:LEU:HD13	1:C:625:LEU:N	2.24	0.51
1:A:3:ILE:HG21	1:A:621:TYR:CZ	2.46	0.51
1:B:180:MET:HB2	1:B:314:LEU:CD2	2.40	0.51
1:B:627:LEU:HD11	1:B:655:LEU:HG	1.92	0.51
1:C:385:VAL:N	1:C:386:PRO:HD2	2.24	0.51
1:A:3:ILE:N	1:A:3:ILE:HD13	2.25	0.51
1:B:60:MET:O	1:B:63:GLN:HB2	2.09	0.51
1:B:60:MET:HE1	1:B:506:THR:C	2.36	0.51
1:B:113:GLU:OE1	1:B:117:ARG:HD2	2.11	0.51
1:B:215:GLU:HG3	1:B:265:ASN:ND2	2.26	0.51
1:B:509:ALA:O	1:B:513:ARG:HG3	2.10	0.51
1:C:297:GLN:O	1:C:301:GLU:HB2	2.11	0.51
1:A:544:LEU:C	1:A:544:LEU:HD13	2.36	0.51
1:B:373:PRO:HB3	1:B:377:VAL:HG21	1.91	0.51
1:A:20:THR:HB	1:A:41:ASN:HB2	1.92	0.51
1:C:233:ASN:CG	1:C:259:GLY:HA3	2.36	0.51
1:C:248:ASP:O	1:C:252:MET:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:LYS:HG3	1:C:558:ASN:ND2	2.26	0.51
1:A:50:THR:HB	1:A:520:LEU:CD2	2.41	0.51
1:B:144:VAL:HG11	3:B:835:HOH:O	2.11	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:C:112:ILE:HG23	1:C:113:GLU:N	2.25	0.51
1:B:497:ILE:HD12	1:B:497:ILE:N	2.26	0.50
1:C:45:ARG:HE	1:C:82:GLU:CD	2.19	0.50
1:A:367:VAL:N	1:A:389:THR:HG21	2.12	0.50
1:A:672:GLN:HG3	1:A:682:SER:O	2.11	0.50
1:B:228:VAL:HG12	1:B:229:LEU:N	2.25	0.50
1:C:188:ILE:HD13	1:C:193:VAL:CB	2.41	0.50
1:A:220:VAL:O	1:A:261:LEU:HA	2.11	0.50
1:A:263:ASN:HD22	1:A:266:GLU:H	1.59	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:C:20:THR:HB	1:C:41:ASN:HB2	1.92	0.50
1:C:289:GLU:HG2	1:C:322:ALA:HA	1.92	0.50
1:C:204:LEU:O	1:C:264:VAL:HG11	2.10	0.50
1:B:72:ILE:O	1:B:74:PRO:HD3	2.11	0.50
1:B:623:ARG:HG2	1:B:625:LEU:HD21	1.94	0.50
1:C:238:LEU:C	1:C:240:GLN:N	2.68	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:180:MET:HE3	1:C:312:LEU:HB3	1.92	0.49
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:522:ASN:HD22	1:A:616:THR:CG2	2.24	0.49
1:B:334:ARG:HG2	1:B:334:ARG:HH11	1.76	0.49
1:B:377:VAL:HG12	1:B:377:VAL:O	2.11	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:B:300:MET:HE1	1:B:304:LYS:CE	2.43	0.49
1:A:250:ALA:HA	1:A:325:PRO:CG	2.42	0.49
1:A:625:LEU:HG	1:A:638:PRO:HG2	1.94	0.49
1:B:29:LEU:H	1:B:29:LEU:HD22	1.77	0.49
1:C:311:LYS:HA	1:C:366:CYS:O	2.12	0.49
1:C:662:LEU:HD13	1:C:709:ILE:HG23	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ASN:ND2	1:B:265:ASN:H	2.10	0.49
1:C:289:GLU:CG	1:C:322:ALA:HA	2.42	0.49
1:A:641:VAL:HG12	1:A:642:ARG:N	2.27	0.49
1:B:329:LYS:N	1:B:349:GLN:HE22	1.88	0.49
1:C:398:SER:O	1:C:400:GLN:HG3	2.13	0.49
1:A:4:GLN:HG3	1:A:5:VAL:H	1.78	0.49
1:A:516:GLU:OE2	3:A:820:HOH:O	2.20	0.49
1:C:180:MET:HG2	1:C:223:VAL:HB	1.95	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:257:LEU:O	1:A:259:GLY:N	2.39	0.48
1:C:16:GLU:HB3	1:C:17:PRO:CD	2.42	0.48
1:A:321:ILE:HD13	1:A:321:ILE:H	1.77	0.48
1:A:387:GLN:HB2	1:A:606:GLN:OE1	2.13	0.48
1:A:597:THR:HB	1:A:600:ASP:OD1	2.13	0.48
1:B:470:ASP:CG	1:B:471:ARG:H	2.21	0.48
1:C:60:MET:HE1	1:C:506:THR:C	2.38	0.48
1:A:657:GLU:HG3	1:A:720:MET:SD	2.53	0.48
1:A:632:VAL:O	1:A:632:VAL:HG13	2.13	0.48
1:B:255:PRO:HB2	1:B:257:LEU:CD1	2.43	0.48
1:B:447:ASN:ND2	1:B:449:THR:H	2.12	0.48
1:B:577:LEU:HB3	1:B:578:PRO:HD3	1.94	0.48
1:B:597:THR:CG2	1:B:598:THR:N	2.76	0.48
1:C:44:PRO:HA	1:C:47:ILE:O	2.13	0.48
1:C:213:ALA:C	1:C:215:GLU:H	2.19	0.48
1:C:270:VAL:HG23	3:C:807:HOH:O	2.13	0.48
1:C:415:ASP:HA	1:C:418:LYS:HD2	1.94	0.48
1:C:522:ASN:O	1:C:526:LYS:HG3	2.13	0.48
1:C:557:LYS:HE3	1:C:558:ASN:ND2	2.28	0.48
1:A:533:LEU:HD12	1:A:533:LEU:N	2.28	0.48
1:C:195:LEU:O	1:C:198:GLU:HB2	2.13	0.48
1:C:311:LYS:HG3	1:C:422:PHE:HE1	1.78	0.48
1:C:496:ARG:C	1:C:497:ILE:HD12	2.39	0.48
1:C:656:LEU:HD23	1:C:657:GLU:N	2.29	0.48
1:C:81:GLU:CD	1:C:81:GLU:H	2.22	0.48
1:C:612:ASP:HB3	1:C:615:GLU:HG3	1.96	0.48
1:A:200:LEU:HG	1:A:204:LEU:HD11	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:633:GLU:HG3	1:A:634:SER:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:PRO:C	1:B:133:TYR:H	2.21	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:415:ASP:HA	1:A:418:LYS:CD	2.40	0.48
1:C:149:ARG:HG3	1:C:149:ARG:NH1	2.25	0.48
1:C:293:VAL:HB	1:C:325:PRO:O	2.14	0.48
1:B:180:MET:HE3	1:B:314:LEU:CD2	2.34	0.47
1:B:552:LEU:HB2	1:B:762:ILE:HD11	1.96	0.47
1:A:743:LYS:HD2	1:A:750:SER:HB2	1.95	0.47
1:B:249:VAL:C	1:B:251:ASP:N	2.72	0.47
1:C:268:ARG:HG3	1:C:268:ARG:HH11	1.78	0.47
1:A:461:THR:HG21	1:A:611:MET:O	2.14	0.47
1:A:595:GLU:HB2	3:A:898:HOH:O	2.14	0.47
1:C:557:LYS:HE3	1:C:558:ASN:HD21	1.80	0.47
1:A:59:ASP:O	1:A:63:GLN:HG3	2.15	0.47
1:A:655:LEU:HD23	1:A:663:PHE:O	2.15	0.47
1:B:297:GLN:HG2	1:B:356:LEU:HD13	1.96	0.47
1:C:209:ARG:HH11	1:C:209:ARG:HG2	1.79	0.47
1:C:612:ASP:OD1	1:C:613:VAL:N	2.48	0.47
1:C:756:CYS:C	1:C:758:MET:H	2.21	0.47
1:A:465:GLU:OE2	1:A:467:LYS:HE3	2.15	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:B:246:VAL:HG21	3:B:871:HOH:O	2.14	0.47
1:B:323:GLU:OE1	1:B:327:LYS:HD3	2.14	0.47
1:B:337:ILE:O	1:B:342:GLU:HB2	2.15	0.47
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:120:CYS:O	1:A:124:SER:HA	2.15	0.47
1:A:156:SER:HA	1:A:497:ILE: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:517:THR:OG1	1:A:574:MET:HA	2.15	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:B:657:GLU:CD	1:B:716:ARG:NH1	2.73	0.47
1:C:554:CYS:HA	1:C:557:LYS:HG2	1.96	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:B:23:ARG:HD2	1:B:503:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:GLU:HG3	1:B:720:MET:SD	2.55	0.46
1:C:32:THR:C	1:C:33:ASN:HD22	2.23	0.46
1:C:98:CYS:O	1:C:102:LYS:HA	2.15	0.46
1:A:647:ARG:HA	1:A:647:ARG:HH11	1.80	0.46
1:A:699:ASN:HD21	1:A:702:SER:H	1.62	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:B:88:VAL:HG12	1:B:89:ASP:N	2.30	0.46
1:C:572:GLU:HA	1:C:575:LYS:HE3	1.97	0.46
1:C:625:LEU:HB3	1:C:640:ALA:HA	1.98	0.46
1:A:551:ILE:HG13	1:A:552:LEU:N	2.31	0.46
1:B:182:ASP:OD2	1:B:317:THR:HG23	2.14	0.46
1:B:350:THR:CG2	1:B:351:GLY:N	2.78	0.46
1:C:187:ALA:HB2	1:C:317:THR:HG21	1.97	0.46
1:C:625:LEU:HD13	1:C:625:LEU:H	1.80	0.46
1:B:595:GLU:OE2	1:B:734:LEU:HD21	2.16	0.46
1:B:636:THR:O	1:B:637:GLU:C	2.58	0.46
1:C:204:LEU:HD22	3:C:830:HOH:O	2.15	0.46
1:C:213:ALA:C	1:C:215:GLU:N	2.74	0.46
1:C:267:SER:O	1:C:271:ILE:HG13	2.15	0.46
1:C:275:LEU:HD11	3:C:830:HOH:O	2.15	0.46
1:A:385:VAL:HB	1:A:386:PRO:HD3	1.97	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:C:636:THR:HG22	1:C:637:GLU:N	2.30	0.46
1:A:249:VAL:HG12	1:A:325:PRO:HD2	1.98	0.46
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:B:555:TYR:O	1:B:559:CYS:HB2	2.16	0.46
1:A:2:PRO:HD2	1:A:642:ARG:NH1	2.29	0.46
1:A:627:LEU:CD1	1:A:664:LEU:HD11	2.46	0.46
1:C:81:GLU:CD	1:C:81:GLU:N	2.74	0.46
1:C:112:ILE:CG2	1:C:113:GLU:HG3	2.40	0.46
1:C:368:ASP:OD1	1:C:392:SER:N	2.43	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:556:ARG:CZ	1:A:569:ILE:HG12	2.45	0.46
1:B:145:ASP:OD1	1:B:146:ALA:N	2.49	0.46
1:C:541:ARG:CD	1:C:585:LEU:HD22	2.45	0.46
1:B:138:ASP:OD1	1:B:140:THR:N	2.49	0.45
1:A:447:ASN:ND2	1:A:447:ASN:C	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:2:PRO:C	1:A:3:ILE:CG1	2.89	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:C:15:THR:CA	3:C:831:HOH:O	2.62	0.45
1:A:377:VAL:HG12	1:A:382:LEU:CD1	2.46	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:A:252:MET:O	1:A:253:PHE:CB	2.65	0.45
1:A:323:GLU:O	1:A:324:ALA:HB2	2.17	0.45
1:B:623:ARG:HG2	1:B:625:LEU:CD2	2.47	0.45
1:C:512:TYR:CD2	3:C:823:HOH:O	2.55	0.45
1:A:232:TYR:HE1	1:A:243:MET:HE2	1.79	0.45
1:A:278:ILE:HB	1:A:279:PRO:HD3	1.99	0.45
1:C:6:ILE:HG13	1:C:576:LEU:CD1	2.44	0.45
1:A:90:HIS:CE1	1:A:133:TYR:CZ	3.05	0.45
1:A:634:SER:O	1:A:635:THR:C	2.60	0.45
1:B:326:GLY:O	1:B:327:LYS:C	2.60	0.45
1:C:178:ILE:CG2	1:C:180:MET:HE2	2.46	0.45
1:C:222:PHE:O	1:C:223:VAL:HG23	2.17	0.45
1:C:511:LEU:C	1:C:511:LEU:HD13	2.42	0.45
1:A:557:LYS:HE3	3:A:839:HOH:O	2.16	0.45
1:B:337:ILE:O	1:B:342:GLU:CD	2.60	0.45
1:C:65:GLN:HG3	1:C:550:GLN:CD	2.42	0.45
1:C:224:THR:OG1	1:C:230:HIS:HB2	2.17	0.45
1:C:244:MET:SD	1:C:257:LEU:HD22	2.57	0.45
1:C:656:LEU:HD23	1:C:656:LEU:C	2.42	0.45
1:C:694:LEU:HD23	1:C:706:ARG:HG2	1.98	0.45
1:C:401:VAL:O	1:C:401:VAL:HG22	2.16	0.45
1:C:743:LYS:CG	1:C:750:SER:HB2	2.37	0.45
1:A:10:ARG:CG	1:A:29:LEU:HD23	2.47	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: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:7:GLU:OE2	1:A:31:THR:HG21	2.18	0.44
1:A:727:GLN:O	1:A:727:GLN:HG3	2.16	0.44
1:C:90:HIS:HE1	1:C:151:GLU:OE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASP:C	1:C:138:ASP:OD1	2.60	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:B:337:ILE:N	1:B:337:ILE:HD12	2.32	0.44
1:A:238:LEU:O	1:A:270:VAL:CG2	2.65	0.44
1:B:117:ARG:CA	1:B:129:VAL:HG23	2.48	0.44
1:B:666:VAL:HG13	1:B:670:VAL:HG21	1.99	0.44
1:C:300:MET:HE2	1:C:301:GLU:HA	1.98	0.44
1:C:642:ARG:HG3	1:C:741:GLU:OE2	2.17	0.44
1:A:533:LEU:HD11	1:A:605:ARG:CZ	2.48	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:C:541:ARG:HH11	1:C:541:ARG:HG2	1.82	0.44
1:A:175:PRO:HG2	1:A:218:ILE:CD1	2.47	0.44
1:A:533:LEU:HD11	1:A:605:ARG:NH2	2.33	0.44
1:B:632:VAL:HG12	1:B:635:THR:HG23	2.00	0.44
1:A:6:ILE:HG13	1:A:576:LEU:HD11	1.99	0.44
1:A:180:MET:CE	1:A:312:LEU:HB3	2.41	0.44
1:B:511:LEU:HD13	1:B:511:LEU:C	2.43	0.44
1:B:625:LEU:HD12	1:B:638:PRO:O	2.18	0.44
1:C:143:ARG:CG	1:C:145:ASP:OD1	2.66	0.44
1:C:559:CYS:SG	3:C:823:HOH:O	2.60	0.44
1:B:41:ASN:N	1:B:41:ASN:ND2	2.58	0.44
1:B:371:LEU:C	1:B:373:PRO:HD3	2.43	0.44
1:C:10:ARG:HG2	1:C:29:LEU:HG	2.00	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:C:252:MET:HE2	1:C:252:MET:HA	2.00	0.44
1:C:407:ARG:HA	1:C:719:TYR:CD2	2.53	0.44
1:A:220:VAL:HG12	1:A:221:GLY:N	2.33	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:C:386:PRO:CA	1:C:389:THR:HG22	2.47	0.44
1:C:758:MET:O	1:C:762:ILE:HG13	2.18	0.44
1:B:175:PRO:HG3	1:B:422:PHE:CE2	2.53	0.43
1:C:387:GLN:CB	1:C:606:GLN:HE22	2.26	0.43
1:C:389:THR:O	1:C:454:ALA:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:568:LEU:HD23	1:A:568:LEU:H	1.82	0.43
1:B:634:SER:C	1:B:636:THR:H	2.26	0.43
1:C:233:ASN:ND2	1:C:259:GLY:HA3	2.33	0.43
1:B:612:ASP:CB	1:B:615:GLU:HG3	2.48	0.43
1:B:106:CYS:HB2	1:B:107:PRO:CD	2.49	0.43
1:B:475:GLU:HG3	1:B:476:SER:N	2.34	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:A:46:TYR:OH	1:A:78:LEU:HD11	2.19	0.43
1:A:231:PHE:CZ	1:A:298:ALA:HB1	2.39	0.43
1:A:419:VAL:HG13	3:A:853:HOH:O	2.18	0.43
1:B:23:ARG:C	3:B:837:HOH:O	2.61	0.43
1:B:72:ILE:C	1:B:74:PRO:HD3	2.44	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:2:PRO:O	1:A:4:GLN:HG2	2.18	0.43
1:A:750:SER:O	1:A:751:TYR:C	2.62	0.43
1:B:591:GLN:NE2	1:B:748:GLY:HA2	2.33	0.43
1:B:604:VAL:O	1:B:608:VAL:HG23	2.19	0.43
1:A:244:MET:HE3	1:A:257:LEU:HD22	1.99	0.43
1:A:533:LEU:N	1:A:533:LEU:CD1	2.82	0.43
1:C:367:VAL:H	1:C:389:THR:HG21	1.84	0.43
1:A:112:ILE:HG13	1:A:113:GLU:HG3	2.00	0.43
1:A:730:LYS:C	1:A:732:GLU:H	2.26	0.43
1:B:556:ARG:CD	1:B:569:ILE:HD11	2.48	0.43
1:A:36:VAL:HG11	1:A:43:SER:HB2	2.00	0.43
1:A:300:MET:HE2	1:A:300:MET:C	2.43	0.43
1:A:533:LEU:HD11	1:A:605:ARG:HH21	1.83	0.43
1:A:623:ARG:HG2	1:A:625:LEU:HD13	2.00	0.43
1:B:135:GLN:HB3	1:B:142:LYS:CE	2.43	0.43
1:C:6:ILE:HG22	1:C:29:LEU:HD11	2.01	0.43
1:C:334:ARG:HA	1:C:337:ILE:HD12	2.01	0.43
1:C:471:ARG:HB2	1:C:471:ARG:NH1	2.34	0.43
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:638:PRO:HA	1:B:639:PRO:HD2	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ARG:HG3	1:C:268:ARG:NH1	2.34	0.42
1:C:274:LEU:HD11	1:C:278:ILE:HD11	2.00	0.42
1:C:439:PHE:CE2	1:C:445:MET:HE1	2.53	0.42
1:C:494:ARG:NE	3:C:801:HOH:O	2.51	0.42
1:C:566:GLY:N	1:C:763:ARG:NH1	2.66	0.42
1:A:16:GLU:HG3	3:A:874:HOH:O	2.18	0.42
1:A:182:ASP:OD1	1:A:182:ASP:C	2.62	0.42
1:A:402:GLU:CD	1:A:402:GLU:H	2.26	0.42
1:C:117:ARG:HG2	1:C:128:ASP:HA	2.00	0.42
1:C:265:ASN:N	1:C:265:ASN:ND2	2.63	0.42
1:C:611:MET:HB2	1:C:615:GLU:CB	2.46	0.42
1:A:544:LEU:CD1	1:A:581:LEU:HD11	2.50	0.42
1:B:334:ARG:HA	1:B:337:ILE:CD1	2.49	0.42
1:B:385:VAL:N	1:B:386:PRO:HD2	2.34	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:C:297:GLN:NE2	3:C:834:HOH:O	2.53	0.42
1:A:366:CYS:HA	1:A:389:THR:CG2	2.49	0.42
1:B:372:PHE:N	1:B:373:PRO:HD3	2.34	0.42
1:C:151:GLU:HA	1:C:157:TYR:CE2	2.54	0.42
1:C:350:THR:HG22	1:C:352:ALA:H	1.85	0.42
1:A:106:CYS:HB2	1:A:107:PRO:CD	2.49	0.42
1:B:319:LEU:HD11	1:B:328:LEU:HB2	2.02	0.42
1:B:613:VAL:HA	1:B:616:THR:HG22	2.00	0.42
1:B:716:ARG:HD3	1:B:716:ARG:HA	1.83	0.42
1:C:137:LEU:O	1:C:144:VAL:HB	2.19	0.42
1:C:380:ALA:O	1:C:384:VAL:HG23	2.19	0.42
1:C:538:LYS:O	1:C:538:LYS:HD3	2.19	0.42
1:B:187:ALA:HB2	1:B:317:THR:HG21	2.02	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:B:704:LYS:NZ	3:B:833:HOH:O	2.53	0.42
1:C:106:CYS:HB2	1:C:107:PRO:CD	2.49	0.42
1:C:207:LEU:O	1:C:209:ARG:NE	2.51	0.42
1:C:642:ARG:NH1	1:C:741:GLU:OE1	2.52	0.42
1:A:4:GLN:HG3	1:A:5:VAL:HG13	2.02	0.42
1:A:135:GLN:HG3	1:C:99:ASN:HB2	2.02	0.42
1:A:443:PHE:CD1	1:A:443:PHE:C	2.98	0.42
1:A:632:VAL:O	1:A:633:GLU:C	2.63	0.42
1:B:255:PRO:HB2	1:B:257:LEU:HD11	2.02	0.42
1:B:479:LEU:HD23	1:B:501:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:GLN:HG3	1:B:682:SER:O	2.19	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:A:130:PRO:HB2	1:A:133:TYR:HB2	2.02	0.42
1:B:90:HIS:CD2	1:B:95:PRO:HA	2.54	0.42
1:B:166:CYS:SG	1:B:493:ARG:HG2	2.60	0.42
1:B:373:PRO:HB3	1:B:377:VAL:HG23	2.01	0.42
1:B:522:ASN:HD22	1:B:616:THR:HG21	1.85	0.42
1:A:35:LEU:HD21	3:C:806:HOH:O	2.18	0.41
1:A:149:ARG:HG3	3:C:818:HOH:O	2.20	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:B:482:CYS:O	1:B:497:ILE:HA	2.20	0.41
1:C:180:MET:CE	1:C:312:LEU:HB3	2.50	0.41
1:C:295:VAL:O	1:C:298:ALA:HB3	2.19	0.41
1:A:335:LYS:O	1:A:335:LYS:HG3	2.21	0.41
1:A:474:GLU:HA	1:A:504:CYS:HB2	2.01	0.41
1:A:657:GLU:HG3	1:A:720:MET:CE	2.49	0.41
1:B:210:GLU:OE2	1:B:488:SER:HB2	2.20	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:A:90:HIS:CE1	1:A:137:LEU:CD1	3.03	0.41
1:B:336:LEU:O	1:B:342:GLU:HB2	2.21	0.41
1:B:433:GLY:C	1:B:469:ASP:OD1	2.64	0.41
1:C:73:LYS:HD2	1:C:76:ALA:HB2	2.02	0.41
1:C:316:HIS:NE2	1:C:318:SER:O	2.53	0.41
1:A:73:LYS:HE2	1:A:458:GLY:O	2.21	0.41
1:A:461:THR:HG22	1:A:610:SER:C	2.45	0.41
1:A:626:PRO:HA	1:A:654:TYR:CD2	2.55	0.41
1:B:102:LYS:HE2	1:B:102:LYS:HB3	1.93	0.41
1:B:180:MET:HA	1:B:223:VAL:O	2.21	0.41
1:B:755:LEU:HA	1:B:755:LEU:HD23	1.86	0.41
1:C:165:TYR:CE1	1:C:495:LEU:HD11	2.55	0.41
1:A:2:PRO:O	1:A:4:GLN:N	2.54	0.41
1:B:168:ASN:O	1:B:169:ASN:C	2.64	0.41
1:B:263:ASN:HD22	1:B:265:ASN:N	2.19	0.41
1:B:656:LEU:C	1:B:656:LEU:HD23	2.45	0.41
1:B:756:CYS:SG	1:B:760:LYS:HE3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:VAL:HG12	1:C:5:VAL:O	2.20	0.41
1:A:257:LEU:C	1:A:259:GLY:H	2.28	0.41
1:B:138:ASP:C	1:B:140:THR:N	2.77	0.41
1:C:387:GLN:OE1	1:C:606:GLN:NE2	2.54	0.41
1:C:497:ILE:N	1:C:497:ILE:CD1	2.84	0.41
1:C:517:THR:OG1	1:C:574:MET:HA	2.21	0.41
1:A:4:GLN:CG	1:A:5:VAL:N	2.84	0.41
1:A:15:THR:O	1:A:15:THR:HG22	2.21	0.41
1:B:244:MET:CE	1:B:255:PRO:HD2	2.51	0.41
1:B:469:ASP:CG	3:B:836:HOH:O	2.63	0.41
1:C:17:PRO:HA	1:C:35:LEU:O	2.21	0.41
1:A:484:LEU:O	1:A:495:LEU:HA	2.21	0.41
1:A:632:VAL:CG1	1:A:635:THR:HB	2.51	0.41
1:B:151:GLU:OE1	1:B:151:GLU:N	2.53	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: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:B:568:LEU:HD12	1:B:568:LEU:C	2.45	0.41
1:B:591:GLN:HE21	1:B:748:GLY:HA2	1.84	0.41
1:C:264:VAL:HG12	1:C:268:ARG:NH2	2.36	0.41
1:C:370:PHE:CE1	1:C:394:TYR:CD2	3.09	0.41
1:C:556:ARG:HG3	1:C:569:ILE:HD11	2.03	0.41
1:C:606:GLN:C	1:C:609:THR:HG22	2.46	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: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:C:259:GLY:O	1:C:262:VAL:HG13	2.21	0.41
1:C:531:GLY:C	1:C:533:LEU:H	2.29	0.41
1:A:249:VAL:HG12	1:A:325:PRO:CD	2.51	0.40
1:A:623:ARG:HH12	1:A:715:GLN:NE2	2.19	0.40
1:B:533:LEU:CD1	1:B:605:ARG:HE	2.20	0.40
1:C:167:LYS:NZ	1:C:362:ALA:O	2.46	0.40
1:C:686:GLN:HG2	1:C:726:LYS:NZ	2.35	0.40
1:A:319:LEU:HD23	1:A:320:PRO:CD	2.46	0.40
1:B:180:MET:HE2	1:B:312:LEU:HD13	1.99	0.40
1:B:637:GLU:HA	1:B:638:PRO:HD2	1.91	0.40
1:B:657:GLU:HG2	1:B:659:GLY:H	1.86	0.40
1:C:576:LEU:HB3	1:C:580:TYR:CE2	2.56	0.40
1:B:68:LEU:HD22	1:B:68:LEU:H	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:VAL:N	1:B:294:PRO:CD	2.84	0.40
1:B:300:MET:HE3	1:B:363:GLN:HG3	2.03	0.40
1:B:533:LEU:N	1:B:533:LEU:HD12	2.36	0.40
1:B:555:TYR:CZ	1:B:571:PRO:HB3	2.56	0.40
1:C:112:ILE:CG2	1:C:113:GLU:N	2.83	0.40
1:C:252:MET:CE	1:C:294:PRO:HB3	2.49	0.40
1:C:289:GLU:HG2	1:C:322:ALA:CB	2.52	0.40
1:C:497:ILE:HD12	1:C:497:ILE:N	2.36	0.40
1:A:496:ARG:C	1:A:497:ILE:HD12	2.47	0.40
1:A:533:LEU:HD21	1:A:605:ARG:NH2	2.35	0.40
1:A:626:PRO:HB3	1:A:654:TYR:CE2	2.56	0.40
1:A:656:LEU:C	1:A:656:LEU:HD23	2.46	0.40
1:B:108:PHE:O	1:B:121:CYS:HB3	2.22	0.40
1:B:249:VAL:CG1	1:B:250:ALA:H	2.07	0.40
1:B:343:LYS:CD	1:B:347:GLN:HE22	2.34	0.40
1:C:8:ASP:O	1:C:11:ASN:HB2	2.22	0.40
1:A:46:TYR:CG	1:A:498:HIS:CE1	3.10	0.40
1:A:678:LEU:HD13	1:A:678:LEU:O	2.22	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%)	7	6
1	B	733/766 (96%)	673 (92%)	40 (6%)	20 (3%)	4	2
1	C	729/766 (95%)	626 (86%)	79 (11%)	24 (3%)	3	1
All	All	2214/2298 (96%)	2004 (90%)	153 (7%)	57 (3%)	4	2

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
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%)	633 (95%)	34 (5%)	21	26
1	B	650/673 (97%)	611 (94%)	39 (6%)	17	21
1	C	649/673 (96%)	622 (96%)	27 (4%)	26	35
All	All	1966/2019 (97%)	1866 (95%)	100 (5%)	21	26

All (100) 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	339	THR
1	A	371	LEU
1	A	389	THR
1	A	395	LYS
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	716	ARG
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	73	LYS
1	B	90	HIS
1	B	110	GLN
1	B	145	ASP
1	B	200	LEU
1	B	204	LEU
1	B	252	MET
1	B	263	ASN
1	B	287	GLU
1	B	300	MET
1	B	318	SER
1	B	319	LEU

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Mol	Chain	Res	Type
1	B	367	VAL
1	B	371	LEU
1	B	389	THR
1	B	419	VAL
1	B	438	ASP
1	B	449	THR
1	B	461	THR
1	B	475	GLU
1	B	544	LEU
1	B	569	ILE
1	B	579	VAL
1	B	591	GLN
1	B	625	LEU
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	68	LEU
1	C	90	HIS
1	C	110	GLN
1	C	112	ILE
1	C	139	HIS
1	C	143	ARG
1	C	144	VAL
1	C	149	ARG
1	C	164	ASP
1	C	256	LEU
1	C	300	MET
1	C	321	ILE
1	C	331	ARG
1	C	392	SER
1	C	429	ARG
1	C	447	ASN
1	C	497	ILE
1	C	579	VAL
1	C	610	SER

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Mol	Chain	Res	Type
1	C	616	THR
1	C	625	LEU
1	C	638	PRO
1	C	641	VAL
1	C	642	ARG
1	C	716	ARG
1	C	743	LYS
1	C	755	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
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	374	ASN
1	A	400	GLN
1	A	447	ASN
1	A	507	GLN
1	A	550	GLN
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	39	GLN
1	B	41	ASN
1	B	53	ASN
1	B	90	HIS
1	B	119	GLN
1	B	242	GLN
1	B	263	ASN
1	B	338	ASN
1	B	347	GLN
1	B	349	GLN
1	B	363	GLN
1	B	387	GLN

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Mol	Chain	Res	Type
1	B	400	GLN
1	B	405	GLN
1	B	417	GLN
1	B	492	GLN
1	B	507	GLN
1	B	550	GLN
1	B	606	GLN
1	B	672	GLN
1	B	699	ASN
1	B	715	GLN
1	C	33	ASN
1	C	90	HIS
1	C	119	GLN
1	C	139	HIS
1	C	169	ASN
1	C	230	HIS
1	C	240	GLN
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	405	GLN
1	C	417	GLN
1	C	447	ASN
1	C	492	GLN
1	C	547	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 [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](#)

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%)	0.19	46 (6%) 27 31	13, 29, 65, 105	0
1	B	738/766 (96%)	0.61	80 (10%) 11 12	20, 40, 79, 104	0
1	C	732/766 (95%)	1.57	273 (37%) 1 0	22, 64, 98, 111	0
All	All	2228/2298 (96%)	0.78	399 (17%) 3 4	13, 41, 91, 111	0

All (399) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	LEU	6.8
1	A	257	LEU	6.7
1	B	568	LEU	6.6
1	B	147	TYR	6.5
1	B	566	GLY	6.4
1	B	146	ALA	6.2
1	C	288	THR	6.2
1	C	566	GLY	6.2
1	A	568	LEU	6.2
1	C	697	LEU	5.9
1	A	729	ASP	5.4
1	C	371	LEU	5.3
1	C	250	ALA	5.3
1	C	668	ALA	5.2
1	C	282	PHE	5.2
1	B	632	VAL	5.2
1	C	696	VAL	5.2
1	C	568	LEU	5.0
1	C	275	LEU	4.8
1	A	5	VAL	4.8
1	B	729	ASP	4.7
1	C	701	LEU	4.7
1	C	256	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	144	VAL	4.6
1	A	631	PRO	4.6
1	B	749	ALA	4.6
1	C	567	GLN	4.5
1	C	253	PHE	4.5
1	C	137	LEU	4.4
1	C	628	THR	4.4
1	C	372	PHE	4.4
1	C	257	LEU	4.4
1	A	2	PRO	4.3
1	C	245	VAL	4.3
1	C	635	THR	4.3
1	C	403	ASN	4.2
1	B	131	PRO	4.2
1	C	594	ALA	4.2
1	C	734	LEU	4.2
1	C	755	LEU	4.2
1	C	259	GLY	4.1
1	B	764	GLN	4.1
1	C	693	VAL	4.1
1	B	256	LEU	4.1
1	A	258	ASP	4.1
1	A	254	VAL	4.1
1	A	632	VAL	4.1
1	C	602	ALA	4.1
1	C	178	ILE	4.1
1	C	249	VAL	4.1
1	C	655	LEU	4.0
1	C	719	TYR	4.0
1	A	250	ALA	4.0
1	C	345	LEU	4.0
1	C	705	VAL	4.0
1	C	261	LEU	4.0
1	C	745	LEU	3.9
1	C	692	SER	3.9
1	B	145	ASP	3.9
1	C	737	HIS	3.9
1	A	749	ALA	3.9
1	C	239	ALA	3.9
1	C	749	ALA	3.9
1	C	231	PHE	3.9
1	C	592	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	336	LEU	3.8
1	C	138	ASP	3.8
1	C	264	VAL	3.8
1	C	401	VAL	3.8
1	C	725	VAL	3.8
1	C	551	ILE	3.8
1	A	6	ILE	3.7
1	A	629	LYS	3.7
1	A	635	THR	3.7
1	C	15	THR	3.7
1	C	689	SER	3.7
1	C	408	PHE	3.7
1	C	728	GLU	3.7
1	B	139	HIS	3.7
1	C	322	ALA	3.7
1	B	730	LYS	3.7
1	C	326	GLY	3.6
1	C	236	SER	3.6
1	B	567	GLN	3.6
1	C	271	ILE	3.6
1	C	254	VAL	3.6
1	A	638	PRO	3.6
1	C	4	GLN	3.6
1	C	206	PHE	3.6
1	C	687	ILE	3.6
1	A	7	GLU	3.6
1	B	569	ILE	3.6
1	A	566	GLY	3.5
1	C	211	GLY	3.5
1	A	15	THR	3.5
1	C	598	THR	3.5
1	C	746	SER	3.5
1	C	665	TRP	3.5
1	B	148	ASP	3.5
1	C	292	PHE	3.5
1	C	601	ARG	3.5
1	B	559	CYS	3.5
1	B	337	ILE	3.5
1	C	760	LYS	3.4
1	B	249	VAL	3.4
1	C	374	ASN	3.4
1	B	254	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	686	GLN	3.4
1	C	225	TYR	3.4
1	A	141	GLY	3.4
1	C	197	CYS	3.4
1	A	733	MET	3.3
1	C	278	ILE	3.3
1	A	252	MET	3.3
1	B	731	MET	3.3
1	C	180	MET	3.3
1	C	695	PRO	3.3
1	C	187	ALA	3.3
1	B	141	GLY	3.3
1	C	317	THR	3.3
1	C	726	LYS	3.3
1	B	99	ASN	3.3
1	C	469	ASP	3.3
1	C	722	LEU	3.3
1	C	575	LYS	3.3
1	C	270	VAL	3.3
1	C	213	ALA	3.2
1	A	630	SER	3.2
1	C	666	VAL	3.2
1	C	724	VAL	3.2
1	C	704	LYS	3.2
1	C	320	PRO	3.2
1	B	363	GLN	3.2
1	C	738	PHE	3.2
1	B	743	LYS	3.1
1	C	757	HIS	3.1
1	C	369	LEU	3.1
1	C	181	ILE	3.1
1	C	344	THR	3.1
1	C	398	SER	3.1
1	B	169	ASN	3.1
1	C	5	VAL	3.1
1	C	752	VAL	3.1
1	A	745	LEU	3.1
1	C	691	LEU	3.1
1	C	663	PHE	3.1
1	C	193	VAL	3.1
1	C	373	PRO	3.1
1	C	700	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	629	LYS	3.1
1	C	244	MET	3.1
1	A	337	ILE	3.1
1	C	688	THR	3.1
1	C	699	ASN	3.1
1	A	249	VAL	3.1
1	C	596	VAL	3.1
1	C	232	TYR	3.0
1	B	140	THR	3.0
1	A	255	PRO	3.0
1	A	550	GLN	3.0
1	C	226	ASN	3.0
1	C	588	ASP	3.0
1	C	667	GLY	3.0
1	C	625	LEU	3.0
1	A	3	ILE	3.0
1	C	252	MET	3.0
1	C	733	MET	3.0
1	B	633	GLU	3.0
1	C	385	VAL	3.0
1	A	728	GLU	3.0
1	B	253	PHE	2.9
1	C	188	ILE	2.9
1	C	569	ILE	2.9
1	B	15	THR	2.9
1	C	627	LEU	2.9
1	C	227	LYS	2.9
1	C	723	THR	2.9
1	C	14	GLY	2.9
1	C	593	GLY	2.9
1	C	260	PHE	2.9
1	C	281	MET	2.9
1	C	634	SER	2.9
1	A	14	GLY	2.9
1	C	258	ASP	2.9
1	C	139	HIS	2.9
1	C	195	LEU	2.9
1	C	203	LEU	2.9
1	C	269	ALA	2.9
1	C	314	LEU	2.9
1	A	338	ASN	2.9
1	B	252	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	729	ASP	2.8
1	B	631	PRO	2.8
1	C	255	PRO	2.8
1	C	765	LEU	2.8
1	A	253	PHE	2.8
1	A	633	GLU	2.8
1	C	291	VAL	2.8
1	C	224	THR	2.8
1	C	331	ARG	2.8
1	C	762	ILE	2.8
1	B	124	SER	2.8
1	A	238	LEU	2.8
1	C	664	LEU	2.8
1	C	246	VAL	2.8
1	B	635	THR	2.8
1	C	191	GLY	2.8
1	C	241	PRO	2.8
1	C	590	LEU	2.8
1	C	324	ALA	2.8
1	B	143	ARG	2.8
1	C	116	ARG	2.8
1	C	190	THR	2.7
1	C	276	ASP	2.7
1	C	199	GLU	2.7
1	C	572	GLU	2.7
1	C	708	LEU	2.7
1	C	185	TYR	2.7
1	C	302	ALA	2.7
1	C	352	ALA	2.7
1	C	346	PHE	2.7
1	C	237	SER	2.7
1	C	342	GLU	2.7
1	C	228	VAL	2.7
1	C	6	ILE	2.7
1	C	218	ILE	2.7
1	C	649	SER	2.7
1	C	204	LEU	2.7
1	C	298	ALA	2.7
1	C	397	ALA	2.7
1	C	643	ALA	2.7
1	C	654	TYR	2.7
1	A	140	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	612	ASP	2.7
1	C	265	ASN	2.7
1	B	212	GLY	2.7
1	C	229	LEU	2.7
1	B	594	ALA	2.6
1	C	251	ASP	2.6
1	C	290	THR	2.6
1	C	748	GLY	2.6
1	C	318	SER	2.6
1	B	56	CYS	2.6
1	B	765	LEU	2.6
1	B	475	GLU	2.6
1	A	10	ARG	2.6
1	B	133	TYR	2.6
1	C	335	LYS	2.6
1	C	703	LYS	2.6
1	C	177	PHE	2.6
1	C	262	VAL	2.6
1	C	694	LEU	2.6
1	B	214	GLU	2.6
1	C	637	GLU	2.6
1	C	640	ALA	2.6
1	C	12	ASN	2.6
1	C	599	ASP	2.6
1	B	748	GLY	2.6
1	C	377	VAL	2.6
1	C	393	VAL	2.6
1	C	230	HIS	2.6
1	A	16	GLU	2.5
1	C	192	LEU	2.5
1	B	116	ARG	2.5
1	C	559	CYS	2.5
1	C	399	PHE	2.5
1	B	136	HIS	2.5
1	B	630	SER	2.5
1	C	744	SER	2.5
1	B	533	LEU	2.5
1	C	238	LEU	2.5
1	A	612	ASP	2.5
1	C	263	ASN	2.5
1	C	639	PRO	2.5
1	C	293	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	334	ARG	2.5
1	A	11	ASN	2.5
1	C	747	GLY	2.5
1	C	240	GLN	2.5
1	C	13	ARG	2.5
1	C	375	GLN	2.5
1	C	536	PRO	2.5
1	C	10	ARG	2.4
1	C	339	THR	2.4
1	C	597	THR	2.4
1	C	267	SER	2.4
1	C	404	ASP	2.4
1	C	380	ALA	2.4
1	C	7	GLU	2.4
1	C	605	ARG	2.4
1	C	235	LYS	2.4
1	C	524	MET	2.4
1	B	257	LEU	2.4
1	C	396	TYR	2.4
1	A	334	ARG	2.4
1	B	100	ARG	2.4
1	C	205	ASP	2.4
1	C	350	THR	2.4
1	B	634	SER	2.4
1	C	328	LEU	2.4
1	C	333	ASP	2.4
1	C	742	ASP	2.4
1	C	690	GLY	2.4
1	B	551	ILE	2.4
1	C	179	PHE	2.4
1	C	353	TYR	2.3
1	C	612	ASP	2.3
1	C	736	LYS	2.3
1	B	472	LEU	2.3
1	C	363	GLN	2.3
1	C	382	LEU	2.3
1	B	638	PRO	2.3
1	C	86	TYR	2.3
1	C	407	ARG	2.3
1	C	379	VAL	2.3
1	C	727	GLN	2.3
1	B	554	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	274	LEU	2.3
1	C	248	ASP	2.3
1	C	332	ASP	2.3
1	C	378	ASP	2.3
1	C	279	PRO	2.3
1	C	272	THR	2.3
1	B	637	GLU	2.3
1	C	400	GLN	2.3
1	C	405	GLN	2.3
1	C	527	PHE	2.3
1	C	756	CYS	2.3
1	B	86	TYR	2.3
1	C	541	ARG	2.3
1	B	242	GLN	2.3
1	C	740	VAL	2.3
1	C	376	TYR	2.2
1	C	557	LYS	2.2
1	C	653	ILE	2.2
1	C	754	PHE	2.2
1	A	639	PRO	2.2
1	C	243	MET	2.2
1	C	327	LYS	2.2
1	B	152	LEU	2.2
1	B	345	LEU	2.2
1	B	766	LEU	2.2
1	C	409	LEU	2.2
1	C	9	ASP	2.2
1	C	698	ASP	2.2
1	B	747	GLY	2.2
1	B	557	LYS	2.2
1	C	636	THR	2.2
1	C	645	GLU	2.2
1	C	550	GLN	2.2
1	A	504	CYS	2.2
1	B	446	SER	2.2
1	C	268	ARG	2.1
1	C	412	LEU	2.1
1	C	660	LEU	2.1
1	C	662	LEU	2.1
1	C	419	VAL	2.1
1	C	650	ASN	2.1
1	C	731	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	531	GLY	2.1
1	C	217	ALA	2.1
1	C	394	TYR	2.1
1	C	648	LEU	2.1
1	C	739	LEU	2.1
1	A	251	ASP	2.1
1	B	164	ASP	2.1
1	B	233	ASN	2.1
1	B	248	ASP	2.1
1	C	330	ASN	2.1
1	C	474	GLU	2.1
1	C	606	GLN	2.1
1	B	250	ALA	2.1
1	B	374	ASN	2.1
1	B	473	ASN	2.1
1	C	321	ILE	2.1
1	C	277	GLN	2.1
1	C	349	GLN	2.1
1	B	17	PRO	2.1
1	B	114	GLY	2.1
1	A	634	SER	2.1
1	C	767	SER	2.1
1	C	266	GLU	2.1
1	C	633	GLU	2.1
1	B	137	LEU	2.1
1	C	200	LEU	2.1
1	C	591	GLN	2.1
1	C	147	TYR	2.1
1	B	763	ARG	2.1
1	A	730	LYS	2.0
1	C	280	GLU	2.0
1	B	745	LEU	2.0
1	C	303	LEU	2.0
1	C	183	VAL	2.0
1	C	537	VAL	2.0
1	B	134	PHE	2.0
1	B	671	GLN	2.0
1	C	207	LEU	2.0
1	C	413	ARG	2.0
1	C	743	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	800	1/1	0.97	0.05	27,27,27,27	0
2	ZN	B	800	1/1	1.00	0.01	40,40,40,40	0
2	ZN	C	800	1/1	1.00	0.01	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.