



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:59 PM UTC

PDB ID : 1JSW / pdb_00001jsw
Title : NATIVE L-ASPARTATE AMMONIA LYASE
Authors : Shi, W.; Dunbar, J.; Farber, G.K.
Deposited on : 1997-02-19
Resolution : 2.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

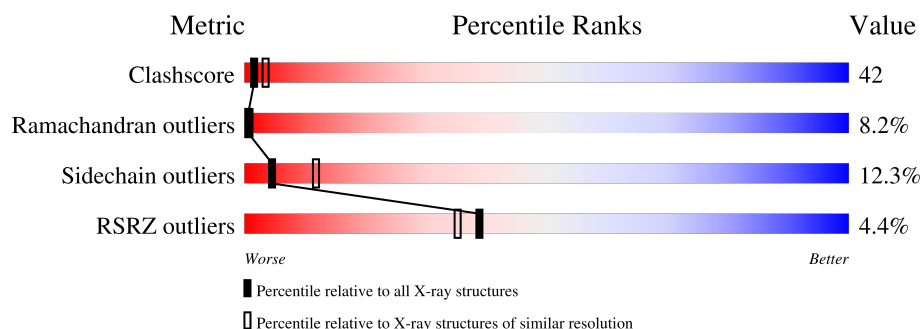
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	478	
1	B	478	
1	C	478	
1	D	478	

2 Entry composition [i](#)

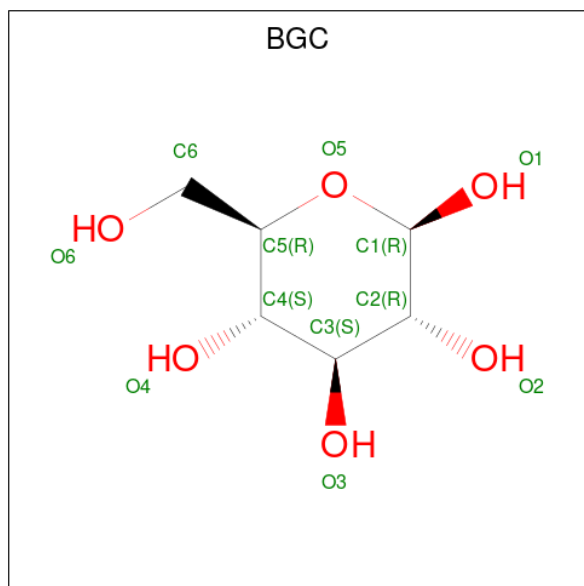
There are 4 unique types of molecules in this entry. The entry contains 13764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-ASPARTATE AMMONIA-LYASE.

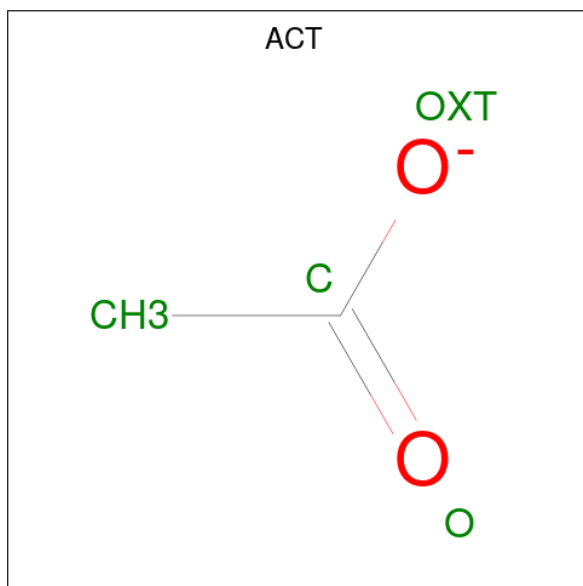
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3502	2205	595	676	26			
1	B	460	Total	C	N	O	S	0	0	0
			3511	2210	597	678	26			
1	C	413	Total	C	N	O	S	0	0	0
			3152	1988	534	606	24			
1	D	459	Total	C	N	O	S	0	0	0
			3502	2205	595	676	26			

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

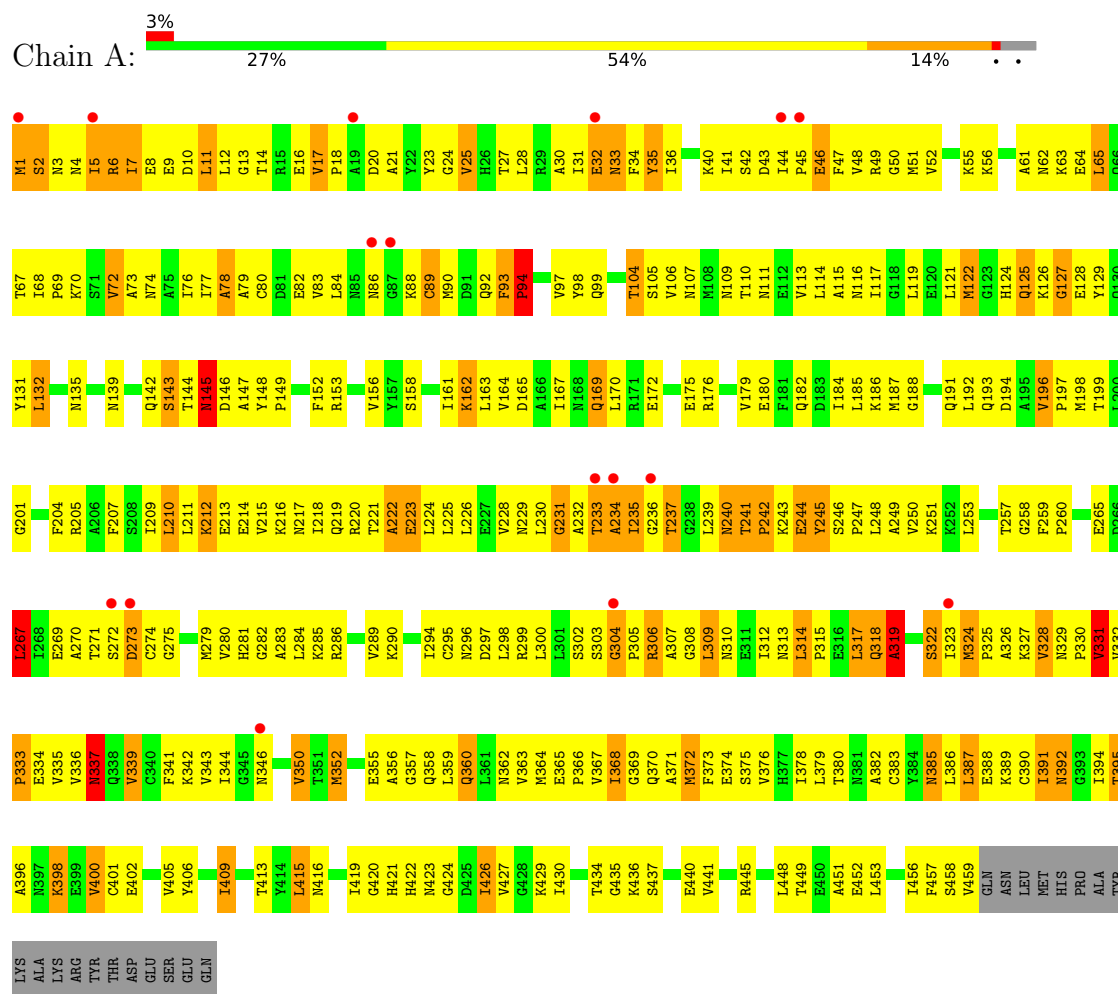
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	16	Total	O	0	0
			16	16		
4	C	11	Total	O	0	0
			11	11		
4	D	23	Total	O	0	0
			23	23		

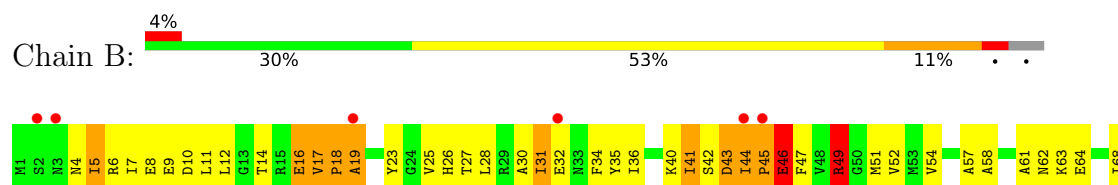
3 Residue-property plots

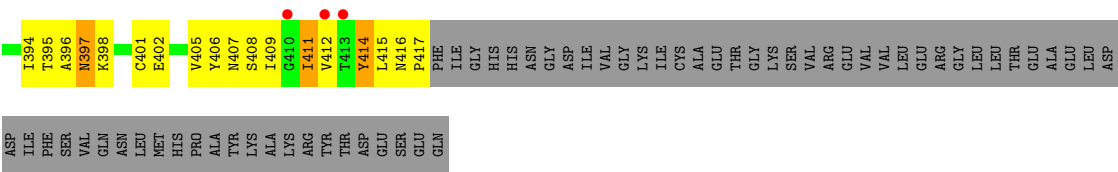
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: L-ASPARTATE AMMONIA-LYASE

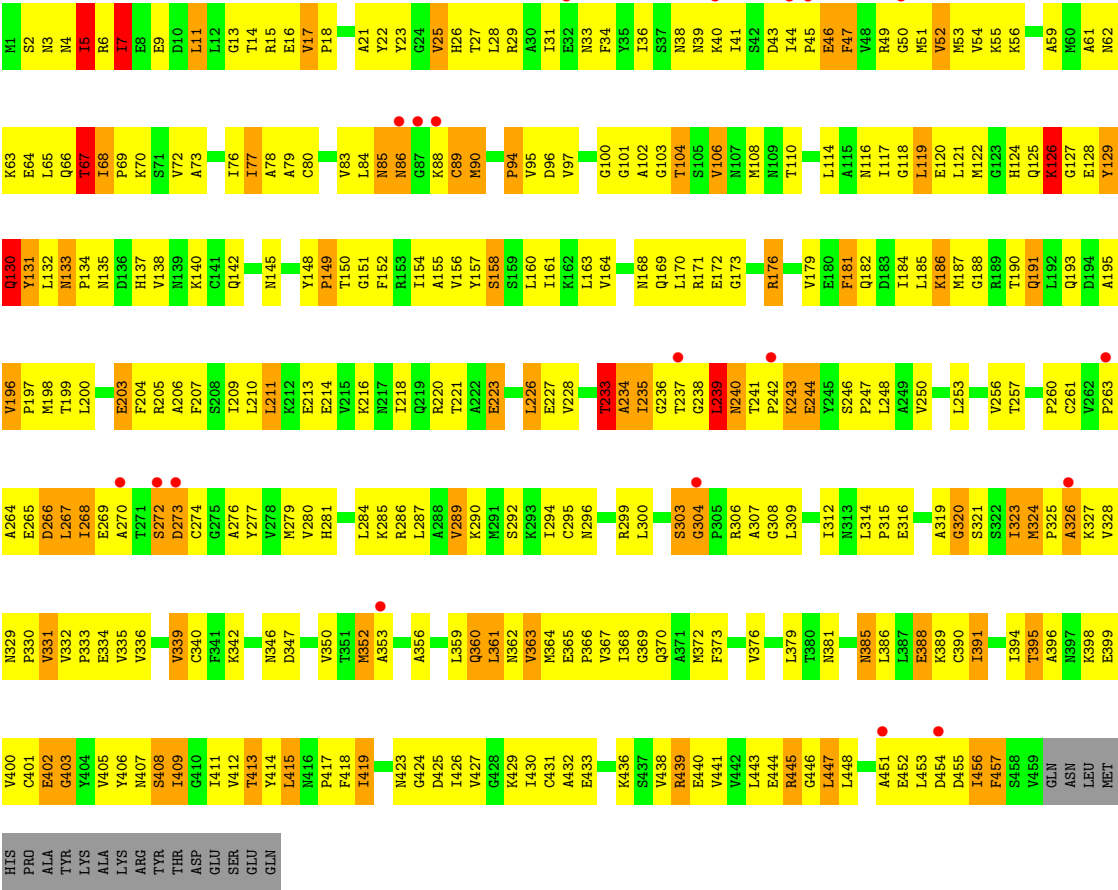


• Molecule 1: L-ASPARTATE AMMONIA-LYASE





● Molecule 1: L-ASPARTATE AMMONIA-LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.50Å 146.20Å 103.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 73.5 (10.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.216 , 0.371 0.256 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13764	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: BGC, ACT

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	0.61	0/3553	1.22	35/4815 (0.7%)
1	B	0.60	0/3562	1.21	32/4827 (0.7%)
1	C	0.60	0/3199	1.20	38/4338 (0.9%)
1	D	0.61	0/3553	1.19	30/4815 (0.6%)
All	All	0.61	0/13867	1.21	135/18795 (0.7%)

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	TYR	N-CA-C	-10.10	99.67	112.90
1	B	241	THR	N-CA-C	-9.89	100.39	113.25
1	A	331	VAL	N-CA-C	9.42	121.36	110.62
1	B	127	GLY	N-CA-C	9.32	120.24	111.67
1	D	131	TYR	N-CA-C	-9.21	101.35	112.59
1	B	331	VAL	N-CA-C	9.09	119.08	110.53
1	D	3	ASN	N-CA-C	8.62	123.55	112.34
1	B	43	ASP	N-CA-C	8.27	122.92	109.85
1	B	276	ALA	N-CA-C	-8.18	103.19	113.01
1	D	67	THR	N-CA-C	-8.16	102.77	112.89
1	A	329	ASN	N-CA-C	8.05	119.87	109.64
1	C	233	THR	N-CA-C	8.04	122.20	109.50
1	A	368	ILE	N-CA-C	-8.02	103.08	111.58
1	C	234	ALA	N-CA-C	-7.96	103.17	113.12
1	D	90	MET	N-CA-C	7.70	119.75	111.36
1	D	7	ILE	N-CA-C	7.68	119.72	107.73
1	D	2	SER	N-CA-C	-7.64	104.01	112.72
1	C	46	GLU	N-CA-C	7.62	127.02	110.80
1	A	104	THR	N-CA-C	-7.59	103.01	111.28
1	C	329	ASN	CA-C-N	7.54	129.26	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	329	ASN	C-N-CA	7.54	129.26	119.84
1	A	388	GLU	N-CA-C	7.43	119.37	111.28
1	C	240	ASN	N-CA-C	7.24	126.21	110.80
1	C	251	LYS	N-CA-C	-7.22	103.41	111.28
1	B	324	MET	CA-C-N	7.09	128.71	119.84
1	B	324	MET	C-N-CA	7.09	128.71	119.84
1	C	232	ALA	N-CA-C	7.03	118.68	108.34
1	C	337	ASN	N-CA-C	-7.03	103.55	111.07
1	B	86	ASN	N-CA-C	-6.92	104.15	112.59
1	A	3	ASN	N-CA-C	6.87	121.08	108.58
1	D	176	ARG	N-CA-C	-6.78	103.97	111.36
1	C	304	GLY	CA-C-N	6.74	128.26	119.84
1	C	304	GLY	C-N-CA	6.74	128.26	119.84
1	D	268	ILE	N-CA-C	6.73	119.63	109.20
1	B	459	VAL	N-CA-C	6.67	123.22	109.34
1	A	391	ILE	N-CA-C	6.62	117.38	110.62
1	B	131	TYR	N-CA-C	-6.60	105.09	113.01
1	D	244	GLU	N-CA-C	-6.54	105.84	113.88
1	D	63	LYS	N-CA-C	-6.44	103.95	110.97
1	C	259	PHE	CA-C-N	6.43	127.88	119.84
1	C	259	PHE	C-N-CA	6.43	127.88	119.84
1	C	317	LEU	N-CA-C	6.42	120.42	111.56
1	A	309	LEU	N-CA-C	-6.42	103.57	111.40
1	C	241	THR	CA-C-N	6.39	127.82	119.84
1	C	241	THR	C-N-CA	6.39	127.82	119.84
1	B	404	TYR	N-CA-C	-6.38	103.84	111.69
1	C	389	LYS	N-CA-C	6.35	120.64	113.02
1	A	93	PHE	CA-C-N	6.23	127.63	119.84
1	A	93	PHE	C-N-CA	6.23	127.63	119.84
1	B	458	SER	N-CA-C	6.22	120.35	110.70
1	C	39	ASN	N-CA-C	6.21	118.41	108.41
1	C	91	ASP	N-CA-C	6.19	123.99	110.80
1	D	402	GLU	N-CA-C	-6.19	105.55	113.23
1	A	395	THR	N-CA-C	-6.19	99.93	109.52
1	C	37	SER	N-CA-C	6.19	118.02	110.41
1	A	210	LEU	N-CA-C	-6.18	104.24	110.97
1	D	126	LYS	N-CA-C	-6.17	101.15	110.28
1	A	258	GLY	N-CA-C	-6.16	106.42	115.72
1	A	337	ASN	N-CA-C	-6.16	104.48	111.07
1	D	361	LEU	N-CA-C	6.13	118.38	108.32
1	A	43	ASP	N-CA-C	6.12	118.75	108.23
1	C	197	PRO	N-CA-C	6.10	119.76	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	THR	N-CA-C	6.10	118.17	110.24
1	C	368	ILE	N-CA-C	-6.00	103.59	111.09
1	B	104	THR	N-CA-C	-6.00	104.83	111.36
1	C	258	GLY	N-CA-C	-5.98	107.96	115.08
1	A	322	SER	N-CA-C	5.92	118.62	111.40
1	D	169	GLN	N-CA-C	-5.90	104.92	111.71
1	B	258	GLY	N-CA-C	-5.89	107.12	115.43
1	A	350	VAL	N-CA-C	-5.88	105.12	110.82
1	A	435	GLY	N-CA-C	-5.88	107.28	114.92
1	B	174	PHE	N-CA-C	-5.88	105.77	113.12
1	D	78	ALA	N-CA-C	-5.87	104.48	111.69
1	D	191	GLN	N-CA-C	-5.86	105.43	112.58
1	C	184	ILE	N-CA-C	5.85	116.03	107.37
1	D	388	GLU	N-CA-C	5.78	120.47	113.41
1	C	150	THR	N-CA-C	5.74	117.54	111.28
1	B	183	ASP	N-CA-C	5.72	117.38	109.54
1	A	344	ILE	N-CA-C	-5.71	104.95	110.72
1	D	68	ILE	CA-C-N	5.67	126.55	119.98
1	D	68	ILE	C-N-CA	5.67	126.55	119.98
1	B	244	GLU	N-CA-C	-5.66	106.46	113.19
1	D	368	ILE	N-CA-C	-5.65	104.03	111.09
1	A	409	ILE	N-CA-C	5.64	120.02	111.89
1	A	241	THR	CA-C-N	5.62	126.87	119.84
1	A	241	THR	C-N-CA	5.62	126.87	119.84
1	C	281	HIS	N-CA-C	-5.60	105.17	112.23
1	B	16	GLU	N-CA-C	5.59	117.59	109.71
1	D	38	ASN	N-CA-C	-5.58	106.26	112.57
1	A	196	VAL	CA-C-N	5.58	125.89	119.93
1	A	196	VAL	C-N-CA	5.58	125.89	119.93
1	B	363	VAL	N-CA-C	5.57	118.01	111.05
1	D	130	GLN	N-CA-C	5.57	118.47	108.17
1	B	92	GLN	N-CA-C	-5.56	105.19	112.41
1	D	104	THR	N-CA-C	-5.54	105.24	111.28
1	D	415	LEU	N-CA-C	-5.52	106.39	113.01
1	D	233	THR	N-CA-C	5.46	122.44	110.80
1	A	333	PRO	N-CA-C	-5.45	105.67	113.47
1	D	196	VAL	CA-C-N	5.44	125.74	119.92
1	D	196	VAL	C-N-CA	5.44	125.74	119.92
1	B	107	ASN	N-CA-C	-5.43	105.52	111.82
1	C	161	ILE	N-CA-C	-5.42	105.25	110.72
1	B	445	ARG	N-CA-C	-5.42	106.51	113.23
1	C	271	THR	N-CA-C	-5.38	105.98	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	LEU	N-CA-C	-5.34	96.33	107.37
1	B	281	HIS	N-CA-C	-5.34	104.89	111.40
1	B	359	LEU	N-CA-C	5.33	117.57	108.67
1	A	169	GLN	N-CA-C	-5.33	105.64	111.82
1	C	104	THR	N-CA-C	-5.31	104.73	111.11
1	C	318	GLN	N-CA-C	5.29	122.07	110.80
1	C	40	LYS	N-CA-C	-5.28	101.68	109.86
1	D	403	GLY	N-CA-C	-5.27	106.41	112.73
1	B	252	LYS	N-CA-C	-5.25	105.16	112.45
1	A	360	GLN	N-CA-C	5.25	119.85	112.72
1	D	106	VAL	N-CA-C	-5.24	106.03	111.58
1	A	78	ALA	N-CA-C	-5.24	104.99	111.33
1	A	415	LEU	N-CA-C	-5.21	107.09	113.50
1	B	329	ASN	CA-C-N	5.21	126.35	119.84
1	B	329	ASN	C-N-CA	5.21	126.35	119.84
1	C	133	ASN	CA-C-N	5.20	126.34	119.84
1	C	133	ASN	C-N-CA	5.20	126.34	119.84
1	C	176	ARG	N-CA-C	-5.18	103.63	111.56
1	C	348	THR	N-CA-C	-5.18	104.58	112.04
1	B	83	VAL	N-CA-C	-5.17	108.46	113.53
1	B	49	ARG	N-CA-C	-5.15	105.57	111.14
1	A	196	VAL	N-CA-C	5.15	114.83	109.01
1	B	329	ASN	N-CA-C	5.13	115.88	109.57
1	A	122	MET	N-CA-C	-5.09	106.91	113.02
1	A	319	ALA	N-CA-C	5.08	121.61	110.80
1	B	422	HIS	N-CA-C	5.08	118.25	111.75
1	A	64	GLU	N-CA-C	-5.06	105.76	111.28
1	C	414	TYR	N-CA-C	-5.06	107.28	113.50
1	B	347	ASP	N-CA-C	-5.05	105.47	110.97
1	C	328	VAL	N-CA-C	-5.04	98.86	109.34
1	D	94	PRO	N-CA-C	5.01	120.61	114.35

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	3502	0	3539	351	0
1	B	3511	0	3547	313	0
1	C	3152	0	3191	283	0
1	D	3502	0	3539	327	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	4	0	3	0	0
4	A	19	0	0	1	0
4	B	16	0	0	0	0
4	C	11	0	0	0	0
4	D	23	0	0	1	0
All	All	13764	0	13843	1158	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 42.

All (1158) 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:A:269:GLU:HG3	1:A:270:ALA:H	1.20	1.05
1:D:273:ASP:HB2	1:D:362:ASN:HD22	1.22	1.04
1:B:319:ALA:HB2	1:D:26:HIS:CE1	1.94	1.02
1:B:119:LEU:HG	1:B:132:LEU:HB3	1.42	1.01
1:A:83:VAL:HG13	1:A:90:MET:HB3	1.43	1.01
1:A:284:LEU:HD21	1:A:376:VAL:HG22	1.40	1.00
1:A:323:ILE:HB	1:A:324:MET:SD	2.02	0.99
1:A:241:THR:N	1:A:242:PRO:HD2	1.78	0.98
1:D:431:CYS:SG	1:D:441:VAL:HG21	2.05	0.95
1:B:314:LEU:HD12	1:B:390:CYS:SG	2.07	0.93
1:A:416:ASN:HD21	1:A:424:GLY:HA3	1.32	0.93
1:C:185:LEU:HB3	1:C:405:VAL:HG11	1.50	0.93
1:D:235:ILE:HD12	1:D:236:GLY:H	1.34	0.92
1:B:439:ARG:HH22	1:B:454:ASP:HB3	1.35	0.91
1:D:287:LEU:HD23	1:D:379:LEU:HD13	1.53	0.91
1:C:200:LEU:HD22	1:C:401:CYS:SG	2.11	0.91
1:D:253:LEU:HD12	1:D:261:CYS:SG	2.11	0.91
1:A:52:VAL:HG21	1:A:83:VAL:HG11	1.53	0.91
1:A:5:ILE:HG22	1:A:18:PRO:HA	1.53	0.89
1:A:226:LEU:HD11	1:A:259:PHE:HB3	1.52	0.89
1:D:323:ILE:HG12	1:D:324:MET:SD	2.12	0.89
1:C:185:LEU:HB2	1:C:402:GLU:HG2	1.54	0.89
1:B:93:PHE:HA	1:B:109:ASN:HD21	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:CG	1:A:270:ALA:H	1.87	0.88
1:D:445:ARG:HG2	1:D:445:ARG:HH11	1.36	0.88
1:D:233:THR:HA	1:D:238:GLY:HA2	1.55	0.88
1:B:44:ILE:H	1:B:45:PRO:HD2	1.38	0.88
1:C:152:PHE:HE2	1:C:369:GLY:HA2	1.37	0.87
1:C:172:GLU:HB3	1:C:176:ARG:HH21	1.38	0.87
1:B:323:ILE:HB	1:B:324:MET:SD	2.16	0.86
1:B:12:LEU:HD13	1:D:319:ALA:HA	1.58	0.86
1:B:35:TYR:CE1	1:D:385:ASN:HA	2.11	0.85
1:A:135:ASN:HA	1:A:139:ASN:HB3	1.59	0.84
1:B:199:THR:HG23	1:B:202:GLN:H	1.41	0.84
1:B:35:TYR:HE1	1:D:385:ASN:HA	1.43	0.84
1:B:319:ALA:HB2	1:D:26:HIS:HE1	1.38	0.83
1:D:409:ILE:H	1:D:409:ILE:HD12	1.40	0.83
1:D:409:ILE:O	1:D:412:VAL:HG23	1.78	0.83
1:C:179:VAL:O	1:C:182:GLN:HG2	1.79	0.82
1:C:104:THR:HG22	1:C:144:THR:HG21	1.60	0.82
1:B:277:TYR:HA	1:B:280:VAL:HG22	1.61	0.82
1:C:408:SER:O	1:C:411:ILE:HG23	1.80	0.82
1:A:416:ASN:ND2	1:A:424:GLY:HA3	1.95	0.81
1:D:85:ASN:OD1	1:D:88:LYS:HB2	1.79	0.81
1:B:238:GLY:HA3	1:B:242:PRO:HG2	1.59	0.81
1:C:352:MET:SD	1:D:352:MET:HE3	2.20	0.81
1:D:49:ARG:HG2	1:D:84:LEU:HD23	1.63	0.81
1:B:9:GLU:HB2	1:B:14:THR:HG22	1.62	0.80
1:B:104:THR:HA	1:B:144:THR:HG21	1.63	0.80
1:B:338:GLN:HE21	1:D:367:VAL:HB	1.46	0.80
1:B:119:LEU:HA	1:B:122:MET:HE2	1.64	0.79
1:A:6:ARG:HH11	1:A:17:VAL:HG13	1.47	0.79
1:C:119:LEU:HD23	1:C:132:LEU:HB3	1.64	0.79
1:C:51:MET:HE2	1:C:106:VAL:HG12	1.63	0.79
1:C:247:PRO:O	1:C:251:LYS:HG2	1.83	0.79
1:A:270:ALA:HA	1:A:274:CYS:HG	1.47	0.79
1:C:152:PHE:CE2	1:C:369:GLY:HA2	2.18	0.79
1:A:270:ALA:HA	1:A:274:CYS:SG	2.23	0.78
1:B:239:LEU:O	1:B:242:PRO:HD2	1.83	0.78
1:D:40:LYS:HA	1:D:96:ASP:HA	1.65	0.78
1:C:8:GLU:HB2	1:C:25:VAL:HG13	1.63	0.78
1:C:412:VAL:HA	1:C:415:LEU:HB3	1.65	0.78
1:C:235:ILE:HA	1:C:360:GLN:HG2	1.66	0.78
1:B:243:LYS:HE3	1:B:244:GLU:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:PHE:O	1:D:210:LEU:HB3	1.84	0.77
1:A:215:VAL:HG12	1:A:219:GLN:HE21	1.49	0.77
1:B:364:MET:O	1:B:367:VAL:HG12	1.84	0.77
1:B:439:ARG:HG3	1:B:439:ARG:HH11	1.49	0.77
1:D:272:SER:HA	1:D:361:LEU:HA	1.66	0.77
1:A:204:PHE:HA	1:A:207:PHE:HD2	1.49	0.77
1:D:242:PRO:HA	1:D:246:SER:OG	1.85	0.76
1:C:300:LEU:HD11	1:D:300:LEU:HD11	1.64	0.76
1:D:72:VAL:HB	1:D:132:LEU:HD13	1.67	0.76
1:A:99:GLN:OE1	1:A:105:SER:HB2	1.86	0.76
1:C:327:LYS:O	1:C:328:VAL:HG23	1.86	0.75
1:D:323:ILE:HD13	1:D:323:ILE:H	1.51	0.75
1:D:425:ASP:O	1:D:429:LYS:HG2	1.85	0.75
1:B:93:PHE:HA	1:B:109:ASN:ND2	2.01	0.75
1:D:414:TYR:O	1:D:417:PRO:HD2	1.87	0.75
1:A:217:ASN:HD21	1:D:279:MET:HG3	1.52	0.74
1:A:305:PRO:HD3	1:B:193:GLN:HE22	1.53	0.74
1:A:93:PHE:HA	1:A:109:ASN:HD21	1.52	0.74
1:A:343:VAL:HG21	1:A:379:LEU:HG	1.67	0.73
1:B:49:ARG:HA	1:B:52:VAL:HG22	1.69	0.73
1:B:150:THR:O	1:B:154:ILE:HG12	1.88	0.73
1:A:10:ASP:HB3	1:A:25:VAL:HG11	1.68	0.73
1:A:47:PHE:HE2	1:A:106:VAL:HG11	1.53	0.73
1:B:198:MET:HE2	1:C:235:ILE:HB	1.69	0.73
1:D:210:LEU:HD21	1:D:290:LYS:HB3	1.71	0.73
1:D:436:LYS:HB3	1:D:440:GLU:HG3	1.70	0.73
1:B:8:GLU:HB3	1:B:25:VAL:HG22	1.69	0.73
1:D:11:LEU:HD22	1:D:11:LEU:H	1.53	0.73
1:D:130:GLN:HE21	1:D:130:GLN:N	1.86	0.73
1:A:198:MET:HB3	1:D:235:ILE:HD13	1.71	0.72
1:D:204:PHE:HA	1:D:207:PHE:HD2	1.54	0.72
1:A:21:ALA:HA	1:A:92:GLN:OE1	1.90	0.72
1:A:152:PHE:O	1:A:156:VAL:HG23	1.89	0.72
1:A:290:LYS:HZ3	1:D:273:ASP:CG	1.97	0.72
1:B:275:GLY:HA3	1:C:290:LYS:HZ1	1.53	0.72
1:C:324:MET:SD	1:C:324:MET:N	2.62	0.72
1:A:285:LYS:O	1:A:289:VAL:HG23	1.90	0.72
1:A:230:LEU:HD23	1:A:249:ALA:HB1	1.71	0.72
1:D:204:PHE:HA	1:D:207:PHE:CD2	2.25	0.72
1:C:416:ASN:HB2	1:C:417:PRO:HD3	1.72	0.72
1:D:28:LEU:HA	1:D:31:ILE:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LEU:HD21	1:D:376:VAL:HG12	1.70	0.71
1:B:5:ILE:H	1:B:5:ILE:HD13	1.54	0.71
1:D:241:THR:N	1:D:242:PRO:HD2	2.05	0.71
1:B:210:LEU:HD21	1:B:290:LYS:HD2	1.72	0.71
1:C:152:PHE:HE2	1:C:369:GLY:CA	2.03	0.71
1:B:341:PHE:CE2	1:D:353:ALA:HA	2.26	0.71
1:C:202:GLN:O	1:C:205:ARG:HG2	1.89	0.71
1:D:414:TYR:CD2	1:D:456:ILE:HG12	2.26	0.71
1:A:8:GLU:HB3	1:A:25:VAL:HG22	1.71	0.71
1:A:359:LEU:HD11	1:D:300:LEU:HD23	1.73	0.71
1:B:456:ILE:HG13	1:B:457:PHE:H	1.55	0.71
1:B:51:MET:O	1:B:54:VAL:HG12	1.89	0.71
1:C:40:LYS:HD3	1:C:94:PRO:HA	1.71	0.71
1:A:61:ALA:O	1:A:65:LEU:HB2	1.89	0.71
1:A:69:PRO:HB2	1:A:72:VAL:HG13	1.73	0.71
1:D:296:ASN:HA	1:D:299:ARG:HE	1.55	0.70
1:A:449:THR:HG22	1:A:451:ALA:H	1.56	0.70
1:D:51:MET:O	1:D:54:VAL:HG12	1.91	0.70
1:A:51:MET:O	1:A:55:LYS:HG2	1.92	0.70
1:C:182:GLN:HG3	1:C:183:ASP:H	1.57	0.70
1:A:230:LEU:HD22	1:A:253:LEU:HD12	1.72	0.70
1:D:56:LYS:HD3	1:D:256:VAL:HG21	1.73	0.70
1:B:63:LYS:HZ2	1:B:74:ASN:HD21	1.38	0.70
1:C:279:MET:HA	1:C:279:MET:HE2	1.72	0.70
1:D:47:PHE:HA	1:D:155:ALA:CB	2.21	0.70
1:D:129:TYR:CD2	1:D:131:TYR:HE2	2.10	0.70
1:A:269:GLU:HG3	1:A:270:ALA:N	2.01	0.69
1:B:85:ASN:CG	1:B:86:ASN:H	2.00	0.69
1:D:76:ILE:HG13	1:D:132:LEU:HD11	1.73	0.69
1:B:235:ILE:HG13	1:C:196:VAL:HG13	1.74	0.69
1:B:176:ARG:O	1:B:179:VAL:HG12	1.93	0.69
1:B:221:THR:O	1:B:224:LEU:HG	1.92	0.69
1:A:56:LYS:HB2	1:A:80:CYS:SG	2.31	0.69
1:B:233:THR:HB	1:B:238:GLY:HA2	1.73	0.69
1:C:323:ILE:HG22	1:C:324:MET:SD	2.31	0.69
1:A:339:VAL:HG21	1:A:382:ALA:HB2	1.74	0.69
1:B:187:MET:HE3	1:B:405:VAL:HA	1.75	0.69
1:D:130:GLN:HE21	1:D:130:GLN:CA	2.06	0.69
1:D:250:VAL:HG21	1:D:263:PRO:HG3	1.74	0.69
1:C:189:ARG:HH21	1:C:309:LEU:HD11	1.58	0.69
1:C:53:MET:SD	1:C:257:THR:HA	2.33	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:MET:SD	1:A:132:LEU:CD1	2.81	0.68
1:C:146:ASP:HB2	1:C:229:ASN:OD1	1.92	0.68
1:A:109:ASN:O	1:A:113:VAL:HG23	1.93	0.68
1:B:7:ILE:HA	1:B:16:GLU:HA	1.74	0.68
1:B:87:GLY:C	1:B:89:CYS:H	2.02	0.68
1:C:235:ILE:HD12	1:C:236:GLY:N	2.09	0.68
1:D:150:THR:O	1:D:154:ILE:HG12	1.94	0.68
1:D:6:ARG:NH1	1:D:127:GLY:HA2	2.07	0.68
1:B:341:PHE:HE2	1:D:353:ALA:HA	1.59	0.67
1:D:285:LYS:HD3	1:D:347:ASP:CG	2.19	0.67
1:B:72:VAL:HG21	1:B:137:HIS:CD2	2.29	0.67
1:B:90:MET:HG3	1:B:91:ASP:H	1.58	0.67
1:C:182:GLN:HG3	1:C:183:ASP:N	2.09	0.67
1:C:164:VAL:HG21	1:C:219:GLN:OE1	1.95	0.67
1:A:11:LEU:H	1:A:11:LEU:HD22	1.60	0.67
1:C:22:TYR:HB2	1:C:92:GLN:HG3	1.76	0.67
1:D:23:TYR:HB2	1:D:27:THR:HB	1.76	0.67
1:A:215:VAL:HG12	1:A:219:GLN:NE2	2.10	0.67
1:A:336:VAL:HA	1:A:339:VAL:HG13	1.75	0.67
1:C:44:ILE:H	1:C:45:PRO:HD2	1.60	0.66
1:A:9:GLU:HG3	1:A:13:GLY:O	1.95	0.66
1:C:281:HIS:HA	1:C:284:LEU:HD22	1.76	0.66
1:A:305:PRO:HD3	1:B:193:GLN:NE2	2.10	0.66
1:B:322:SER:O	1:B:325:PRO:HG3	1.96	0.66
1:A:187:MET:SD	1:A:197:PRO:HD3	2.35	0.66
1:A:212:LYS:O	1:A:216:LYS:HG3	1.96	0.66
1:B:431:CYS:SG	1:B:441:VAL:HG21	2.35	0.66
1:A:318:GLN:HG3	1:A:319:ALA:H	1.61	0.66
1:C:273:ASP:HB2	1:C:362:ASN:HD22	1.61	0.66
1:A:34:PHE:HZ	1:C:331:VAL:HG22	1.60	0.66
1:C:409:ILE:HD11	1:D:306:ARG:HB2	1.77	0.66
1:D:414:TYR:CE2	1:D:456:ILE:HG12	2.30	0.66
1:C:101:GLY:O	1:C:104:THR:HG23	1.96	0.66
1:A:318:GLN:CG	1:A:319:ALA:H	2.08	0.65
1:B:314:LEU:CD1	1:B:390:CYS:SG	2.83	0.65
1:D:246:SER:HB2	1:D:247:PRO:HD3	1.76	0.65
1:B:63:LYS:NZ	1:B:74:ASN:HD21	1.93	0.65
1:B:85:ASN:ND2	1:B:88:LYS:HZ1	1.93	0.65
1:D:188:GLY:O	1:D:195:ALA:HB3	1.96	0.65
1:B:44:ILE:H	1:B:45:PRO:CD	2.09	0.65
1:B:439:ARG:HH21	1:B:450:GLU:HG3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PHE:CZ	1:C:331:VAL:HG22	2.31	0.65
1:A:122:MET:SD	1:A:132:LEU:HD13	2.37	0.65
1:C:126:LYS:HG2	1:C:127:GLY:H	1.62	0.65
1:A:241:THR:N	1:A:242:PRO:CD	2.58	0.65
1:D:158:SER:HA	1:D:161:ILE:HD12	1.79	0.65
1:D:210:LEU:HD13	1:D:294:ILE:HD11	1.77	0.65
1:D:285:LYS:O	1:D:289:VAL:HG23	1.97	0.65
1:D:323:ILE:HD13	1:D:323:ILE:N	2.12	0.65
1:B:220:ARG:O	1:B:223:GLU:HG2	1.96	0.65
1:B:425:ASP:O	1:B:429:LYS:HG2	1.97	0.64
1:D:332:VAL:O	1:D:335:VAL:HG12	1.96	0.64
1:A:68:ILE:HD12	1:A:72:VAL:HG23	1.78	0.64
1:B:34:PHE:HZ	1:D:331:VAL:HG22	1.62	0.64
1:A:122:MET:HE2	1:A:124:HIS:HE1	1.61	0.64
1:A:214:GLU:O	1:A:218:ILE:HG12	1.97	0.64
1:A:286:ARG:HH11	1:D:279:MET:HG2	1.63	0.64
1:C:267:LEU:HD23	1:C:267:LEU:H	1.63	0.64
1:A:92:GLN:O	1:A:94:PRO:HD3	1.98	0.64
1:B:163:LEU:O	1:B:167:ILE:HG13	1.96	0.64
1:B:381:ASN:O	1:B:385:ASN:HB2	1.98	0.64
1:B:317:LEU:HB3	1:D:33:ASN:ND2	2.13	0.64
1:D:47:PHE:HA	1:D:155:ALA:HB1	1.78	0.64
1:D:150:THR:HG23	1:D:228:VAL:HB	1.78	0.64
1:D:220:ARG:O	1:D:223:GLU:HB3	1.97	0.64
1:B:239:LEU:HD21	1:C:196:VAL:HG11	1.80	0.64
1:A:63:LYS:HE3	1:A:70:LYS:HG3	1.79	0.64
1:B:324:MET:SD	1:B:324:MET:N	2.71	0.64
1:B:235:ILE:CG1	1:C:196:VAL:HG13	2.28	0.63
1:B:443:LEU:HD13	1:B:453:LEU:HD22	1.79	0.63
1:D:145:ASN:O	1:D:149:PRO:HG2	1.97	0.63
1:C:189:ARG:NH2	1:C:309:LEU:HD11	2.13	0.63
1:A:379:LEU:O	1:A:382:ALA:HB3	1.99	0.63
1:B:108:MET:HE2	1:B:111:ASN:ND2	2.12	0.63
1:D:323:ILE:H	1:D:323:ILE:CD1	2.11	0.63
1:C:407:ASN:ND2	1:D:306:ARG:HH21	1.97	0.63
1:D:158:SER:O	1:D:161:ILE:HB	1.99	0.63
1:A:332:VAL:O	1:A:335:VAL:HG12	1.99	0.63
1:A:30:ALA:HA	1:A:33:ASN:HD22	1.63	0.63
1:B:209:ILE:HG13	1:C:268:ILE:HD12	1.80	0.63
1:C:372:MET:O	1:C:376:VAL:HG23	1.98	0.63
1:C:402:GLU:HB3	1:C:406:TYR:HE2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:VAL:HG23	1:C:372:MET:SD	2.39	0.63
1:A:331:VAL:HG22	1:C:100:GLY:HA3	1.79	0.63
1:B:231:GLY:HA2	1:B:241:THR:HG22	1.81	0.63
1:C:72:VAL:HG21	1:C:137:HIS:CD2	2.34	0.63
1:D:7:ILE:HA	1:D:16:GLU:HA	1.81	0.63
1:C:82:GLU:O	1:C:88:LYS:HB3	1.99	0.62
1:B:119:LEU:N	1:B:132:LEU:HD23	2.14	0.62
1:C:343:VAL:CG2	1:C:378:ILE:HD11	2.28	0.62
1:D:129:TYR:C	1:D:130:GLN:HE21	2.07	0.62
1:A:145:ASN:HD22	1:A:234:ALA:HB2	1.64	0.62
1:A:182:GLN:HA	1:A:201:GLY:HA3	1.80	0.62
1:A:207:PHE:CE1	1:A:294:ILE:HG23	2.34	0.62
1:C:130:GLN:NE2	1:C:133:ASN:HA	2.14	0.62
1:B:257:THR:HB	1:B:259:PHE:CD2	2.34	0.62
1:A:409:ILE:HG23	1:B:306:ARG:HD2	1.81	0.62
1:B:141:CYS:HB3	1:B:245:TYR:CE2	2.34	0.62
1:B:313:ASN:O	1:B:394:ILE:HA	2.00	0.62
1:B:319:ALA:HB1	1:D:11:LEU:HD23	1.81	0.62
1:D:184:ILE:O	1:D:200:LEU:N	2.31	0.62
1:B:415:LEU:HD22	1:B:448:LEU:HD21	1.81	0.62
1:D:31:ILE:HD11	1:D:94:PRO:HG2	1.82	0.62
1:B:416:ASN:HB2	1:B:417:PRO:HD3	1.81	0.62
1:D:52:VAL:HG13	1:D:114:LEU:HD11	1.82	0.62
1:C:212:LYS:O	1:C:216:LYS:HG2	2.00	0.61
1:D:221:THR:HG22	1:D:280:VAL:HG12	1.82	0.61
1:A:218:ILE:HD13	1:A:283:ALA:HB1	1.80	0.61
1:A:341:PHE:CD1	1:C:352:MET:HB3	2.36	0.61
1:A:343:VAL:HG23	1:A:378:ILE:HD11	1.82	0.61
1:B:150:THR:HG23	1:B:228:VAL:HB	1.80	0.61
1:D:156:VAL:O	1:D:160:LEU:HG	1.99	0.61
1:B:119:LEU:CG	1:B:132:LEU:HB3	2.24	0.61
1:B:108:MET:HE2	1:B:111:ASN:HD22	1.65	0.61
1:D:11:LEU:H	1:D:11:LEU:CD2	2.14	0.61
1:C:128:GLU:O	1:C:130:GLN:HG2	2.01	0.61
1:D:173:GLY:O	1:D:176:ARG:HB3	2.00	0.61
1:A:437:SER:OG	1:A:440:GLU:HG3	2.01	0.61
1:B:102:ALA:HB2	1:B:363:VAL:HA	1.82	0.61
1:D:127:GLY:C	1:D:129:TYR:H	2.09	0.61
1:D:323:ILE:HG12	1:D:324:MET:H	1.65	0.61
1:B:88:LYS:C	1:B:89:CYS:SG	2.84	0.61
1:C:53:MET:SD	1:C:257:THR:HG22	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:GLU:HA	1:C:272:SER:OG	2.00	0.61
1:D:119:LEU:HB2	1:D:124:HIS:HB2	1.83	0.61
1:B:225:LEU:HG	1:B:280:VAL:HG11	1.83	0.61
1:C:281:HIS:CD2	1:C:350:VAL:HG21	2.36	0.60
1:D:292:SER:HB2	1:D:340:CYS:SG	2.40	0.60
1:B:254:ALA:HB2	1:B:261:CYS:SG	2.41	0.60
1:D:423:ASN:HD22	1:D:447:LEU:HD11	1.66	0.60
1:B:6:ARG:HD2	1:B:17:VAL:CG1	2.31	0.60
1:B:363:VAL:O	1:B:366:PRO:HD2	2.01	0.60
1:A:416:ASN:O	1:A:420:GLY:N	2.34	0.60
1:B:211:LEU:O	1:B:215:VAL:HG23	2.01	0.60
1:C:218:ILE:HD11	1:C:287:LEU:HD22	1.83	0.60
1:A:47:PHE:HZ	1:A:148:TYR:CE1	2.18	0.60
1:A:119:LEU:CD1	1:A:126:LYS:HA	2.32	0.60
1:B:116:ASN:CG	1:B:126:LYS:HB2	2.27	0.60
1:A:152:PHE:CE1	1:A:369:GLY:HA2	2.37	0.60
1:A:176:ARG:O	1:A:180:GLU:HG3	2.01	0.60
1:A:318:GLN:HG3	1:A:319:ALA:N	2.17	0.60
1:C:40:LYS:HD3	1:C:94:PRO:CA	2.32	0.60
1:D:76:ILE:CG1	1:D:132:LEU:HD11	2.31	0.60
1:C:205:ARG:HB2	1:C:205:ARG:NH1	2.17	0.60
1:A:28:LEU:HA	1:A:31:ILE:HD12	1.84	0.60
1:A:346:ASN:O	1:A:350:VAL:HG23	2.02	0.60
1:B:312:ILE:HB	1:B:394:ILE:CG2	2.32	0.60
1:D:73:ALA:O	1:D:77:ILE:HG23	2.02	0.60
1:D:39:ASN:O	1:D:97:VAL:HG22	2.02	0.59
1:D:385:ASN:HD22	1:D:385:ASN:C	2.10	0.59
1:A:119:LEU:HA	1:A:122:MET:HB2	1.85	0.59
1:D:127:GLY:O	1:D:129:TYR:N	2.35	0.59
1:D:148:TYR:HB3	1:D:149:PRO:HD3	1.84	0.59
1:A:369:GLY:O	1:A:373:PHE:HD1	1.84	0.59
1:B:295:CYS:O	1:B:299:ARG:HG3	2.02	0.59
1:C:248:LEU:O	1:C:252:LYS:HG2	2.02	0.59
1:A:8:GLU:OE1	1:A:17:VAL:HG11	2.03	0.59
1:B:149:PRO:O	1:B:153:ARG:HG3	2.02	0.59
1:D:49:ARG:O	1:D:53:MET:HG3	2.02	0.59
1:D:226:LEU:HD23	1:D:260:PRO:HG2	1.84	0.59
1:D:314:LEU:HD23	1:D:394:ILE:HD12	1.83	0.59
1:A:306:ARG:NE	1:A:306:ARG:HA	2.18	0.59
1:C:364:MET:O	1:C:367:VAL:HG12	2.03	0.59
1:A:122:MET:HE2	1:A:124:HIS:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ILE:HD12	1:C:72:VAL:HG23	1.85	0.59
1:C:69:PRO:O	1:C:72:VAL:HG22	2.02	0.59
1:A:241:THR:H	1:A:242:PRO:HD2	1.66	0.59
1:C:130:GLN:NE2	1:C:130:GLN:HA	2.17	0.59
1:A:244:GLU:HB3	1:A:248:LEU:HD22	1.85	0.59
1:B:62:ASN:HB3	1:B:68:ILE:HG12	1.85	0.58
1:C:327:LYS:NZ	1:C:329:ASN:HD21	2.00	0.58
1:A:223:GLU:HA	1:A:226:LEU:HD23	1.85	0.58
1:A:334:GLU:O	1:A:337:ASN:HB2	2.03	0.58
1:A:370:GLN:HG3	1:A:371:ALA:N	2.16	0.58
1:B:233:THR:CB	1:B:238:GLY:HA2	2.34	0.58
1:B:324:MET:N	1:B:325:PRO:HD3	2.18	0.58
1:B:343:VAL:HG21	1:B:379:LEU:HD21	1.84	0.58
1:A:65:LEU:HD22	1:A:245:TYR:HD1	1.68	0.58
1:C:343:VAL:HG21	1:C:379:LEU:HG	1.85	0.58
1:D:234:ALA:CB	1:D:239:LEU:HD23	2.33	0.58
1:A:405:VAL:HG23	1:A:406:TYR:N	2.18	0.58
1:B:314:LEU:HD13	1:B:394:ILE:HG12	1.86	0.58
1:D:186:LYS:HA	1:D:401:CYS:O	2.03	0.58
1:D:402:GLU:HA	1:D:405:VAL:HG12	1.84	0.58
1:D:427:VAL:HG11	1:D:438:VAL:HG13	1.86	0.58
1:B:6:ARG:HD2	1:B:17:VAL:HG13	1.85	0.58
1:C:241:THR:O	1:C:243:LYS:N	2.37	0.58
1:D:221:THR:CG2	1:D:280:VAL:HA	2.34	0.58
1:A:72:VAL:O	1:A:76:ILE:HG12	2.03	0.58
1:B:181:PHE:CZ	1:B:395:THR:HA	2.39	0.58
1:D:132:LEU:O	1:D:137:HIS:HB2	2.03	0.58
1:A:451:ALA:C	1:A:453:LEU:H	2.11	0.58
1:B:353:ALA:O	1:B:356:ALA:HB3	2.03	0.58
1:D:426:ILE:O	1:D:430:ILE:HG12	2.03	0.58
1:A:146:ASP:HB2	1:A:229:ASN:O	2.04	0.57
1:C:20:ASP:HA	1:C:126:LYS:NZ	2.19	0.57
1:D:130:GLN:HG3	1:D:133:ASN:HA	1.85	0.57
1:A:441:VAL:O	1:A:445:ARG:HG3	2.04	0.57
1:B:35:TYR:OH	1:D:389:LYS:HG2	2.04	0.57
1:B:285:LYS:O	1:B:288:ALA:HB3	2.04	0.57
1:A:330:PRO:O	1:A:333:PRO:HD2	2.04	0.57
1:A:389:LYS:NZ	1:C:33:ASN:HA	2.19	0.57
1:C:313:ASN:N	1:C:395:THR:O	2.34	0.57
1:D:221:THR:HG21	1:D:280:VAL:HA	1.85	0.57
1:A:204:PHE:HA	1:A:207:PHE:CD2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:TYR:CD2	1:D:339:VAL:HG12	2.40	0.57
1:C:11:LEU:H	1:C:11:LEU:HD22	1.69	0.57
1:C:189:ARG:HH11	1:C:189:ARG:HB2	1.68	0.57
1:A:97:VAL:HG23	1:A:98:TYR:CE1	2.38	0.57
1:A:162:LYS:HD2	4:A:709:HOH:O	2.04	0.57
1:B:452:GLU:O	1:B:455:ASP:HB2	2.05	0.57
1:C:45:PRO:HB2	1:C:159:SER:OG	2.04	0.57
1:C:177:LYS:HE3	1:C:391:ILE:O	2.04	0.57
1:D:295:CYS:SG	1:D:336:VAL:HB	2.43	0.57
1:D:445:ARG:HG2	1:D:445:ARG:NH1	2.14	0.57
1:B:235:ILE:HG12	1:C:196:VAL:O	2.04	0.57
1:B:323:ILE:C	1:B:325:PRO:HD3	2.30	0.57
1:C:214:GLU:OE1	1:C:287:LEU:HA	2.05	0.57
1:D:52:VAL:HG21	1:D:83:VAL:HG11	1.87	0.57
1:D:346:ASN:O	1:D:350:VAL:HG23	2.05	0.57
1:B:365:GLU:N	1:B:366:PRO:HD2	2.20	0.57
1:D:124:HIS:HB3	1:D:129:TYR:HD2	1.70	0.57
1:A:21:ALA:HB1	1:A:23:TYR:CE1	2.40	0.56
1:A:248:LEU:HD12	1:A:251:LYS:HD3	1.86	0.56
1:B:104:THR:HA	1:B:144:THR:CG2	2.34	0.56
1:B:107:ASN:ND2	1:B:147:ALA:HB3	2.19	0.56
1:C:94:PRO:HD2	1:C:109:ASN:HD21	1.69	0.56
1:A:56:LYS:HB2	1:A:80:CYS:CB	2.35	0.56
1:A:79:ALA:O	1:A:82:GLU:HB2	2.05	0.56
1:A:358:GLN:NE2	1:C:299:ARG:HH12	2.03	0.56
1:B:200:LEU:HD11	1:B:204:PHE:HE1	1.70	0.56
1:C:241:THR:O	1:C:243:LYS:HG2	2.05	0.56
1:D:200:LEU:HD21	1:D:312:ILE:CG2	2.36	0.56
1:A:234:ALA:O	1:A:235:ILE:HG23	2.05	0.56
1:C:311:GLU:HB3	1:C:401:CYS:SG	2.46	0.56
1:D:119:LEU:HD23	1:D:132:LEU:HB3	1.87	0.56
1:D:120:GLU:HA	1:D:124:HIS:O	2.05	0.56
1:C:88:LYS:C	1:C:90:MET:H	2.14	0.56
1:D:419:ILE:HD11	1:D:424:GLY:HA2	1.88	0.56
1:B:161:ILE:O	1:B:164:VAL:HG22	2.05	0.56
1:A:391:ILE:HA	1:A:394:ILE:HG13	1.88	0.56
1:B:108:MET:O	1:B:112:GLU:HG3	2.05	0.56
1:B:159:SER:HB3	1:B:376:VAL:HG11	1.87	0.56
1:B:350:VAL:HG13	1:B:368:ILE:HG12	1.86	0.56
1:D:204:PHE:HZ	1:D:312:ILE:HD13	1.71	0.56
1:D:391:ILE:HA	1:D:394:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD23	1:C:319:ALA:HA	1.87	0.56
1:A:240:ASN:C	1:A:242:PRO:HD2	2.31	0.56
1:A:257:THR:HB	1:A:259:PHE:CD2	2.40	0.56
1:D:6:ARG:O	1:D:17:VAL:N	2.39	0.56
1:A:34:PHE:HZ	1:C:331:VAL:CG2	2.19	0.56
1:B:189:ARG:HB2	1:C:359:LEU:HD12	1.86	0.56
1:C:247:PRO:HA	1:C:250:VAL:HG22	1.87	0.56
1:D:295:CYS:SG	1:D:336:VAL:CG1	2.94	0.56
1:A:40:LYS:HD3	1:A:94:PRO:O	2.06	0.55
1:A:107:ASN:OD1	1:A:147:ALA:HB3	2.05	0.55
1:A:237:THR:HA	1:A:267:LEU:HD23	1.88	0.55
1:A:419:ILE:O	1:A:423:ASN:HB2	2.06	0.55
1:D:6:ARG:HG2	1:D:17:VAL:O	2.06	0.55
1:D:13:GLY:HA3	1:D:15:ARG:HH12	1.70	0.55
1:C:11:LEU:HD22	1:C:11:LEU:N	2.21	0.55
1:A:196:VAL:HG23	1:D:235:ILE:HG12	1.87	0.55
1:A:423:ASN:O	1:A:426:ILE:HG23	2.07	0.55
1:C:173:GLY:O	1:C:177:LYS:HG2	2.07	0.55
1:C:302:SER:HB3	1:C:314:LEU:HD13	1.87	0.55
1:B:268:ILE:HD13	1:C:205:ARG:HD3	1.88	0.55
1:C:81:ASP:O	1:C:85:ASN:HB3	2.06	0.55
1:C:90:MET:O	1:C:92:GLN:N	2.38	0.55
1:C:329:ASN:O	1:C:331:VAL:N	2.39	0.55
1:D:168:ASN:HD22	1:D:171:ARG:HD3	1.71	0.55
1:D:356:ALA:HB3	1:D:364:MET:HG3	1.88	0.55
1:A:97:VAL:HG23	1:A:98:TYR:CD1	2.41	0.55
1:B:350:VAL:HG13	1:B:368:ILE:HG23	1.87	0.55
1:C:241:THR:OG1	1:C:242:PRO:HD3	2.06	0.55
1:B:419:ILE:HG21	1:B:448:LEU:HD21	1.87	0.55
1:D:315:PRO:HD3	1:D:394:ILE:HD13	1.87	0.55
1:A:119:LEU:HD12	1:A:126:LYS:HA	1.88	0.55
1:A:314:LEU:HD21	1:A:333:PRO:HG2	1.89	0.55
1:A:328:VAL:HG12	1:A:328:VAL:O	2.06	0.55
1:B:288:ALA:HB1	1:B:344:ILE:HG13	1.89	0.55
1:B:156:VAL:O	1:B:160:LEU:HG	2.07	0.55
1:C:267:LEU:O	1:C:268:ILE:HG23	2.06	0.55
1:C:402:GLU:HB3	1:C:406:TYR:CE2	2.41	0.55
1:D:11:LEU:HD22	1:D:11:LEU:N	2.20	0.55
1:B:51:MET:HE2	1:B:106:VAL:HG12	1.88	0.55
1:B:116:ASN:OD1	1:B:126:LYS:HB2	2.06	0.55
1:B:327:LYS:O	1:B:328:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PHE:O	1:A:211:LEU:HG	2.08	0.55
1:A:364:MET:HG2	1:C:341:PHE:CE2	2.42	0.55
1:D:281:HIS:CD2	1:D:350:VAL:HG21	2.42	0.55
1:C:120:GLU:C	1:C:122:MET:H	2.15	0.54
1:A:110:THR:HG22	1:A:114:LEU:HD11	1.89	0.54
1:A:332:VAL:O	1:A:336:VAL:HG23	2.07	0.54
1:B:6:ARG:HH21	1:B:126:LYS:HZ3	1.55	0.54
1:B:370:GLN:O	1:B:374:GLU:HB2	2.08	0.54
1:B:431:CYS:SG	1:B:441:VAL:CG2	2.95	0.54
1:C:134:PRO:HA	1:C:138:VAL:HG23	1.90	0.54
1:C:267:LEU:H	1:C:267:LEU:CD2	2.21	0.54
1:D:170:LEU:HD23	1:D:211:LEU:HG	1.90	0.54
1:A:122:MET:C	1:A:124:HIS:H	2.14	0.54
1:C:386:LEU:O	1:C:390:CYS:HB3	2.06	0.54
1:D:40:LYS:HE2	1:D:94:PRO:O	2.06	0.54
1:D:168:ASN:O	1:D:172:GLU:HG3	2.07	0.54
1:D:241:THR:N	1:D:242:PRO:CD	2.66	0.54
1:A:415:LEU:O	1:A:419:ILE:HG12	2.08	0.54
1:B:36:ILE:HG12	1:D:339:VAL:HG11	1.88	0.54
1:B:102:ALA:HB2	1:B:363:VAL:HG12	1.90	0.54
1:B:23:TYR:HB2	1:B:27:THR:HG21	1.90	0.54
1:B:308:GLY:O	1:B:310:ASN:N	2.40	0.54
1:B:187:MET:HE2	1:B:197:PRO:HG3	1.90	0.54
1:A:115:ALA:O	1:A:119:LEU:HG	2.08	0.54
1:A:199:THR:C	1:A:201:GLY:H	2.16	0.54
1:A:378:ILE:HG13	1:A:379:LEU:N	2.23	0.54
1:B:243:LYS:CE	1:B:244:GLU:H	2.18	0.54
1:B:423:ASN:O	1:B:426:ILE:HG22	2.06	0.54
1:D:246:SER:HB2	1:D:247:PRO:CD	2.37	0.54
1:A:272:SER:HA	1:A:362:ASN:N	2.22	0.54
1:A:281:HIS:CD2	1:A:350:VAL:HG21	2.43	0.54
1:B:339:VAL:O	1:B:343:VAL:HG23	2.08	0.54
1:A:237:THR:HA	1:A:267:LEU:CD2	2.38	0.53
1:D:152:PHE:CE1	1:D:369:GLY:HA2	2.43	0.53
1:A:331:VAL:HG13	1:C:34:PHE:HE1	1.72	0.53
1:B:88:LYS:O	1:B:89:CYS:SG	2.66	0.53
1:B:363:VAL:CG1	1:C:191:GLN:HG2	2.38	0.53
1:A:34:PHE:HA	1:C:385:ASN:OD1	2.08	0.53
1:B:439:ARG:HG3	1:B:439:ARG:NH1	2.22	0.53
1:C:6:ARG:HH11	1:C:127:GLY:HA3	1.73	0.53
1:C:325:PRO:O	1:D:409:ILE:HD13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ALA:C	1:D:266:ASP:H	2.15	0.53
1:D:280:VAL:HG23	1:D:281:HIS:N	2.24	0.53
1:D:321:SER:OG	1:D:325:PRO:HA	2.09	0.53
1:A:295:CYS:O	1:A:299:ARG:HG3	2.08	0.53
1:C:406:TYR:C	1:C:408:SER:H	2.15	0.53
1:D:303:SER:HG	1:D:309:LEU:H	1.54	0.53
1:D:436:LYS:HZ1	1:D:440:GLU:HB2	1.73	0.53
1:A:153:ARG:HD3	1:A:228:VAL:HG12	1.91	0.53
1:A:324:MET:SD	1:A:324:MET:N	2.82	0.53
1:B:5:ILE:HD13	1:B:5:ILE:N	2.22	0.53
1:B:52:VAL:HG12	1:B:114:LEU:HD21	1.90	0.53
1:B:173:GLY:C	1:B:391:ILE:HD12	2.34	0.53
1:B:205:ARG:O	1:B:209:ILE:HG12	2.07	0.53
1:C:27:THR:O	1:C:31:ILE:HG13	2.08	0.53
1:C:62:ASN:HD22	1:C:67:THR:HG21	1.72	0.53
1:C:154:ILE:HG13	1:C:259:PHE:HD2	1.73	0.53
1:A:146:ASP:CG	1:A:231:GLY:H	2.17	0.53
1:A:359:LEU:N	1:A:359:LEU:HD12	2.23	0.53
1:B:191:GLN:O	1:B:192:LEU:HB2	2.09	0.53
1:D:246:SER:O	1:D:250:VAL:HG13	2.09	0.53
1:C:193:GLN:HB2	1:D:327:LYS:NZ	2.23	0.53
1:C:200:LEU:O	1:C:203:GLU:HB3	2.09	0.53
1:D:22:TYR:O	1:D:116:ASN:ND2	2.40	0.53
1:D:233:THR:OG1	1:D:234:ALA:N	2.37	0.53
1:A:35:TYR:HE1	1:C:389:LYS:HD2	1.73	0.52
1:A:299:ARG:HB3	1:B:192:LEU:HD12	1.92	0.52
1:A:327:LYS:O	1:A:328:VAL:HG23	2.09	0.52
1:A:370:GLN:HG3	1:A:371:ALA:H	1.75	0.52
1:B:45:PRO:O	1:B:46:GLU:HB2	2.09	0.52
1:D:185:LEU:HA	1:D:198:MET:O	2.09	0.52
1:C:276:ALA:O	1:C:280:VAL:HG13	2.09	0.52
1:D:28:LEU:O	1:D:31:ILE:HB	2.09	0.52
1:D:46:GLU:OE2	1:D:155:ALA:HA	2.09	0.52
1:D:210:LEU:HD22	1:D:294:ILE:HD11	1.91	0.52
1:D:296:ASN:HA	1:D:299:ARG:NE	2.24	0.52
1:A:275:GLY:HA3	1:D:286:ARG:NE	2.24	0.52
1:B:85:ASN:HD22	1:B:88:LYS:HZ1	1.56	0.52
1:B:87:GLY:C	1:B:89:CYS:N	2.67	0.52
1:B:181:PHE:HZ	1:B:395:THR:HA	1.73	0.52
1:D:101:GLY:O	1:D:104:THR:HG23	2.09	0.52
1:D:242:PRO:HA	1:D:246:SER:HG	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:ARG:HA	1:D:453:LEU:HD21	1.91	0.52
1:A:294:ILE:O	1:A:298:LEU:HG	2.09	0.52
1:B:199:THR:HG23	1:B:202:GLN:N	2.18	0.52
1:B:305:PRO:O	1:B:306:ARG:HB3	2.09	0.52
1:D:365:GLU:N	1:D:366:PRO:CD	2.72	0.52
1:A:235:ILE:HD13	1:D:196:VAL:HG23	1.91	0.52
1:B:189:ARG:HA	1:B:193:GLN:O	2.09	0.52
1:D:247:PRO:O	1:D:250:VAL:HG22	2.09	0.52
1:A:188:GLY:HA2	1:D:360:GLN:OE1	2.10	0.52
1:A:322:SER:CB	1:B:429:LYS:HZ1	2.23	0.52
1:D:279:MET:HE2	1:D:279:MET:HA	1.91	0.52
1:D:314:LEU:HD23	1:D:394:ILE:CD1	2.40	0.52
1:A:267:LEU:N	1:A:267:LEU:HD22	2.24	0.52
1:A:275:GLY:HA3	1:D:286:ARG:CZ	2.39	0.52
1:A:327:LYS:HG2	1:A:328:VAL:H	1.73	0.52
1:C:44:ILE:HB	1:C:45:PRO:HD3	1.91	0.52
1:D:119:LEU:HD22	1:D:129:TYR:O	2.09	0.52
1:C:148:TYR:HB3	1:C:149:PRO:HD3	1.92	0.52
1:A:9:GLU:HG3	1:A:13:GLY:C	2.34	0.52
1:A:350:VAL:HG13	1:A:368:ILE:HG23	1.92	0.52
1:B:31:ILE:HG22	1:B:31:ILE:O	2.10	0.52
1:B:196:VAL:O	1:C:235:ILE:HG21	2.10	0.52
1:C:332:VAL:O	1:C:335:VAL:HG12	2.10	0.52
1:C:391:ILE:HA	1:C:394:ILE:HG13	1.90	0.52
1:D:117:ILE:O	1:D:121:LEU:HG	2.10	0.52
1:A:68:ILE:HD11	1:A:73:ALA:HA	1.92	0.52
1:C:11:LEU:H	1:C:11:LEU:CD2	2.22	0.52
1:D:55:LYS:HG3	1:D:110:THR:CG2	2.39	0.52
1:D:295:CYS:SG	1:D:336:VAL:HG11	2.50	0.52
1:D:415:LEU:HA	1:D:418:PHE:HD2	1.74	0.52
1:A:5:ILE:N	1:A:5:ILE:HD13	2.25	0.51
1:C:323:ILE:C	1:C:324:MET:SD	2.92	0.51
1:A:74:ASN:O	1:A:78:ALA:HB2	2.10	0.51
1:A:359:LEU:HD11	1:D:300:LEU:CD2	2.40	0.51
1:A:365:GLU:N	1:A:366:PRO:HD2	2.25	0.51
1:A:434:THR:HB	1:A:436:LYS:HG3	1.92	0.51
1:B:83:VAL:HA	1:B:87:GLY:HA2	1.92	0.51
1:B:323:ILE:C	1:B:324:MET:SD	2.93	0.51
1:C:149:PRO:O	1:C:152:PHE:HB3	2.10	0.51
1:A:458:SER:O	1:A:459:VAL:HB	2.09	0.51
1:B:41:ILE:HD11	1:B:99:GLN:HE22	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HB3	1:B:405:VAL:HG21	1.93	0.51
1:C:119:LEU:CD2	1:C:132:LEU:HB3	2.37	0.51
1:A:286:ARG:HH11	1:D:279:MET:CG	2.22	0.51
1:A:342:LYS:NZ	1:C:342:LYS:NZ	2.58	0.51
1:A:364:MET:HG2	1:C:341:PHE:HE2	1.74	0.51
1:B:187:MET:HE3	1:B:405:VAL:HG22	1.92	0.51
1:B:281:HIS:O	1:B:284:LEU:N	2.43	0.51
1:B:302:SER:HB3	1:B:312:ILE:HG13	1.92	0.51
1:B:413:THR:HA	1:B:416:ASN:OD1	2.11	0.51
1:C:220:ARG:O	1:C:223:GLU:HG3	2.09	0.51
1:D:415:LEU:O	1:D:419:ILE:HG23	2.10	0.51
1:A:125:GLN:NE2	1:A:129:TYR:HB2	2.25	0.51
1:A:389:LYS:HZ3	1:C:33:ASN:HA	1.75	0.51
1:A:271:THR:HG23	1:A:272:SER:N	2.25	0.51
1:C:175:GLU:O	1:C:179:VAL:HG23	2.10	0.51
1:C:402:GLU:O	1:C:405:VAL:HG12	2.10	0.51
1:A:163:LEU:O	1:A:167:ILE:HG13	2.10	0.51
1:D:55:LYS:HG3	1:D:110:THR:HG21	1.93	0.51
1:D:323:ILE:HG12	1:D:324:MET:N	2.25	0.51
1:A:23:TYR:HB2	1:A:27:THR:HG21	1.92	0.51
1:A:269:GLU:CG	1:A:270:ALA:N	2.63	0.51
1:A:387:LEU:HA	1:A:391:ILE:HG13	1.93	0.51
1:B:69:PRO:HB2	1:B:72:VAL:HG13	1.93	0.51
1:B:186:LYS:HE3	1:B:203:GLU:OE1	2.10	0.51
1:B:445:ARG:HB3	1:B:447:LEU:HD13	1.93	0.51
1:D:235:ILE:CD1	1:D:236:GLY:H	2.13	0.51
1:B:200:LEU:CD2	1:B:396:ALA:HB2	2.41	0.50
1:C:139:ASN:ND2	1:C:142:GLN:HB2	2.27	0.50
1:C:168:ASN:O	1:C:171:ARG:HB2	2.11	0.50
1:A:5:ILE:HG13	1:A:16:GLU:HB3	1.93	0.50
1:A:185:LEU:H	1:A:402:GLU:HG2	1.75	0.50
1:C:274:CYS:HB2	1:C:277:TYR:CE2	2.46	0.50
1:A:113:VAL:O	1:A:117:ILE:HG13	2.10	0.50
1:C:26:HIS:ND1	1:C:108:MET:HG2	2.26	0.50
1:D:273:ASP:CB	1:D:362:ASN:HD22	2.08	0.50
1:D:381:ASN:O	1:D:385:ASN:HB2	2.10	0.50
1:D:431:CYS:SG	1:D:441:VAL:CG2	2.91	0.50
1:B:40:LYS:O	1:B:42:SER:N	2.44	0.50
1:B:157:TYR:O	1:B:161:ILE:HG13	2.10	0.50
1:B:231:GLY:HA2	1:B:241:THR:CG2	2.41	0.50
1:B:401:CYS:O	1:B:404:TYR:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LEU:HB3	1:B:419:ILE:CD1	2.40	0.50
1:D:413:THR:O	1:D:417:PRO:HD3	2.10	0.50
1:A:339:VAL:HG21	1:A:382:ALA:CB	2.40	0.50
1:A:355:GLU:C	1:A:357:GLY:H	2.19	0.50
1:B:250:VAL:HA	1:B:253:LEU:CB	2.42	0.50
1:D:244:GLU:OE2	1:D:248:LEU:HD22	2.12	0.50
1:B:250:VAL:HA	1:B:253:LEU:HB3	1.92	0.50
1:D:214:GLU:OE1	1:D:287:LEU:HA	2.12	0.50
1:A:131:TYR:O	1:A:132:LEU:HD12	2.11	0.50
1:A:302:SER:OG	1:A:314:LEU:HD13	2.11	0.50
1:A:172:GLU:O	1:A:176:ARG:HG3	2.11	0.50
1:B:85:ASN:ND2	1:B:88:LYS:NZ	2.60	0.50
1:B:324:MET:C	1:B:326:ALA:H	2.20	0.50
1:C:10:ASP:HB3	1:C:29:ARG:HH21	1.77	0.50
1:D:130:GLN:HE21	1:D:130:GLN:HA	1.76	0.50
1:A:216:LYS:O	1:A:220:ARG:HB2	2.12	0.50
1:B:285:LYS:HD3	1:B:347:ASP:CG	2.37	0.50
1:D:85:ASN:O	1:D:86:ASN:HB3	2.12	0.50
1:D:210:LEU:HD22	1:D:294:ILE:CD1	2.42	0.50
1:B:72:VAL:O	1:B:75:ALA:HB3	2.11	0.49
1:B:439:ARG:HG2	1:B:453:LEU:HD21	1.94	0.49
1:C:117:ILE:O	1:C:121:LEU:HG	2.11	0.49
1:D:134:PRO:HG2	1:D:135:ASN:H	1.77	0.49
1:D:187:MET:HE3	1:D:195:ALA:O	2.12	0.49
1:A:152:PHE:CZ	1:A:369:GLY:HA2	2.47	0.49
1:A:222:ALA:O	1:A:224:LEU:N	2.45	0.49
1:A:413:THR:HG22	1:A:413:THR:O	2.12	0.49
1:C:108:MET:HA	1:C:111:ASN:HD22	1.78	0.49
1:D:445:ARG:HH11	1:D:445:ARG:CG	2.12	0.49
1:A:192:LEU:HD13	1:B:300:LEU:HA	1.93	0.49
1:C:45:PRO:HG2	1:C:373:PHE:CD1	2.47	0.49
1:C:48:VAL:O	1:C:52:VAL:HG12	2.12	0.49
1:D:323:ILE:CG1	1:D:324:MET:SD	2.94	0.49
1:A:92:GLN:C	1:A:94:PRO:HD3	2.37	0.49
1:A:247:PRO:O	1:A:250:VAL:HG22	2.13	0.49
1:B:281:HIS:HB2	1:B:372:MET:HE1	1.95	0.49
1:D:373:PHE:HA	1:D:376:VAL:HG22	1.94	0.49
1:A:68:ILE:HD12	1:A:72:VAL:CG2	2.40	0.49
1:A:110:THR:O	1:A:114:LEU:HG	2.12	0.49
1:A:235:ILE:HG22	1:D:188:GLY:HA3	1.94	0.49
1:A:191:GLN:HG2	1:D:363:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:VAL:HG23	1:D:101:GLY:N	2.28	0.49
1:C:304:GLY:HA2	1:D:193:GLN:HA	1.93	0.49
1:D:444:GLU:HG3	1:D:445:ARG:N	2.27	0.49
1:A:126:LYS:HG3	1:A:127:GLY:N	2.28	0.49
1:A:191:GLN:HG2	1:D:363:VAL:HG11	1.95	0.49
1:B:85:ASN:CG	1:B:86:ASN:N	2.69	0.49
1:B:336:VAL:HA	1:B:339:VAL:HG13	1.94	0.49
1:B:354:ALA:CB	1:C:289:VAL:HG11	2.42	0.49
1:B:442:VAL:HG11	1:B:448:LEU:HD23	1.93	0.49
1:C:205:ARG:HB2	1:C:205:ARG:CZ	2.43	0.49
1:C:257:THR:HB	1:C:259:PHE:CD2	2.47	0.49
1:A:296:ASN:O	1:A:300:LEU:HB2	2.13	0.49
1:B:273:ASP:O	1:C:290:LYS:NZ	2.38	0.49
1:B:456:ILE:O	1:B:457:PHE:HB2	2.12	0.49
1:C:69:PRO:HB2	1:C:72:VAL:HG13	1.94	0.49
1:C:119:LEU:O	1:C:122:MET:HB2	2.13	0.49
1:C:196:VAL:HG23	1:C:197:PRO:HD2	1.94	0.49
1:D:161:ILE:O	1:D:164:VAL:HG22	2.13	0.49
1:A:405:VAL:CG2	1:A:406:TYR:N	2.76	0.49
1:B:5:ILE:HA	1:B:19:ALA:HB2	1.95	0.49
1:D:241:THR:H	1:D:242:PRO:HD2	1.78	0.49
1:D:269:GLU:HA	1:D:272:SER:OG	2.13	0.49
1:A:272:SER:HA	1:A:362:ASN:H	1.78	0.49
1:A:322:SER:HA	1:B:429:LYS:HZ3	1.78	0.49
1:B:275:GLY:HA3	1:C:290:LYS:NZ	2.25	0.49
1:B:281:HIS:C	1:B:283:ALA:N	2.70	0.49
1:D:274:CYS:SG	1:D:276:ALA:HB3	2.53	0.49
1:A:111:ASN:CG	1:A:139:ASN:HB2	2.38	0.48
1:A:125:GLN:HE22	1:A:131:TYR:HE1	1.61	0.48
1:A:327:LYS:HG2	1:A:328:VAL:N	2.28	0.48
1:B:324:MET:O	1:B:326:ALA:N	2.46	0.48
1:A:145:ASN:HB2	1:A:233:THR:O	2.13	0.48
1:B:52:VAL:HG23	1:B:84:LEU:HD21	1.95	0.48
1:D:83:VAL:HG22	1:D:89:CYS:HB2	1.95	0.48
1:A:36:ILE:HG23	1:C:378:ILE:HB	1.93	0.48
1:A:93:PHE:HA	1:A:109:ASN:ND2	2.24	0.48
1:B:58:ALA:HB1	1:B:142:GLN:HE22	1.79	0.48
1:B:273:ASP:OD1	1:C:290:LYS:NZ	2.46	0.48
1:D:56:LYS:HB2	1:D:80:CYS:SG	2.53	0.48
1:D:129:TYR:CD2	1:D:131:TYR:CE2	2.97	0.48
1:A:307:ALA:HB3	1:B:194:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:VAL:HG22	1:A:375:SER:HA	1.94	0.48
1:C:272:SER:HA	1:C:362:ASN:N	2.29	0.48
1:D:13:GLY:HA3	1:D:15:ARG:NH1	2.28	0.48
1:D:47:PHE:N	1:D:155:ALA:HB1	2.27	0.48
1:D:273:ASP:HB2	1:D:362:ASN:ND2	2.07	0.48
1:B:419:ILE:CG2	1:B:448:LEU:HD21	2.43	0.48
1:D:79:ALA:HB1	1:D:117:ILE:HB	1.95	0.48
1:B:293:LYS:HA	1:B:296:ASN:HB2	1.95	0.48
1:B:387:LEU:HG	1:B:388:GLU:N	2.29	0.48
1:D:23:TYR:HB2	1:D:27:THR:CB	2.43	0.48
1:A:98:TYR:CD1	1:A:98:TYR:N	2.80	0.48
1:A:184:ILE:HG23	1:A:398:LYS:HA	1.95	0.48
1:A:226:LEU:CD1	1:A:259:PHE:HB3	2.35	0.48
1:B:49:ARG:HA	1:B:52:VAL:CG2	2.43	0.48
1:B:177:LYS:HE3	1:B:391:ILE:O	2.13	0.48
1:B:227:GLU:HB3	1:B:264:ALA:HA	1.96	0.48
1:C:5:ILE:HG22	1:C:18:PRO:HA	1.93	0.48
1:D:41:ILE:HG13	1:D:95:VAL:O	2.13	0.48
1:B:241:THR:HB	1:B:242:PRO:HD3	1.95	0.48
1:B:459:VAL:HG22	1:B:460:GLN:H	1.77	0.48
1:A:47:PHE:CZ	1:A:148:TYR:CE1	3.01	0.48
1:A:126:LYS:HG3	1:A:127:GLY:H	1.79	0.48
1:B:176:ARG:NH2	1:B:392:ASN:ND2	2.62	0.48
1:D:274:CYS:SG	1:D:276:ALA:CB	3.02	0.48
1:D:325:PRO:O	1:D:326:ALA:HB2	2.14	0.48
1:A:242:PRO:O	1:A:243:LYS:HB3	2.14	0.48
1:B:108:MET:CE	1:B:111:ASN:HD22	2.26	0.48
1:B:124:HIS:HD2	1:B:131:TYR:CE1	2.32	0.48
1:D:190:THR:O	1:D:191:GLN:HB2	2.14	0.48
1:D:234:ALA:HB2	1:D:239:LEU:HD23	1.96	0.48
1:A:235:ILE:HG13	1:A:236:GLY:H	1.79	0.47
1:A:364:MET:O	1:A:367:VAL:HG12	2.14	0.47
1:C:285:LYS:HD3	1:C:347:ASP:CB	2.44	0.47
1:A:331:VAL:HG13	1:C:34:PHE:CE1	2.49	0.47
1:C:8:GLU:HA	1:C:128:GLU:HG2	1.96	0.47
1:C:126:LYS:HG2	1:C:127:GLY:N	2.28	0.47
1:C:166:ALA:HA	1:C:384:TYR:CE1	2.49	0.47
1:C:241:THR:N	1:C:242:PRO:HD2	2.30	0.47
1:D:9:GLU:HB2	1:D:14:THR:HG22	1.97	0.47
1:D:26:HIS:HD2	1:D:108:MET:HG3	1.79	0.47
1:A:368:ILE:O	1:A:372:MET:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLY:O	1:A:372:MET:HB3	2.14	0.47
1:C:295:CYS:SG	1:C:336:VAL:HG11	2.54	0.47
1:D:185:LEU:HA	1:D:199:THR:HA	1.96	0.47
1:D:423:ASN:O	1:D:427:VAL:HG23	2.14	0.47
1:A:185:LEU:HD22	1:A:406:TYR:HE1	1.78	0.47
1:A:243:LYS:O	1:A:244:GLU:C	2.56	0.47
1:C:8:GLU:HB2	1:C:25:VAL:CG1	2.39	0.47
1:C:79:ALA:HB2	1:C:118:GLY:CA	2.43	0.47
1:D:423:ASN:HD22	1:D:447:LEU:HD21	1.80	0.47
1:B:152:PHE:CE1	1:B:369:GLY:HA2	2.48	0.47
1:C:327:LYS:HZ1	1:C:329:ASN:HD21	1.62	0.47
1:C:378:ILE:HD13	1:C:379:LEU:H	1.80	0.47
1:A:342:LYS:HZ2	1:C:342:LYS:NZ	2.12	0.47
1:B:225:LEU:CG	1:B:280:VAL:HG11	2.44	0.47
1:B:415:LEU:HD13	1:B:442:VAL:HG21	1.97	0.47
1:C:47:PHE:O	1:C:50:GLY:N	2.47	0.47
1:D:102:ALA:HB2	1:D:363:VAL:HB	1.94	0.47
1:D:204:PHE:CZ	1:D:312:ILE:HD13	2.49	0.47
1:D:214:GLU:O	1:D:218:ILE:HG13	2.15	0.47
1:D:399:GLU:O	1:D:403:GLY:N	2.48	0.47
1:D:456:ILE:O	1:D:457:PHE:CG	2.67	0.47
1:A:56:LYS:HB2	1:A:80:CYS:HB3	1.96	0.47
1:A:194:ASP:OD2	1:B:305:PRO:O	2.33	0.47
1:A:205:ARG:HH21	1:A:209:ILE:HD11	1.80	0.47
1:A:419:ILE:O	1:A:423:ASN:ND2	2.47	0.47
1:C:280:VAL:O	1:C:284:LEU:HD13	2.15	0.47
1:A:83:VAL:CG1	1:A:90:MET:HB3	2.31	0.47
1:C:170:LEU:HA	1:C:387:LEU:HD13	1.96	0.47
1:C:299:ARG:HG2	1:C:330:PRO:HB2	1.97	0.47
1:D:5:ILE:N	1:D:5:ILE:HD13	2.30	0.47
1:A:145:ASN:ND2	1:A:234:ALA:HB2	2.30	0.47
1:B:51:MET:HB3	1:B:110:THR:HG21	1.97	0.47
1:C:104:THR:HG22	1:C:144:THR:CG2	2.37	0.47
1:D:168:ASN:ND2	1:D:171:ARG:HD3	2.30	0.47
1:A:196:VAL:HG23	1:D:235:ILE:CG1	2.44	0.46
1:A:243:LYS:HG2	1:A:244:GLU:N	2.30	0.46
1:B:9:GLU:CG	1:B:10:ASP:N	2.78	0.46
1:B:439:ARG:NH2	1:B:450:GLU:HG3	2.28	0.46
1:C:327:LYS:HE2	1:C:329:ASN:OD1	2.15	0.46
1:D:27:THR:O	1:D:31:ILE:HG13	2.15	0.46
1:D:54:VAL:HG13	1:D:55:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:CE1	1:C:389:LYS:HD2	2.51	0.46
1:A:45:PRO:O	1:A:46:GLU:HB2	2.15	0.46
1:A:164:VAL:HB	1:A:215:VAL:HG13	1.97	0.46
1:A:330:PRO:O	1:A:334:GLU:HG3	2.16	0.46
1:B:63:LYS:HG3	1:B:64:GLU:N	2.30	0.46
1:C:157:TYR:CE2	1:C:226:LEU:HD11	2.51	0.46
1:D:372:MET:O	1:D:376:VAL:HG13	2.15	0.46
1:B:99:GLN:HE22	1:B:106:VAL:CG2	2.29	0.46
1:D:197:PRO:HB3	1:D:405:VAL:HG23	1.97	0.46
1:A:241:THR:O	1:A:242:PRO:O	2.33	0.46
1:B:45:PRO:HB2	1:B:159:SER:OG	2.16	0.46
1:B:61:ALA:O	1:B:64:GLU:HB3	2.16	0.46
1:B:118:GLY:O	1:B:122:MET:HG3	2.15	0.46
1:B:280:VAL:O	1:B:284:LEU:HD22	2.14	0.46
1:C:146:ASP:C	1:C:149:PRO:HD2	2.41	0.46
1:D:324:MET:SD	1:D:324:MET:N	2.88	0.46
1:B:281:HIS:HA	1:B:284:LEU:CD2	2.46	0.46
1:C:365:GLU:HB2	1:C:366:PRO:HD3	1.98	0.46
1:A:199:THR:C	1:A:201:GLY:N	2.73	0.46
1:B:330:PRO:O	1:B:334:GLU:HG3	2.16	0.46
1:D:69:PRO:O	1:D:72:VAL:HG22	2.15	0.46
1:D:116:ASN:O	1:D:120:GLU:HB2	2.15	0.46
1:D:186:LYS:O	1:D:405:VAL:HB	2.15	0.46
1:D:207:PHE:CD1	1:D:294:ILE:HG23	2.50	0.46
1:D:250:VAL:HG21	1:D:263:PRO:CG	2.45	0.46
1:B:101:GLY:O	1:B:104:THR:HG23	2.15	0.46
1:D:264:ALA:C	1:D:266:ASP:N	2.72	0.46
1:D:439:ARG:HH22	1:D:454:ASP:HB3	1.80	0.46
1:A:204:PHE:O	1:A:207:PHE:HB2	2.16	0.46
1:A:352:MET:HE3	1:B:352:MET:HE3	1.98	0.46
1:D:127:GLY:C	1:D:129:TYR:N	2.74	0.46
1:A:175:GLU:O	1:A:179:VAL:HG23	2.15	0.46
1:A:290:LYS:NZ	1:D:273:ASP:CG	2.69	0.46
1:B:186:LYS:HG2	1:B:187:MET:N	2.29	0.46
1:D:50:GLY:HA2	1:D:53:MET:HE3	1.98	0.46
1:A:35:TYR:N	1:A:35:TYR:CD1	2.84	0.46
1:A:342:LYS:NZ	1:C:342:LYS:HZ2	2.14	0.46
1:B:431:CYS:SG	1:B:438:VAL:HA	2.56	0.46
1:C:223:GLU:O	1:C:226:LEU:HB2	2.16	0.46
1:C:231:GLY:CA	1:C:241:THR:HG21	2.46	0.46
1:A:273:ASP:OD1	1:A:274:CYS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ALA:O	1:B:327:LYS:HG3	2.16	0.45
1:C:233:THR:HB	1:C:237:THR:O	2.16	0.45
1:A:48:VAL:C	1:A:50:GLY:N	2.72	0.45
1:B:170:LEU:HD12	1:B:391:ILE:HD13	1.97	0.45
1:C:116:ASN:O	1:C:120:GLU:HG3	2.16	0.45
1:C:186:LYS:HD3	1:C:200:LEU:HA	1.99	0.45
1:C:277:TYR:HA	1:C:280:VAL:HG22	1.98	0.45
1:D:253:LEU:CD1	1:D:261:CYS:SG	2.94	0.45
1:A:46:GLU:HG2	1:A:49:ARG:HD3	1.97	0.45
1:A:170:LEU:HD11	1:A:386:LEU:HD23	1.99	0.45
1:A:318:GLN:O	1:C:12:LEU:HD22	2.16	0.45
1:B:49:ARG:CA	1:B:52:VAL:HG22	2.43	0.45
1:C:92:GLN:O	1:C:94:PRO:HD3	2.17	0.45
1:D:25:VAL:O	1:D:29:ARG:N	2.41	0.45
1:D:100:GLY:C	1:D:102:ALA:H	2.24	0.45
1:A:323:ILE:HG12	1:B:425:ASP:CG	2.42	0.45
1:C:273:ASP:N	1:C:362:ASN:HB2	2.31	0.45
1:C:312:ILE:HG13	1:C:312:ILE:O	2.15	0.45
1:C:328:VAL:HG12	1:C:328:VAL:O	2.16	0.45
1:D:53:MET:SD	1:D:257:THR:HG22	2.57	0.45
1:A:225:LEU:HD21	1:A:280:VAL:HG11	1.98	0.45
1:A:322:SER:HA	1:B:429:LYS:NZ	2.32	0.45
1:B:241:THR:CB	1:B:242:PRO:HD3	2.47	0.45
1:C:339:VAL:HB	1:C:378:ILE:HG12	1.98	0.45
1:C:348:THR:O	1:C:351:THR:HB	2.15	0.45
1:A:6:ARG:HG2	1:A:7:ILE:N	2.31	0.45
1:C:194:ASP:OD1	1:D:307:ALA:HB3	2.16	0.45
1:D:138:VAL:O	1:D:142:GLN:NE2	2.49	0.45
1:D:187:MET:HE2	1:D:408:SER:CB	2.47	0.45
1:A:125:GLN:CD	1:A:125:GLN:H	2.25	0.45
1:D:239:LEU:HB3	1:D:240:ASN:H	1.64	0.45
1:D:406:TYR:HE1	1:D:457:PHE:HB3	1.82	0.45
1:A:142:GLN:O	1:A:143:SER:HB3	2.16	0.45
1:A:245:TYR:CD2	1:A:246:SER:N	2.85	0.45
1:B:209:ILE:HG13	1:C:268:ILE:CD1	2.47	0.45
1:C:409:ILE:CD1	1:D:306:ARG:HB2	2.47	0.45
1:D:160:LEU:O	1:D:163:LEU:HB3	2.17	0.45
1:D:336:VAL:O	1:D:340:CYS:SG	2.62	0.45
1:A:207:PHE:CD1	1:A:294:ILE:HG23	2.52	0.45
1:A:336:VAL:HA	1:A:339:VAL:CG1	2.46	0.45
1:C:92:GLN:C	1:C:94:PRO:HD3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:LEU:O	1:D:66:GLN:HB2	2.16	0.45
1:D:151:GLY:O	1:D:154:ILE:HB	2.16	0.45
1:A:6:ARG:HD3	1:A:8:GLU:HG3	1.99	0.45
1:A:279:MET:O	1:A:282:GLY:N	2.49	0.45
1:A:312:ILE:HB	1:A:394:ILE:CG2	2.47	0.45
1:A:385:ASN:C	1:A:385:ASN:HD22	2.24	0.45
1:C:416:ASN:CB	1:C:417:PRO:HD3	2.42	0.45
1:A:70:LYS:HG2	1:A:74:ASN:ND2	2.31	0.44
1:B:251:LYS:HD2	1:B:251:LYS:HA	1.83	0.44
1:B:442:VAL:HG11	1:B:453:LEU:HD13	1.99	0.44
1:C:50:GLY:O	1:C:54:VAL:HG23	2.16	0.44
1:A:32:GLU:H	1:A:32:GLU:HG2	1.56	0.44
1:A:191:GLN:C	1:A:193:GLN:H	2.25	0.44
1:B:30:ALA:C	1:B:32:GLU:H	2.25	0.44
1:B:204:PHE:HA	1:B:207:PHE:CD2	2.52	0.44
1:B:423:ASN:O	1:B:427:VAL:HG23	2.17	0.44
1:C:62:ASN:ND2	1:C:245:TYR:HE1	2.15	0.44
1:C:93:PHE:HA	1:C:109:ASN:HD21	1.82	0.44
1:C:323:ILE:CG2	1:C:324:MET:SD	3.03	0.44
1:A:122:MET:SD	1:A:132:LEU:HD11	2.57	0.44
1:A:226:LEU:HD12	1:A:260:PRO:C	2.41	0.44
1:B:235:ILE:CD1	1:B:236:GLY:N	2.81	0.44
1:B:442:VAL:CG1	1:B:448:LEU:HD23	2.47	0.44
1:C:116:ASN:ND2	1:C:127:GLY:HA2	2.32	0.44
1:D:72:VAL:HB	1:D:132:LEU:CD1	2.41	0.44
1:D:132:LEU:O	1:D:133:ASN:O	2.34	0.44
1:D:423:ASN:ND2	1:D:447:LEU:HD11	2.32	0.44
1:A:122:MET:HB3	1:A:124:HIS:ND1	2.32	0.44
1:A:323:ILE:HG12	1:B:425:ASP:OD1	2.17	0.44
1:B:247:PRO:O	1:B:251:LYS:HG2	2.17	0.44
1:B:382:ALA:HA	1:D:36:ILE:HD12	1.99	0.44
1:D:181:PHE:CD1	1:D:184:ILE:HD12	2.52	0.44
1:B:171:ARG:NH2	1:B:212:LYS:NZ	2.65	0.44
1:B:246:SER:CB	1:B:247:PRO:HD3	2.48	0.44
1:C:116:ASN:HA	1:C:119:LEU:HD12	1.98	0.44
1:C:353:ALA:C	1:C:355:GLU:H	2.26	0.44
1:D:47:PHE:CE2	1:D:106:VAL:HG11	2.53	0.44
1:D:157:TYR:CE2	1:D:226:LEU:HD22	2.53	0.44
1:D:226:LEU:HD12	1:D:226:LEU:HA	1.60	0.44
1:D:323:ILE:O	1:D:325:PRO:HD3	2.17	0.44
1:D:451:ALA:O	1:D:455:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLY:C	1:D:279:MET:HE1	2.42	0.44
1:A:323:ILE:HG12	1:B:425:ASP:OD2	2.17	0.44
1:B:118:GLY:HA3	1:B:132:LEU:HD21	2.00	0.44
1:D:205:ARG:O	1:D:209:ILE:HG12	2.18	0.44
1:A:36:ILE:HD12	1:C:339:VAL:HG11	1.99	0.44
1:A:56:LYS:CA	1:A:80:CYS:SG	3.05	0.44
1:A:116:ASN:HB3	1:A:126:LYS:HD2	1.99	0.44
1:C:47:PHE:HA	1:C:155:ALA:CB	2.47	0.44
1:C:230:LEU:HD12	1:C:230:LEU:HA	1.59	0.44
1:C:239:LEU:O	1:C:242:PRO:HD2	2.17	0.44
1:C:285:LYS:HD2	1:C:344:ILE:HG23	2.00	0.44
1:D:72:VAL:HG12	1:D:122:MET:HE1	2.00	0.44
1:A:245:TYR:O	1:A:249:ALA:N	2.46	0.44
1:A:416:ASN:CG	1:A:421:HIS:HA	2.43	0.44
1:B:8:GLU:HB3	1:B:25:VAL:CG2	2.41	0.44
1:B:386:LEU:HD12	1:B:390:CYS:HB3	2.00	0.44
1:C:55:LYS:HD2	1:C:55:LYS:N	2.32	0.44
1:C:191:GLN:C	1:C:193:GLN:H	2.26	0.44
1:D:44:ILE:N	1:D:45:PRO:CD	2.81	0.44
1:A:402:GLU:O	1:A:405:VAL:HG22	2.18	0.44
1:C:47:PHE:HA	1:C:155:ALA:HB1	1.99	0.44
1:A:117:ILE:O	1:A:121:LEU:HD23	2.18	0.43
1:A:158:SER:O	1:A:161:ILE:HB	2.18	0.43
1:A:244:GLU:O	1:A:248:LEU:HB2	2.17	0.43
1:A:313:ASN:HB2	1:A:395:THR:OG1	2.17	0.43
1:A:430:ILE:HD13	1:A:430:ILE:HA	1.84	0.43
1:B:49:ARG:HH11	1:B:49:ARG:HB3	1.82	0.43
1:C:181:PHE:O	1:C:184:ILE:N	2.50	0.43
1:C:324:MET:HB2	1:D:409:ILE:CG2	2.48	0.43
1:D:49:ARG:NH2	4:D:490:HOH:O	2.48	0.43
1:A:380:THR:O	1:A:383:CYS:HB2	2.19	0.43
1:A:421:HIS:CD2	1:A:421:HIS:H	2.36	0.43
1:A:449:THR:HB	1:A:452:GLU:HG2	2.00	0.43
1:B:97:VAL:HG23	1:B:98:TYR:CD1	2.52	0.43
1:C:101:GLY:C	1:C:103:GLY:N	2.76	0.43
1:D:54:VAL:HA	1:D:253:LEU:HD23	2.00	0.43
1:A:179:VAL:O	1:A:182:GLN:HG2	2.19	0.43
1:A:246:SER:O	1:A:250:VAL:HG13	2.18	0.43
1:B:306:ARG:HG3	1:B:306:ARG:O	2.18	0.43
1:C:327:LYS:HD2	1:D:193:GLN:CB	2.48	0.43
1:A:297:ASP:OD2	1:D:359:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ALA:HB2	1:B:253:LEU:HA	2.00	0.43
1:C:40:LYS:O	1:C:42:SER:N	2.51	0.43
1:C:86:ASN:OD1	1:C:88:LYS:HB2	2.18	0.43
1:D:49:ARG:HG3	1:D:90:MET:CE	2.47	0.43
1:D:332:VAL:HB	1:D:333:PRO:HD3	2.00	0.43
1:A:185:LEU:HD23	1:A:405:VAL:HG21	1.99	0.43
1:A:259:PHE:HA	1:A:260:PRO:HD3	1.79	0.43
1:B:92:GLN:O	1:B:94:PRO:HD3	2.19	0.43
1:B:150:THR:CG2	1:B:253:LEU:HD21	2.48	0.43
1:B:243:LYS:C	1:B:245:TYR:H	2.26	0.43
1:B:281:HIS:HB2	1:B:372:MET:CE	2.48	0.43
1:B:439:ARG:NH1	1:B:439:ARG:CG	2.81	0.43
1:C:84:LEU:O	1:C:86:ASN:N	2.51	0.43
1:A:271:THR:HG23	1:A:272:SER:H	1.82	0.43
1:B:424:GLY:O	1:B:427:VAL:HB	2.19	0.43
1:C:6:ARG:HE	1:C:6:ARG:HB3	1.63	0.43
1:D:130:GLN:N	1:D:130:GLN:NE2	2.60	0.43
1:D:429:LYS:O	1:D:432:ALA:HB3	2.18	0.43
1:A:17:VAL:HG23	1:A:18:PRO:HD2	1.99	0.43
1:A:45:PRO:HB2	1:A:373:PHE:HD2	1.83	0.43
1:A:62:ASN:OD1	1:A:245:TYR:HE1	2.02	0.43
1:A:163:LEU:HG	1:A:167:ILE:HD11	1.99	0.43
1:A:212:LYS:HG3	1:A:213:GLU:N	2.31	0.43
1:B:40:LYS:HD3	1:B:94:PRO:O	2.18	0.43
1:B:115:ALA:HB2	1:B:134:PRO:HB3	2.01	0.43
1:C:302:SER:CB	1:C:314:LEU:HD13	2.48	0.43
1:D:152:PHE:CZ	1:D:369:GLY:HA2	2.53	0.43
1:D:304:GLY:O	1:D:308:GLY:N	2.52	0.43
1:B:25:VAL:O	1:B:26:HIS:C	2.61	0.43
1:B:285:LYS:HG3	1:B:344:ILE:HA	2.01	0.43
1:C:63:LYS:O	1:C:65:LEU:N	2.42	0.43
1:D:436:LYS:NZ	1:D:440:GLU:HB2	2.33	0.43
1:D:456:ILE:O	1:D:456:ILE:HG23	2.19	0.43
1:A:196:VAL:CB	1:A:197:PRO:HD2	2.49	0.43
1:A:322:SER:CA	1:B:429:LYS:NZ	2.81	0.43
1:B:323:ILE:O	1:B:323:ILE:HG22	2.19	0.43
1:C:193:GLN:HG3	1:D:329:ASN:OD1	2.18	0.43
1:C:327:LYS:HD2	1:D:193:GLN:HB2	2.01	0.43
1:D:210:LEU:HD13	1:D:294:ILE:CD1	2.48	0.43
1:A:248:LEU:O	1:A:251:LYS:HB3	2.19	0.43
1:B:169:GLN:HG2	1:B:384:TYR:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:PRO:HG2	1:C:373:PHE:HD1	1.83	0.43
1:C:204:PHE:O	1:C:207:PHE:HB2	2.18	0.43
1:C:267:LEU:C	1:C:268:ILE:HG12	2.44	0.43
1:A:40:LYS:O	1:A:42:SER:N	2.45	0.42
1:A:161:ILE:O	1:A:164:VAL:HG22	2.19	0.42
1:C:145:ASN:O	1:C:271:THR:HB	2.18	0.42
1:D:110:THR:HG22	1:D:114:LEU:HD13	2.01	0.42
1:A:65:LEU:HD21	1:A:245:TYR:HB2	2.01	0.42
1:A:65:LEU:HB3	1:A:67:THR:HG23	2.01	0.42
1:B:354:ALA:HB1	1:C:289:VAL:HG11	2.00	0.42
1:B:419:ILE:HG21	1:B:448:LEU:CD2	2.49	0.42
1:C:65:LEU:HD13	1:C:244:GLU:HB2	2.01	0.42
1:C:169:GLN:O	1:C:172:GLU:HB3	2.19	0.42
1:D:119:LEU:HD13	1:D:129:TYR:O	2.20	0.42
1:A:56:LYS:HA	1:A:80:CYS:SG	2.59	0.42
1:A:70:LYS:NZ	1:A:74:ASN:HD21	2.17	0.42
1:A:144:THR:O	1:A:149:PRO:HD2	2.19	0.42
1:B:336:VAL:O	1:B:339:VAL:HG13	2.19	0.42
1:C:44:ILE:N	1:C:45:PRO:HD2	2.31	0.42
1:C:130:GLN:HE21	1:C:133:ASN:HA	1.84	0.42
1:C:139:ASN:HD22	1:C:142:GLN:HB2	1.84	0.42
1:C:265:GLU:H	1:C:265:GLU:HG3	1.49	0.42
1:C:272:SER:HB3	1:C:361:LEU:HA	2.01	0.42
1:D:388:GLU:O	1:D:389:LYS:HD2	2.20	0.42
1:A:318:GLN:CG	1:A:319:ALA:N	2.75	0.42
1:A:359:LEU:HD12	1:A:359:LEU:H	1.83	0.42
1:B:370:GLN:OE1	1:D:342:LYS:HE2	2.19	0.42
1:C:62:ASN:HB3	1:C:67:THR:OG1	2.18	0.42
1:C:280:VAL:O	1:C:284:LEU:HD22	2.20	0.42
1:D:103:GLY:HA3	1:D:148:TYR:CD2	2.55	0.42
1:A:125:GLN:CD	1:A:125:GLN:N	2.77	0.42
1:A:284:LEU:HD21	1:A:376:VAL:CG2	2.30	0.42
1:A:334:GLU:OE1	1:C:363:VAL:HB	2.19	0.42
1:B:103:GLY:HA3	1:B:148:TYR:CD2	2.54	0.42
1:B:140:LYS:O	1:B:141:CYS:HB2	2.19	0.42
1:C:45:PRO:O	1:C:159:SER:OG	2.36	0.42
1:C:332:VAL:O	1:C:336:VAL:HG23	2.19	0.42
1:B:124:HIS:CD2	1:B:131:TYR:CD1	3.07	0.42
1:C:304:GLY:HA2	1:C:305:PRO:HD3	1.84	0.42
1:D:18:PRO:HB2	1:D:21:ALA:HB2	2.00	0.42
1:D:170:LEU:HD11	1:D:386:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:SER:O	1:D:273:ASP:CB	2.68	0.42
1:D:330:PRO:C	1:D:333:PRO:HD2	2.45	0.42
1:D:439:ARG:CZ	1:D:453:LEU:HB3	2.48	0.42
1:A:304:GLY:HA2	1:A:305:PRO:HD2	1.94	0.42
1:B:415:LEU:HB3	1:B:419:ILE:HD13	2.01	0.42
1:C:9:GLU:HA	1:C:14:THR:HG22	2.00	0.42
1:C:378:ILE:HD13	1:C:379:LEU:N	2.34	0.42
1:D:453:LEU:HD12	1:D:453:LEU:HA	1.81	0.42
1:A:56:LYS:CB	1:A:80:CYS:SG	3.06	0.42
1:A:300:LEU:O	1:A:303:SER:HB3	2.20	0.42
1:B:10:ASP:OD2	1:D:319:ALA:HB2	2.20	0.42
1:B:160:LEU:O	1:B:161:ILE:C	2.63	0.42
1:B:281:HIS:O	1:B:283:ALA:N	2.53	0.42
1:C:241:THR:N	1:C:242:PRO:CD	2.83	0.42
1:C:313:ASN:OD1	1:C:397:ASN:ND2	2.53	0.42
1:A:5:ILE:HB	1:A:17:VAL:O	2.19	0.42
1:A:99:GLN:O	1:A:99:GLN:HG3	2.20	0.42
1:A:303:SER:HB2	1:B:192:LEU:HB3	2.02	0.42
1:A:312:ILE:HA	1:A:396:ALA:HA	2.02	0.42
1:B:150:THR:CG2	1:B:228:VAL:HB	2.50	0.42
1:B:243:LYS:C	1:B:245:TYR:N	2.78	0.42
1:B:365:GLU:O	1:B:368:ILE:HB	2.20	0.42
1:C:308:GLY:O	1:C:309:LEU:C	2.63	0.42
1:C:373:PHE:O	1:C:374:GLU:C	2.63	0.42
1:C:406:TYR:C	1:C:408:SER:N	2.78	0.42
1:D:76:ILE:O	1:D:79:ALA:HB3	2.19	0.42
1:D:157:TYR:CD2	1:D:226:LEU:HD13	2.55	0.42
1:A:44:ILE:N	1:A:45:PRO:CD	2.83	0.42
1:A:93:PHE:CA	1:A:109:ASN:HD21	2.29	0.42
1:A:400:VAL:HG12	1:A:401:CYS:N	2.34	0.42
1:A:427:VAL:C	1:A:429:LYS:N	2.78	0.42
1:B:5:ILE:N	1:B:5:ILE:CD1	2.82	0.42
1:B:226:LEU:HD12	1:B:226:LEU:HA	1.87	0.42
1:B:231:GLY:O	1:B:241:THR:HB	2.20	0.42
1:B:391:ILE:HG13	1:B:392:ASN:N	2.34	0.42
1:A:194:ASP:H	1:B:305:PRO:HD2	1.85	0.41
1:A:310:ASN:O	1:A:400:VAL:HG11	2.20	0.41
1:A:374:GLU:O	1:A:378:ILE:HG12	2.20	0.41
1:B:100:GLY:HA3	1:D:331:VAL:O	2.20	0.41
1:B:198:MET:HG2	1:B:199:THR:N	2.35	0.41
1:B:286:ARG:O	1:B:289:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:VAL:C	1:B:365:GLU:H	2.28	0.41
1:B:363:VAL:HG11	1:C:191:GLN:HG2	2.01	0.41
1:C:96:ASP:HB3	1:C:98:TYR:O	2.19	0.41
1:C:101:GLY:O	1:C:103:GLY:N	2.53	0.41
1:C:175:GLU:HG2	1:C:208:SER:CB	2.49	0.41
1:D:213:GLU:HA	1:D:216:LYS:HD3	2.02	0.41
1:D:277:TYR:HA	1:D:280:VAL:HG22	2.02	0.41
1:D:280:VAL:HG23	1:D:281:HIS:H	1.84	0.41
1:D:395:THR:HG22	1:D:396:ALA:H	1.85	0.41
1:A:36:ILE:HG21	1:A:98:TYR:CG	2.55	0.41
1:A:74:ASN:O	1:A:78:ALA:CB	2.68	0.41
1:B:445:ARG:CB	1:B:447:LEU:HD13	2.50	0.41
1:D:126:LYS:NZ	1:D:126:LYS:CB	2.83	0.41
1:D:267:LEU:HG	1:D:268:ILE:HG23	2.02	0.41
1:A:27:THR:O	1:A:31:ILE:HG13	2.20	0.41
1:A:153:ARG:NH2	1:A:274:CYS:SG	2.94	0.41
1:B:44:ILE:N	1:B:45:PRO:CD	2.79	0.41
1:B:46:GLU:CG	1:B:47:PHE:H	2.33	0.41
1:B:281:HIS:HA	1:B:284:LEU:HD22	2.02	0.41
1:B:387:LEU:HA	1:B:391:ILE:HG12	2.02	0.41
1:C:59:ALA:O	1:C:60:MET:C	2.63	0.41
1:C:88:LYS:HG3	1:C:89:CYS:N	2.35	0.41
1:C:190:THR:HG23	1:C:195:ALA:HB2	2.02	0.41
1:C:235:ILE:CD1	1:C:236:GLY:N	2.81	0.41
1:C:243:LYS:O	1:C:244:GLU:C	2.62	0.41
1:C:324:MET:HB2	1:D:409:ILE:HB	2.02	0.41
1:D:203:GLU:O	1:D:206:ALA:HB3	2.20	0.41
1:D:226:LEU:CD2	1:D:260:PRO:HG2	2.49	0.41
1:D:403:GLY:O	1:D:407:ASN:HB2	2.19	0.41
1:A:239:LEU:O	1:A:242:PRO:HD2	2.20	0.41
1:A:315:PRO:HG3	1:A:390:CYS:O	2.21	0.41
1:A:324:MET:C	1:A:326:ALA:H	2.28	0.41
1:A:415:LEU:O	1:A:419:ILE:N	2.47	0.41
1:B:83:VAL:C	1:B:87:GLY:HA2	2.46	0.41
1:B:97:VAL:HG23	1:B:98:TYR:N	2.35	0.41
1:B:200:LEU:O	1:B:203:GLU:HB3	2.20	0.41
1:C:63:LYS:NZ	1:C:63:LYS:HB3	2.35	0.41
1:D:172:GLU:O	1:D:176:ARG:HB2	2.19	0.41
1:D:242:PRO:O	1:D:243:LYS:HB2	2.20	0.41
1:D:295:CYS:SG	1:D:336:VAL:CB	3.09	0.41
1:A:286:ARG:HB2	1:D:279:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HG	1:D:320:GLY:C	2.44	0.41
1:B:331:VAL:CG1	1:B:332:VAL:N	2.84	0.41
1:B:340:CYS:O	1:B:343:VAL:HB	2.20	0.41
1:C:6:ARG:NH1	1:C:127:GLY:HA3	2.34	0.41
1:D:414:TYR:O	1:D:418:PHE:CE2	2.74	0.41
1:A:1:MET:SD	1:A:2:SER:N	2.93	0.41
1:C:75:ALA:HB1	1:C:132:LEU:HD22	2.03	0.41
1:C:158:SER:HB3	1:C:259:PHE:CZ	2.56	0.41
1:C:390:CYS:O	1:C:394:ILE:HG13	2.21	0.41
1:A:10:ASP:CG	1:A:12:LEU:H	2.29	0.41
1:A:23:TYR:CD2	1:A:23:TYR:O	2.74	0.41
1:A:104:THR:O	1:A:105:SER:C	2.63	0.41
1:A:241:THR:O	1:A:245:TYR:HB3	2.20	0.41
1:A:405:VAL:CG2	1:A:406:TYR:H	2.34	0.41
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.79	0.41
1:C:293:LYS:HD3	1:C:293:LYS:C	2.45	0.41
1:C:312:ILE:HD12	1:C:394:ILE:HG21	2.02	0.41
1:A:322:SER:CA	1:B:429:LYS:HZ3	2.34	0.41
1:B:17:VAL:HG23	1:B:18:PRO:HD2	2.03	0.41
1:B:17:VAL:HA	1:B:18:PRO:HD3	1.90	0.41
1:B:87:GLY:O	1:B:89:CYS:N	2.54	0.41
1:B:357:GLY:O	1:C:293:LYS:HG2	2.20	0.41
1:B:398:LYS:HG2	1:B:402:GLU:HG3	2.02	0.41
1:C:320:GLY:O	1:C:322:SER:N	2.54	0.41
1:C:323:ILE:HB	1:C:324:MET:SD	2.61	0.41
1:D:62:ASN:HB3	1:D:68:ILE:HG12	2.02	0.41
1:D:62:ASN:HB3	1:D:67:THR:HG1	1.86	0.41
1:D:186:LYS:O	1:D:197:PRO:HA	2.20	0.41
1:A:35:TYR:O	1:C:381:ASN:HB3	2.20	0.41
1:A:196:VAL:HB	1:A:197:PRO:HD2	2.02	0.41
1:A:303:SER:O	1:A:308:GLY:HA3	2.20	0.41
1:A:312:ILE:HB	1:A:394:ILE:HG21	2.03	0.41
1:A:312:ILE:HD12	1:A:394:ILE:HD13	2.03	0.41
1:A:70:LYS:HZ2	1:A:74:ASN:HD21	1.69	0.40
1:C:163:LEU:O	1:C:167:ILE:HG13	2.21	0.40
1:C:272:SER:HA	1:C:362:ASN:H	1.85	0.40
1:D:54:VAL:CG1	1:D:55:LYS:N	2.84	0.40
1:A:89:CYS:HB3	1:A:117:ILE:HD13	2.03	0.40
1:A:317:LEU:N	1:A:317:LEU:CD2	2.84	0.40
1:B:264:ALA:O	1:B:265:GLU:C	2.64	0.40
1:B:264:ALA:O	1:B:266:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:PHE:HA	1:C:109:ASN:ND2	2.36	0.40
1:C:130:GLN:NE2	1:C:132:LEU:O	2.54	0.40
1:C:181:PHE:HZ	1:C:394:ILE:O	2.05	0.40
1:C:343:VAL:HG22	1:C:378:ILE:HD11	2.03	0.40
1:C:414:TYR:O	1:C:417:PRO:HD2	2.21	0.40
1:D:59:ALA:C	1:D:61:ALA:N	2.79	0.40
1:D:243:LYS:HD3	1:D:244:GLU:H	1.86	0.40
1:A:303:SER:O	1:A:304:GLY:O	2.39	0.40
1:A:314:LEU:HG	1:A:390:CYS:SG	2.61	0.40
1:A:317:LEU:N	1:A:317:LEU:HD23	2.37	0.40
1:A:325:PRO:HG2	1:B:409:ILE:CD1	2.52	0.40
1:B:74:ASN:HA	1:B:77:ILE:HG12	2.03	0.40
1:B:199:THR:HG22	1:B:202:GLN:CG	2.51	0.40
1:B:276:ALA:O	1:B:280:VAL:HG13	2.22	0.40
1:D:414:TYR:O	1:D:414:TYR:CD1	2.75	0.40
1:A:164:VAL:HG23	1:A:165:ASP:N	2.37	0.40
1:B:287:LEU:CD1	1:B:291:MET:HG3	2.52	0.40
1:B:343:VAL:HG21	1:B:379:LEU:CD2	2.49	0.40
1:C:124:HIS:CD2	1:C:131:TYR:CE1	3.10	0.40
1:C:172:GLU:CB	1:C:176:ARG:HH21	2.22	0.40
1:D:168:ASN:HD22	1:D:168:ASN:HA	1.70	0.40
1:A:387:LEU:O	1:A:392:ASN:HB2	2.22	0.40
1:C:11:LEU:C	1:C:13:GLY:H	2.30	0.40
1:C:177:LYS:O	1:C:180:GLU:HB3	2.22	0.40
1:D:25:VAL:HB	1:D:29:ARG:HH11	1.87	0.40
1:D:114:LEU:HD12	1:D:114:LEU:N	2.37	0.40
1:D:268:ILE:C	1:D:270:ALA:H	2.29	0.40
1:D:451:ALA:O	1:D:452:GLU:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/478 (96%)	341 (75%)	82 (18%)	34 (7%)	1	1
1	B	458/478 (96%)	352 (77%)	70 (15%)	36 (8%)	1	1
1	C	411/478 (86%)	295 (72%)	77 (19%)	39 (10%)	0	0
1	D	457/478 (96%)	356 (78%)	63 (14%)	38 (8%)	0	1
All	All	1783/1912 (93%)	1344 (75%)	292 (16%)	147 (8%)	0	1

All (147) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	25	VAL
1	A	84	LEU
1	A	88	LYS
1	A	232	ALA
1	A	235	ILE
1	A	242	PRO
1	A	244	GLU
1	A	245	TYR
1	A	267	LEU
1	A	304	GLY
1	A	319	ALA
1	A	328	VAL
1	A	456	ILE
1	A	457	PHE
1	B	41	ILE
1	B	46	GLU
1	B	85	ASN
1	B	237	THR
1	B	264	ALA
1	B	266	ASP
1	B	322	SER
1	B	328	VAL
1	B	459	VAL
1	C	47	PHE
1	C	85	ASN
1	C	90	MET
1	C	91	ASP
1	C	182	GLN
1	C	237	THR
1	C	239	LEU
1	C	242	PRO
1	C	245	TYR

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Mol	Chain	Res	Type
1	C	268	ILE
1	C	328	VAL
1	C	398	LYS
1	D	47	PHE
1	D	86	ASN
1	D	128	GLU
1	D	133	ASN
1	D	233	THR
1	D	239	LEU
1	D	243	LYS
1	D	273	ASP
1	D	303	SER
1	D	326	ALA
1	D	457	PHE
1	A	46	GLU
1	A	223	GLU
1	A	234	ALA
1	A	356	ALA
1	B	4	ASN
1	B	19	ALA
1	B	88	LYS
1	B	135	ASN
1	B	182	GLN
1	B	197	PRO
1	B	235	ILE
1	B	303	SER
1	B	307	ALA
1	B	309	LEU
1	B	325	PRO
1	B	364	MET
1	C	64	GLU
1	C	89	CYS
1	C	240	ASN
1	C	304	GLY
1	C	309	LEU
1	C	321	SER
1	C	396	ALA
1	D	46	GLU
1	D	64	GLU
1	D	234	ALA
1	D	267	LEU
1	D	304	GLY

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Mol	Chain	Res	Type
1	D	320	GLY
1	D	391	ILE
1	D	446	GLY
1	A	145	ASN
1	A	237	THR
1	A	398	LYS
1	B	102	ALA
1	B	234	ALA
1	B	243	LYS
1	B	270	ALA
1	C	102	ALA
1	C	236	GLY
1	C	270	ALA
1	C	359	LEU
1	C	397	ASN
1	D	85	ASN
1	D	186	LYS
1	D	390	CYS
1	D	398	LYS
1	A	4	ASN
1	A	33	ASN
1	A	89	CYS
1	A	128	GLU
1	A	143	SER
1	A	222	ALA
1	A	387	LEU
1	B	18	PRO
1	B	155	ALA
1	B	232	ALA
1	B	265	GLU
1	B	387	LEU
1	C	25	VAL
1	C	65	LEU
1	C	318	GLN
1	C	387	LEU
1	D	237	THR
1	D	411	ILE
1	D	443	LEU
1	A	94	PRO
1	B	44	ILE
1	B	45	PRO
1	B	304	GLY

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Mol	Chain	Res	Type
1	B	456	ILE
1	C	128	GLU
1	C	269	GLU
1	C	273	ASP
1	C	330	PRO
1	D	70	LYS
1	D	181	PHE
1	D	266	ASP
1	D	289	VAL
1	D	328	VAL
1	D	439	ARG
1	A	127	GLY
1	A	372	MET
1	B	90	MET
1	C	235	ILE
1	C	354	ALA
1	D	43	ASP
1	D	149	PRO
1	D	182	GLN
1	A	231	GLY
1	C	41	ILE
1	A	41	ILE
1	C	76	ILE
1	C	101	GLY
1	D	118	GLY
1	B	31	ILE
1	C	308	GLY
1	D	5	ILE
1	C	36	ILE
1	D	456	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	385/402 (96%)	339 (88%)	46 (12%)	5 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	386/402 (96%)	341 (88%)	45 (12%)	5	13
1	C	346/402 (86%)	302 (87%)	44 (13%)	4	11
1	D	385/402 (96%)	335 (87%)	50 (13%)	4	10
All	All	1502/1608 (93%)	1317 (88%)	185 (12%)	4	12

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	5	ILE
1	A	6	ARG
1	A	7	ILE
1	A	11	LEU
1	A	14	THR
1	A	17	VAL
1	A	20	ASP
1	A	32	GLU
1	A	35	TYR
1	A	65	LEU
1	A	72	VAL
1	A	77	ILE
1	A	86	ASN
1	A	94	PRO
1	A	125	GLN
1	A	145	ASN
1	A	162	LYS
1	A	169	GLN
1	A	186	LYS
1	A	210	LEU
1	A	212	LYS
1	A	221	THR
1	A	240	ASN
1	A	265	GLU
1	A	267	LEU
1	A	273	ASP
1	A	306	ARG
1	A	309	LEU
1	A	314	LEU
1	A	317	LEU
1	A	318	GLN

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Mol	Chain	Res	Type
1	A	324	MET
1	A	331	VAL
1	A	337	ASN
1	A	339	VAL
1	A	352	MET
1	A	360	GLN
1	A	363	VAL
1	A	385	ASN
1	A	392	ASN
1	A	400	VAL
1	A	422	HIS
1	A	426	ILE
1	A	448	LEU
1	B	5	ILE
1	B	17	VAL
1	B	28	LEU
1	B	43	ASP
1	B	46	GLU
1	B	49	ARG
1	B	72	VAL
1	B	83	VAL
1	B	88	LYS
1	B	136	ASP
1	B	145	ASN
1	B	162	LYS
1	B	165	ASP
1	B	168	ASN
1	B	169	GLN
1	B	172	GLU
1	B	194	ASP
1	B	197	PRO
1	B	212	LYS
1	B	224	LEU
1	B	226	LEU
1	B	237	THR
1	B	240	ASN
1	B	241	THR
1	B	243	LYS
1	B	246	SER
1	B	248	LEU
1	B	265	GLU
1	B	274	CYS

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Mol	Chain	Res	Type
1	B	284	LEU
1	B	306	ARG
1	B	314	LEU
1	B	324	MET
1	B	331	VAL
1	B	332	VAL
1	B	339	VAL
1	B	352	MET
1	B	355	GLU
1	B	361	LEU
1	B	370	GLN
1	B	385	ASN
1	B	404	TYR
1	B	439	ARG
1	B	443	LEU
1	B	459	VAL
1	C	5	ILE
1	C	6	ARG
1	C	16	GLU
1	C	17	VAL
1	C	18	PRO
1	C	20	ASP
1	C	25	VAL
1	C	39	ASN
1	C	52	VAL
1	C	55	LYS
1	C	63	LYS
1	C	64	GLU
1	C	72	VAL
1	C	77	ILE
1	C	88	LYS
1	C	95	VAL
1	C	107	ASN
1	C	114	LEU
1	C	128	GLU
1	C	139	ASN
1	C	154	ILE
1	C	172	GLU
1	C	185	LEU
1	C	189	ARG
1	C	196	VAL
1	C	210	LEU

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Mol	Chain	Res	Type
1	C	219	GLN
1	C	226	LEU
1	C	237	THR
1	C	241	THR
1	C	242	PRO
1	C	251	LYS
1	C	265	GLU
1	C	266	ASP
1	C	267	LEU
1	C	268	ILE
1	C	272	SER
1	C	284	LEU
1	C	310	ASN
1	C	321	SER
1	C	324	MET
1	C	370	GLN
1	C	378	ILE
1	C	411	ILE
1	D	4	ASN
1	D	5	ILE
1	D	7	ILE
1	D	11	LEU
1	D	17	VAL
1	D	25	VAL
1	D	34	PHE
1	D	52	VAL
1	D	67	THR
1	D	77	ILE
1	D	89	CYS
1	D	119	LEU
1	D	125	GLN
1	D	126	LYS
1	D	129	TYR
1	D	130	GLN
1	D	140	LYS
1	D	158	SER
1	D	179	VAL
1	D	203	GLU
1	D	211	LEU
1	D	223	GLU
1	D	226	LEU
1	D	227	GLU

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Mol	Chain	Res	Type
1	D	235	ILE
1	D	239	LEU
1	D	240	ASN
1	D	265	GLU
1	D	272	SER
1	D	316	GLU
1	D	323	ILE
1	D	324	MET
1	D	331	VAL
1	D	334	GLU
1	D	339	VAL
1	D	352	MET
1	D	360	GLN
1	D	363	VAL
1	D	370	GLN
1	D	385	ASN
1	D	395	THR
1	D	400	VAL
1	D	408	SER
1	D	409	ILE
1	D	413	THR
1	D	419	ILE
1	D	433	GLU
1	D	445	ARG
1	D	447	LEU
1	D	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	74	ASN
1	A	85	ASN
1	A	109	ASN
1	A	124	HIS
1	A	133	ASN
1	A	137	HIS
1	A	191	GLN
1	A	202	GLN
1	A	217	ASN
1	A	219	GLN
1	A	310	ASN

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Mol	Chain	Res	Type
1	A	313	ASN
1	A	318	GLN
1	A	329	ASN
1	A	337	ASN
1	A	358	GLN
1	A	360	GLN
1	A	370	GLN
1	A	381	ASN
1	A	416	ASN
1	A	421	HIS
1	B	3	ASN
1	B	38	ASN
1	B	66	GLN
1	B	74	ASN
1	B	85	ASN
1	B	99	GLN
1	B	124	HIS
1	B	142	GLN
1	B	145	ASN
1	B	191	GLN
1	B	193	GLN
1	B	202	GLN
1	B	346	ASN
1	B	360	GLN
1	B	377	HIS
1	B	421	HIS
1	C	62	ASN
1	C	107	ASN
1	C	109	ASN
1	C	111	ASN
1	C	124	HIS
1	C	125	GLN
1	C	130	GLN
1	C	137	HIS
1	C	139	ASN
1	C	145	ASN
1	C	168	ASN
1	C	202	GLN
1	C	219	GLN
1	C	313	ASN
1	C	329	ASN
1	C	338	GLN

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Mol	Chain	Res	Type
1	C	377	HIS
1	C	397	ASN
1	C	407	ASN
1	C	416	ASN
1	D	26	HIS
1	D	62	ASN
1	D	107	ASN
1	D	130	GLN
1	D	168	ASN
1	D	217	ASN
1	D	310	ASN
1	D	313	ASN
1	D	337	ASN
1	D	338	GLN
1	D	362	ASN
1	D	370	GLN
1	D	397	ASN
1	D	423	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	B	701	-	12,12,12	0.24	0	17,17,17	0.44	0
2	BGC	A	601	-	12,12,12	0.52	0	17,17,17	0.71	0
3	ACT	A	701	-	3,3,3	0.99	0	3,3,3	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	B	701	-	-	0/2/22/22	0/1/1/1
2	BGC	A	601	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BGC	C4-C5-C6-O6
2	A	601	BGC	O5-C5-C6-O6

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	459/478 (96%)	0.34	16 (3%) 47 43	2, 23, 50, 79	0
1	B	460/478 (96%)	0.34	20 (4%) 40 36	4, 22, 50, 69	0
1	C	413/478 (86%)	0.39	24 (5%) 29 25	3, 23, 46, 81	0
1	D	459/478 (96%)	0.35	19 (4%) 41 37	4, 21, 49, 100	0
All	All	1791/1912 (93%)	0.35	79 (4%) 39 35	2, 22, 49, 100	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	87	GLY	8.7
1	B	304	GLY	6.9
1	A	273	ASP	5.8
1	C	87	GLY	5.5
1	B	273	ASP	5.2
1	B	241	THR	4.8
1	D	242	PRO	4.5
1	A	272	SER	4.2
1	D	237	THR	4.1
1	A	87	GLY	4.1
1	A	44	ILE	3.9
1	C	326	ALA	3.8
1	C	86	ASN	3.8
1	C	273	ASP	3.6
1	C	413	THR	3.6
1	C	272	SER	3.5
1	D	326	ALA	3.5
1	A	236	GLY	3.4
1	C	45	PRO	3.4
1	D	32	GLU	3.3
1	A	45	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	86	ASN	3.0
1	C	238	GLY	3.0
1	B	3	ASN	3.0
1	D	454	ASP	3.0
1	A	323	ILE	3.0
1	D	272	SER	2.9
1	C	32	GLU	2.9
1	C	241	THR	2.9
1	D	88	LYS	2.9
1	C	323	ILE	2.8
1	A	233	THR	2.8
1	B	349	THR	2.8
1	C	242	PRO	2.8
1	C	88	LYS	2.8
1	B	323	ILE	2.7
1	B	320	GLY	2.7
1	D	45	PRO	2.6
1	A	5	ILE	2.6
1	A	86	ASN	2.6
1	B	272	SER	2.5
1	C	371	ALA	2.5
1	C	324	MET	2.5
1	D	44	ILE	2.5
1	D	273	ASP	2.5
1	C	410	GLY	2.5
1	A	304	GLY	2.4
1	B	234	ALA	2.4
1	B	45	PRO	2.4
1	A	234	ALA	2.4
1	B	326	ALA	2.4
1	C	44	ILE	2.3
1	C	309	LEU	2.3
1	D	451	ALA	2.3
1	C	234	ALA	2.3
1	B	324	MET	2.2
1	A	19	ALA	2.2
1	D	353	ALA	2.2
1	C	129	TYR	2.2
1	C	412	VAL	2.2
1	B	44	ILE	2.2
1	B	102	ALA	2.2
1	D	270	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	420	GLY	2.2
1	B	2	SER	2.2
1	B	457	PHE	2.1
1	A	32	GLU	2.1
1	D	40	LYS	2.1
1	C	320	GLY	2.1
1	A	346	ASN	2.1
1	D	50	GLY	2.1
1	B	19	ALA	2.1
1	C	271	THR	2.1
1	C	308	GLY	2.1
1	B	32	GLU	2.0
1	B	321	SER	2.0
1	A	1	MET	2.0
1	D	263	PRO	2.0
1	D	304	GLY	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
3	ACT	A	701	4/4	0.74	0.11	31,31,31,31	0
2	BGC	A	601	12/12	0.79	0.08	43,43,43,43	0
2	BGC	B	701	12/12	0.82	0.11	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.