



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:27 PM UTC

PDB ID : 1PO3 / pdb_00001po3
Title : Crystal structure of ferric citrate transporter FecA in complex with ferric citrate
Authors : Yue, W.W.; Grizot, S.; Buchanan, S.K.
Deposited on : 2003-06-13
Resolution : 3.40 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

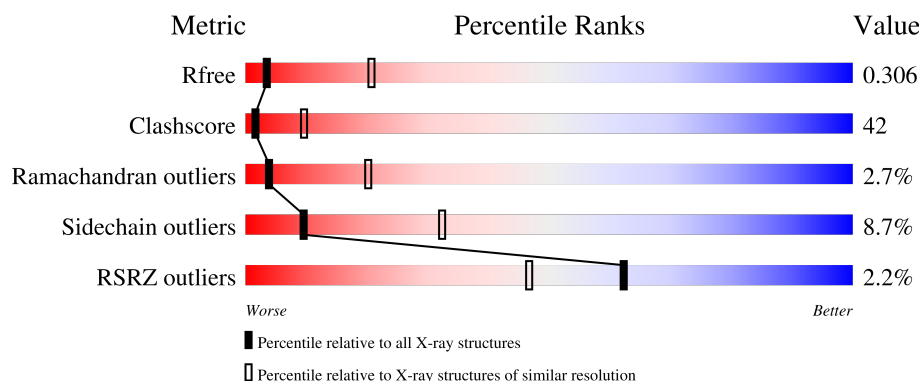
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	751	
1	B	751	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	A	742	-	X	X	-
2	FLC	A	743	-	X	-	-
2	FLC	B	743	-	X	-	-

2 Entry composition [i](#)

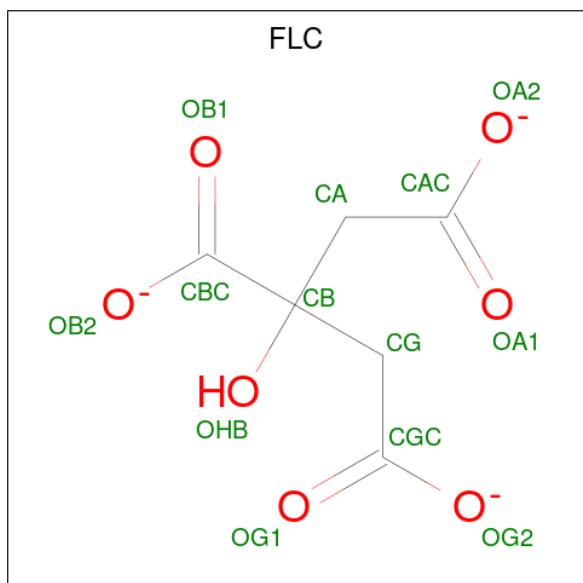
There are 3 unique types of molecules in this entry. The entry contains 10024 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Iron(III) dicitrate transport protein fecA precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	S	0	0	0
			4998	3127	880	979	12			
1	B	645	Total	C	N	O	S	0	0	0
			4970	3107	879	974	10			

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

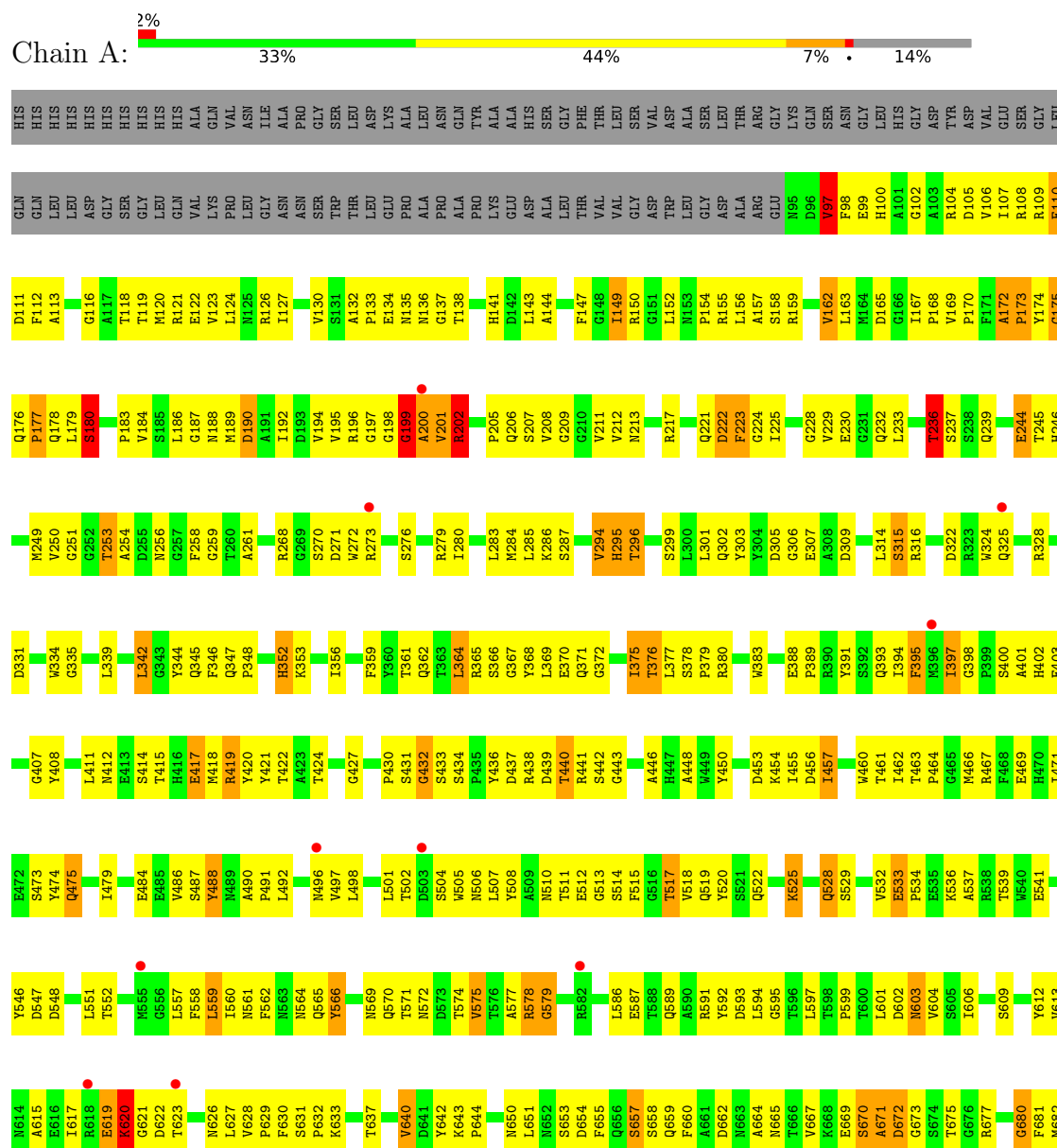
- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Fe 2	0	0
3	B	2	Total 2	Fe 2	0	0

3 Residue-property plots

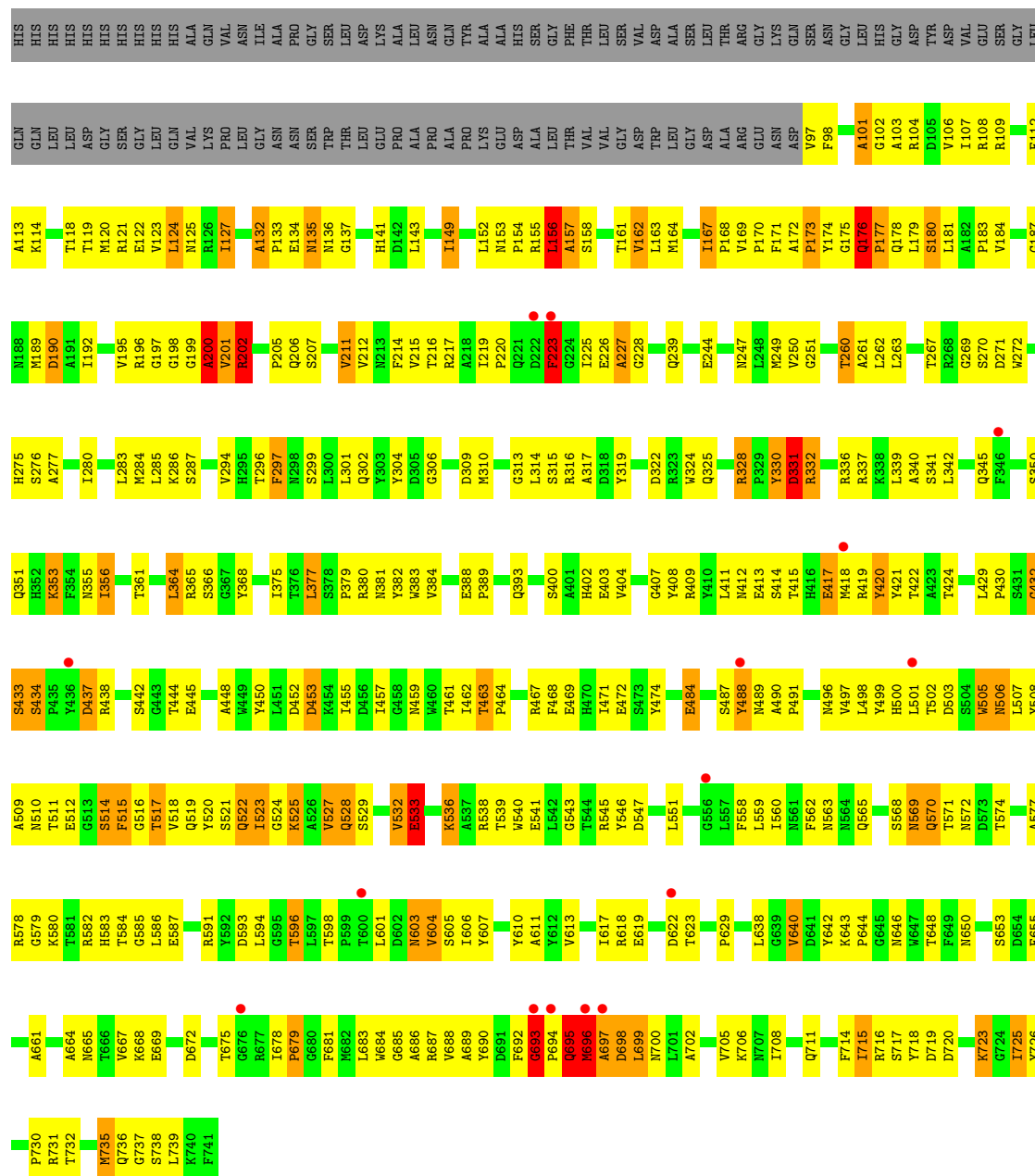
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Iron(III) dicitrate transport protein fecA precursor





- Molecule 1: Iron(III) dicitrate transport protein fecA precursor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.49Å 147.00Å 96.13Å 90.00° 110.58° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40 15.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.40) 98.8 (15.00-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.314 0.242 , 0.306	Depositor DCC
R_{free} test set	1532 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10024	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: FLC, FE

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	0.92	6/5125 (0.1%)	1.25	47/6966 (0.7%)
1	B	0.86	9/5095 (0.2%)	1.28	59/6925 (0.9%)
All	All	0.89	15/10220 (0.1%)	1.26	106/13891 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	PRO	N-CD	-29.82	1.06	1.47
1	B	696	MET	C-N	25.55	1.72	1.33
1	A	173	PRO	N-CA	24.40	1.77	1.47
1	B	697	ALA	N-CA	23.34	1.80	1.46
1	A	200	ALA	N-CA	21.55	1.74	1.46
1	B	533	GLU	C-N	-11.04	1.13	1.34
1	B	697	ALA	C-N	10.76	1.48	1.33
1	B	173	PRO	N-CD	-9.77	1.34	1.47
1	A	158	SER	N-CA	9.70	1.58	1.46
1	B	506	ASN	N-CA	8.21	1.55	1.45
1	B	331	ASP	C-N	7.30	1.42	1.33
1	B	332	ARG	N-CA	6.50	1.53	1.46
1	B	132	ALA	CA-CB	-5.88	1.45	1.53
1	A	295	HIS	CA-C	-5.75	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	PRO	N-CD	-5.61	1.40	1.47

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ALA	CA-C-N	-22.07	95.62	120.12
1	A	172	ALA	C-N-CA	-22.07	95.62	120.12
1	B	332	ARG	N-CA-C	-14.38	86.03	108.76
1	A	200	ALA	N-CA-CB	-14.26	86.40	110.49
1	A	202	ARG	N-CA-C	-14.17	96.89	114.75
1	B	697	ALA	N-CA-CB	-14.10	84.33	110.56
1	B	525	LYS	N-CA-C	13.07	130.50	109.85
1	A	575	VAL	N-CA-C	12.76	119.86	106.21
1	B	433	SER	N-CA-C	-12.41	93.81	111.56
1	B	696	MET	CA-C-N	-12.36	103.83	123.23
1	B	696	MET	C-N-CA	-12.36	103.83	123.23
1	B	331	ASP	CA-C-N	-12.25	98.11	121.63
1	B	331	ASP	C-N-CA	-12.25	98.11	121.63
1	A	173	PRO	N-CA-CB	-11.90	91.29	103.19
1	B	202	ARG	N-CA-C	-11.70	97.42	114.39
1	B	331	ASP	O-C-N	-11.40	107.42	122.59
1	B	533	GLU	O-C-N	11.38	134.40	121.32
1	B	330	TYR	N-CA-C	-10.90	92.99	110.32
1	B	201	VAL	N-CA-CB	-10.35	94.14	111.23
1	A	680	GLY	N-CA-C	-10.30	98.45	112.57
1	A	697	ALA	N-CA-C	10.28	132.69	110.80
1	B	532	VAL	O-C-N	-10.22	109.74	122.52
1	A	672	ASP	N-CA-C	-9.74	101.15	113.23
1	B	696	MET	O-C-N	-9.44	110.04	122.59
1	A	180	SER	N-CA-C	-9.08	101.35	111.07
1	A	97	VAL	N-CA-C	8.70	127.43	109.34
1	B	176	GLN	CA-C-N	-8.68	110.80	119.56
1	B	176	GLN	C-N-CA	-8.68	110.80	119.56
1	A	695	GLN	N-CA-C	-8.62	101.72	108.78
1	B	694	PRO	N-CA-C	-8.43	104.09	114.20
1	A	294	VAL	CB-CA-C	-8.20	103.75	111.05
1	B	532	VAL	CA-C-N	8.19	141.78	121.80
1	B	532	VAL	C-N-CA	8.19	141.78	121.80
1	B	434	SER	CA-C-N	7.71	129.48	119.84
1	B	434	SER	C-N-CA	7.71	129.48	119.84
1	A	294	VAL	N-CA-C	-7.60	105.62	111.62
1	A	620	LYS	N-CA-C	7.49	126.76	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	SER	N-CA-C	-7.10	100.97	110.55
1	A	432	GLY	N-CA-C	-7.08	101.67	112.51
1	A	199	GLY	CA-C-N	-7.08	108.02	121.54
1	A	199	GLY	C-N-CA	-7.08	108.02	121.54
1	B	527	VAL	N-CA-C	-6.93	98.14	108.46
1	A	126	ARG	N-CA-C	-6.92	104.65	113.23
1	B	604	VAL	N-CA-C	-6.91	98.22	108.99
1	A	623	THR	N-CA-C	6.86	121.40	112.89
1	B	532	VAL	N-CA-C	6.85	117.52	110.05
1	B	424	THR	N-CA-C	-6.82	103.87	111.71
1	A	223	PHE	N-CA-C	6.80	119.77	109.23
1	A	376	THR	N-CA-C	6.72	120.35	109.40
1	A	670	SER	N-CA-C	6.63	121.11	112.89
1	B	693	GLY	CA-C-N	-6.52	112.88	120.12
1	B	693	GLY	C-N-CA	-6.52	112.88	120.12
1	B	505	TRP	CA-C-N	-6.46	111.95	122.81
1	B	505	TRP	C-N-CA	-6.46	111.95	122.81
1	B	328	ARG	CA-C-N	6.41	126.17	119.05
1	B	328	ARG	C-N-CA	6.41	126.17	119.05
1	A	621	GLY	N-CA-C	6.36	128.25	113.18
1	A	201	VAL	N-CA-C	-6.32	96.20	109.34
1	A	717	SER	N-CA-C	-6.27	98.69	108.90
1	B	158	SER	N-CA-C	6.24	118.89	111.71
1	B	377	LEU	N-CA-C	-6.20	98.18	108.34
1	B	432	GLY	N-CA-C	-6.12	98.66	113.18
1	A	132	ALA	CA-C-N	6.09	126.11	119.89
1	A	132	ALA	C-N-CA	6.09	126.11	119.89
1	B	157	ALA	N-CA-CB	-6.06	102.93	112.08
1	B	294	VAL	CB-CA-C	-5.95	105.79	111.44
1	B	223	PHE	CA-C-N	5.92	129.66	121.26
1	B	223	PHE	C-N-CA	5.92	129.66	121.26
1	B	158	SER	CA-C-N	-5.82	114.50	123.17
1	B	158	SER	C-N-CA	-5.82	114.50	123.17
1	B	153	ASN	CA-C-N	5.79	125.41	119.56
1	B	153	ASN	C-N-CA	5.79	125.41	119.56
1	A	224	GLY	N-CA-C	5.77	121.84	110.83
1	A	697	ALA	N-CA-CB	-5.74	100.79	110.49
1	B	695	GLN	N-CA-C	-5.64	101.57	109.69
1	A	579	GLY	N-CA-C	5.61	122.01	111.80
1	A	158	SER	N-CA-C	-5.56	106.45	113.18
1	A	575	VAL	CB-CA-C	-5.55	107.00	113.22
1	A	711	GLN	N-CA-C	-5.55	103.06	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	GLU	CA-C-N	5.54	140.28	127.00
1	B	533	GLU	C-N-CA	5.54	140.28	127.00
1	A	138	THR	N-CA-C	-5.45	104.74	111.33
1	A	446	ALA	N-CA-C	5.44	117.28	108.41
1	A	643	LYS	N-CA-C	5.42	118.47	108.94
1	B	725	ILE	N-CA-C	5.42	115.90	107.99
1	A	375	ILE	N-CA-C	-5.41	100.32	108.12
1	B	420	TYR	N-CA-C	-5.40	101.77	110.14
1	B	524	GLY	CA-C-N	-5.40	113.74	122.81
1	B	524	GLY	C-N-CA	-5.40	113.74	122.81
1	A	157	ALA	CA-C-N	-5.38	111.09	121.58
1	A	157	ALA	C-N-CA	-5.38	111.09	121.58
1	B	294	VAL	N-CA-C	-5.38	106.94	111.56
1	B	156	LEU	N-CA-C	5.36	122.22	110.80
1	A	175	GLY	N-CA-C	5.36	120.56	114.67
1	B	137	GLY	N-CA-C	5.35	120.98	111.73
1	A	199	GLY	N-CA-C	5.34	120.21	110.71
1	A	222	ASP	N-CA-C	-5.29	99.53	110.80
1	B	569	ASN	N-CA-CB	5.29	119.42	110.49
1	B	429	LEU	CA-C-N	5.28	126.44	119.84
1	B	429	LEU	C-N-CA	5.28	126.44	119.84
1	A	427	GLY	N-CA-C	-5.25	108.15	114.66
1	B	667	VAL	N-CA-C	5.23	115.89	110.82
1	B	543	GLY	N-CA-C	5.21	120.62	110.73
1	A	597	LEU	N-CA-C	-5.14	107.66	114.04
1	B	269	GLY	N-CA-C	5.06	118.15	110.97
1	A	190	ASP	N-CA-C	-5.05	107.50	113.97

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	GLY	Peptide
1	B	200	ALA	Peptide
1	B	223	PHE	Sidechain

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	4998	0	4673	421	0
1	B	4970	0	4651	390	0
2	A	26	0	9	5	0
2	B	26	0	8	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	10024	0	9341	811	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 (811) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:MET:C	1:B:697:ALA:N	1.72	1.48
1:A:200:ALA:N	1:A:200:ALA:CA	1.74	1.46
1:B:697:ALA:N	1:B:697:ALA:CA	1.80	1.43
1:A:173:PRO:N	1:A:173:PRO:CA	1.77	1.35
1:A:692:PHE:HE1	1:A:701:LEU:HD12	1.17	1.08
1:B:498:LEU:HD11	1:B:506:ASN:HB3	1.37	1.04
1:A:200:ALA:N	1:A:200:ALA:CB	2.23	1.02
1:A:172:ALA:C	1:A:173:PRO:CA	2.32	1.01
1:B:697:ALA:N	1:B:697:ALA:CB	2.22	1.01
1:B:366:SER:HB3	1:B:379:PRO:HA	1.39	1.01
1:A:571:THR:HG21	1:A:723:LYS:HZ1	1.26	0.98
1:B:181:LEU:O	1:B:183:PRO:HD3	1.65	0.97
1:A:619:GLU:HG3	1:A:620:LYS:H	1.30	0.96
1:A:316:ARG:HD3	1:A:669:GLU:OE1	1.65	0.96
1:B:201:VAL:HG13	1:B:467:ARG:HB2	1.48	0.94
1:B:463:THR:HB	1:B:496:ASN:HB2	1.50	0.94
1:B:404:VAL:HG22	1:B:453:ASP:HB2	1.49	0.94
1:B:176:GLN:HE21	1:B:176:GLN:HA	1.31	0.93
1:A:692:PHE:CE1	1:A:701:LEU:HD12	2.02	0.93
1:B:189:MET:HE3	1:B:214:PHE:CB	1.98	0.93
1:A:201:VAL:HG13	1:A:467:ARG:HB2	1.51	0.93
1:B:419:ARG:HH21	1:B:438:ARG:NH2	1.65	0.92
1:A:571:THR:HG21	1:A:723:LYS:NZ	1.84	0.92
1:A:486:VAL:HB	1:A:488:TYR:HE2	1.32	0.91
1:A:362:GLN:NE2	1:A:383:TRP:HE1	1.69	0.91
1:A:239:GLN:HG2	1:A:271:ASP:O	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:GLN:HE21	1:B:570:GLN:HA	1.34	0.91
1:A:239:GLN:NE2	1:A:270:SER:HB2	1.87	0.90
1:B:189:MET:HE3	1:B:214:PHE:HB2	1.55	0.89
1:B:196:ARG:HH21	1:B:587:GLU:CD	1.82	0.88
1:B:316:ARG:HD3	1:B:669:GLU:OE1	1.74	0.88
1:A:487:SER:C	1:A:488:TYR:HD2	1.81	0.87
1:B:697:ALA:O	1:B:698:ASP:C	2.18	0.87
1:A:626:ASN:HB3	1:A:665:ASN:ND2	1.90	0.86
1:A:199:GLY:C	1:A:200:ALA:CA	2.49	0.86
1:B:267:THR:HB	1:B:280:ILE:HB	1.56	0.86
1:A:486:VAL:HB	1:A:488:TYR:CE2	2.12	0.85
1:A:696:MET:HG2	1:A:697:ALA:H	1.38	0.85
1:B:223:PHE:HE1	1:B:251:GLY:N	1.75	0.83
1:A:453:ASP:OD2	1:A:455:ILE:HD11	1.77	0.83
1:A:172:ALA:O	1:A:173:PRO:CA	2.28	0.81
1:A:488:TYR:HD2	1:A:488:TYR:N	1.77	0.81
1:B:422:THR:OG1	1:B:430:PRO:HD3	1.79	0.81
1:B:693:GLY:C	1:B:695:GLN:H	1.87	0.80
1:B:580:LYS:H	1:B:619:GLU:HB2	1.44	0.80
1:A:715:ILE:HD13	1:A:715:ILE:H	1.47	0.80
1:A:431:SER:O	1:A:434:SER:HB3	1.81	0.80
1:B:366:SER:CB	1:B:379:PRO:HA	2.12	0.80
1:A:498:LEU:HD12	1:A:507:LEU:O	1.83	0.79
1:B:136:ASN:HA	1:B:726:TYR:CE2	2.17	0.79
1:A:225:ILE:HG12	1:A:250:VAL:HG22	1.65	0.79
1:A:366:SER:CB	1:A:379:PRO:HA	2.13	0.78
1:B:521:SER:O	1:B:525:LYS:HD2	1.83	0.78
1:A:328:ARG:NH1	1:A:370:GLU:HB3	1.98	0.78
1:A:208:VAL:HB	1:A:514:SER:OG	1.84	0.78
1:B:189:MET:HE3	1:B:214:PHE:HB3	1.66	0.78
1:B:562:PHE:O	1:B:580:LYS:HG3	1.84	0.77
1:B:469:GLU:HB3	1:B:471:ILE:HD11	1.67	0.77
1:B:175:GLY:HA3	1:B:520:TYR:CE2	2.19	0.77
1:B:220:PRO:HG2	1:B:251:GLY:O	1.85	0.77
1:B:143:LEU:CD1	1:B:280:ILE:HD11	2.16	0.76
1:B:223:PHE:CZ	1:B:250:VAL:HG13	2.20	0.76
1:A:504:SER:HB2	1:A:547:ASP:O	1.85	0.76
1:B:220:PRO:CG	1:B:251:GLY:O	2.33	0.76
1:B:98:PHE:HA	1:B:545:ARG:HD2	1.66	0.76
1:B:176:GLN:HA	1:B:176:GLN:NE2	2.01	0.75
1:B:201:VAL:CG1	1:B:467:ARG:HB2	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLY:O	1:B:314:LEU:HD23	1.85	0.75
1:A:107:ILE:N	1:A:107:ILE:HD12	2.02	0.75
1:A:194:VAL:HG13	1:A:212:VAL:HG22	1.68	0.75
1:A:488:TYR:N	1:A:488:TYR:CD2	2.52	0.75
1:A:124:LEU:HD11	1:A:192:ILE:HG21	1.68	0.75
1:A:419:ARG:HD2	1:A:437:ASP:OD1	1.87	0.74
1:B:178:GLN:OE1	1:B:178:GLN:N	2.15	0.74
1:A:366:SER:HB3	1:A:379:PRO:HA	1.67	0.74
1:A:118:THR:HG23	1:A:119:THR:HG23	1.67	0.74
1:A:375:ILE:HD11	1:A:424:THR:HG23	1.69	0.74
1:B:179:LEU:C	1:B:181:LEU:H	1.96	0.73
1:B:223:PHE:HD1	1:B:251:GLY:C	1.95	0.73
1:A:163:LEU:O	1:A:213:ASN:HA	1.88	0.73
1:A:422:THR:HG23	1:A:430:PRO:HB3	1.70	0.73
1:A:705:VAL:HB	1:A:708:ILE:CD1	2.17	0.73
1:B:560:ILE:HB	1:B:583:HIS:HB2	1.70	0.72
1:B:199:GLY:O	1:B:201:VAL:N	2.23	0.72
1:A:362:GLN:HE21	1:A:383:TRP:HE1	1.37	0.71
1:B:163:LEU:HD23	1:B:168:PRO:HA	1.72	0.71
1:A:401:ALA:HB3	1:A:456:ASP:HB2	1.72	0.71
1:A:417:GLU:HG2	1:A:440:THR:HG23	1.73	0.71
1:A:199:GLY:O	1:A:201:VAL:N	2.22	0.71
1:A:201:VAL:CG1	1:A:467:ARG:HB2	2.21	0.71
1:B:109:ARG:HA	1:B:112:PHE:CD2	2.25	0.71
1:A:619:GLU:CG	1:A:620:LYS:H	2.02	0.70
1:B:223:PHE:CZ	1:B:225:ILE:HG13	2.26	0.70
1:B:697:ALA:HB1	1:B:739:LEU:CD1	2.21	0.70
1:B:697:ALA:HB1	1:B:739:LEU:HD11	1.72	0.70
1:A:670:SER:HB3	1:A:675:THR:HB	1.72	0.70
1:B:197:GLY:HA3	1:B:541:GLU:OE1	1.90	0.70
1:B:693:GLY:C	1:B:695:GLN:N	2.46	0.70
1:B:468:PHE:CZ	1:B:489:ASN:HB3	2.27	0.70
1:B:570:GLN:HE21	1:B:570:GLN:CA	2.05	0.70
1:B:184:VAL:HG21	1:B:214:PHE:CD2	2.27	0.70
1:B:565:GLN:OE1	1:B:578:ARG:NH1	2.26	0.69
1:A:152:LEU:HD21	1:A:562:PHE:CZ	2.27	0.69
1:A:533:GLU:CB	1:A:534:PRO:HA	2.21	0.69
1:A:130:VAL:HG22	1:A:149:ILE:HG22	1.74	0.69
1:A:504:SER:O	1:A:546:TYR:HD2	1.76	0.69
1:B:118:THR:HG23	1:B:119:THR:HG23	1.75	0.69
1:B:527:VAL:CG2	1:B:577:ALA:HB2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:PHE:HA	1:A:659:GLN:OE1	1.92	0.68
1:B:692:PHE:H	1:B:692:PHE:HD2	1.41	0.68
1:A:380:ARG:HH22	2:A:742:FLC:HA1	1.59	0.68
1:A:626:ASN:CG	1:A:665:ASN:HD22	2.02	0.68
1:B:155:ARG:HG3	1:B:156:LEU:HD22	1.75	0.68
1:A:244:GLU:CD	1:A:246:HIS:HD1	2.02	0.68
1:B:124:LEU:HA	1:B:127:ILE:HD12	1.76	0.68
1:B:223:PHE:CE1	1:B:251:GLY:N	2.61	0.68
1:A:525:LYS:HB3	1:A:532:VAL:H	1.58	0.67
1:B:468:PHE:HZ	1:B:489:ASN:HB3	1.59	0.67
1:B:384:VAL:HG13	1:B:411:LEU:HD21	1.75	0.67
1:B:638:LEU:C	1:B:638:LEU:HD12	2.19	0.67
1:A:664:ALA:O	1:A:665:ASN:HB2	1.94	0.67
1:A:628:VAL:HG12	1:A:629:PRO:HD2	1.77	0.67
1:A:626:ASN:HB3	1:A:665:ASN:HD22	1.58	0.67
1:B:227:ALA:HA	1:B:247:ASN:O	1.94	0.67
1:B:582:ARG:NH1	1:B:618:ARG:HD2	2.09	0.67
1:A:109:ARG:O	1:A:111:ASP:N	2.28	0.66
1:B:302:GLN:HB3	1:B:339:LEU:HB3	1.76	0.66
1:A:230:GLU:HA	1:A:735:MET:O	1.96	0.66
1:A:411:LEU:HD23	1:A:412:ASN:N	2.11	0.66
1:B:104:ARG:HG3	1:B:195:VAL:HG22	1.75	0.66
1:A:670:SER:O	1:A:671:ALA:HB3	1.96	0.66
1:A:391:TYR:HE1	1:A:393:GLN:HB2	1.61	0.66
1:A:273:ARG:HH12	1:A:726:TYR:CB	2.08	0.65
1:A:589:GLN:HA	1:A:609:SER:HA	1.78	0.65
1:A:487:SER:C	1:A:488:TYR:CD2	2.70	0.65
1:A:667:VAL:HG12	1:A:667:VAL:O	1.94	0.65
1:A:570:GLN:HE21	1:A:570:GLN:HA	1.61	0.65
1:A:198:GLY:N	1:A:512:GLU:OE2	2.30	0.65
1:B:499:TYR:HD2	1:B:501:LEU:HD22	1.61	0.65
1:A:715:ILE:HD13	1:A:715:ILE:N	2.11	0.65
1:B:593:ASP:O	1:B:596:THR:HB	1.97	0.65
1:B:184:VAL:HG23	1:B:189:MET:HE2	1.78	0.65
1:B:223:PHE:CZ	1:B:225:ILE:CG1	2.80	0.65
1:A:176:GLN:NE2	1:A:178:GLN:OE1	2.30	0.64
1:B:569:ASN:HA	1:B:719:ASP:HB3	1.79	0.64
1:A:570:GLN:HB3	2:A:742:FLC:OB1	1.98	0.64
1:A:471:ILE:O	1:A:487:SER:HA	1.97	0.64
1:B:407:GLY:HA3	1:B:450:TYR:CE2	2.32	0.64
1:A:626:ASN:CB	1:A:665:ASN:HD22	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLN:HG3	1:B:239:GLN:O	1.97	0.64
1:A:194:VAL:HG13	1:A:212:VAL:CG2	2.27	0.63
1:B:179:LEU:O	1:B:181:LEU:N	2.31	0.63
1:A:127:ILE:HD13	1:A:194:VAL:HG21	1.79	0.63
1:A:498:LEU:HD11	1:A:506:ASN:HB3	1.79	0.63
1:A:159:ARG:O	1:A:209:GLY:HA3	1.97	0.63
1:B:239:GLN:NE2	1:B:270:SER:HB2	2.14	0.63
1:B:606:ILE:HG22	1:B:640:VAL:HB	1.79	0.63
1:B:383:TRP:HB2	1:B:414:SER:OG	1.99	0.63
1:B:472:GLU:HG2	1:B:487:SER:HB2	1.79	0.63
1:A:324:TRP:CH2	1:A:730:PRO:HG3	2.34	0.63
1:B:190:ASP:N	1:B:215:VAL:O	2.29	0.63
1:B:510:ASN:OD1	1:B:541:GLU:HB2	1.99	0.63
1:B:580:LYS:N	1:B:619:GLU:HB2	2.14	0.62
1:A:229:VAL:HG22	1:A:230:GLU:N	2.13	0.62
1:B:223:PHE:HE1	1:B:251:GLY:H	1.48	0.62
1:B:239:GLN:HE21	1:B:270:SER:CB	2.12	0.62
1:A:708:ILE:O	1:A:731:ARG:NE	2.29	0.62
1:B:368:TYR:CE1	1:B:377:LEU:HD13	2.34	0.62
1:A:380:ARG:NH1	2:A:742:FLC:HG1	2.14	0.62
1:A:443:GLY:HA3	1:A:474:TYR:CE2	2.34	0.62
1:A:711:GLN:NE2	1:A:712:ASP:N	2.48	0.62
1:B:522:GLN:HA	1:B:525:LYS:HD2	1.79	0.62
1:A:662:ASP:OD2	1:A:664:ALA:HB3	2.00	0.62
1:A:109:ARG:C	1:A:111:ASP:H	2.07	0.62
1:A:316:ARG:NH1	1:A:669:GLU:OE2	2.33	0.62
1:A:705:VAL:HB	1:A:708:ILE:HD13	1.80	0.62
1:B:499:TYR:CD2	1:B:501:LEU:HD22	2.35	0.62
1:A:225:ILE:HA	1:A:249:MET:O	1.99	0.61
1:B:167:ILE:N	1:B:167:ILE:HD12	2.16	0.61
1:A:273:ARG:HH12	1:A:726:TYR:HB3	1.64	0.61
1:B:178:GLN:H	1:B:178:GLN:CD	2.08	0.61
1:B:692:PHE:CD2	1:B:692:PHE:N	2.67	0.61
1:A:253:THR:HG23	1:A:259:GLY:HA3	1.82	0.61
1:B:223:PHE:HZ	1:B:250:VAL:HG13	1.64	0.61
1:B:735:MET:HE2	1:B:736:GLN:C	2.24	0.61
1:A:178:GLN:CD	1:A:178:GLN:H	2.09	0.61
1:A:436:TYR:HE1	1:A:479:ILE:HD11	1.65	0.61
1:B:591:ARG:NH1	1:B:607:TYR:HD2	1.99	0.61
1:A:200:ALA:O	1:A:201:VAL:HB	2.00	0.61
1:A:626:ASN:CB	1:A:665:ASN:ND2	2.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PRO:HD2	1:B:251:GLY:C	2.25	0.61
1:A:195:VAL:HB	1:A:211:VAL:CG1	2.31	0.61
1:B:511:THR:HA	1:B:539:THR:O	2.01	0.61
1:B:501:LEU:CD2	1:B:507:LEU:HD13	2.31	0.61
1:A:239:GLN:NE2	1:A:270:SER:CB	2.63	0.61
1:B:223:PHE:HZ	1:B:225:ILE:CG1	2.14	0.61
1:B:512:GLU:N	1:B:512:GLU:OE1	2.33	0.61
1:A:150:ARG:HD3	1:A:560:ILE:HD11	1.83	0.60
1:A:364:LEU:HD22	1:A:365:ARG:N	2.15	0.60
1:B:546:TYR:CD1	1:B:547:ASP:N	2.70	0.60
1:B:120:MET:HE3	1:B:184:VAL:HG22	1.81	0.60
1:B:536:LYS:N	1:B:563:ASN:OD1	2.34	0.60
1:B:569:ASN:C	1:B:569:ASN:HD22	2.08	0.60
1:B:161:THR:HB	1:B:211:VAL:HB	1.83	0.60
1:B:223:PHE:CD1	1:B:251:GLY:C	2.79	0.60
1:A:120:MET:HE3	1:A:184:VAL:HG22	1.83	0.60
1:B:179:LEU:C	1:B:181:LEU:N	2.56	0.60
1:A:149:ILE:HD12	1:A:209:GLY:O	2.02	0.60
1:B:356:ILE:O	1:B:356:ILE:HG23	2.02	0.60
1:B:572:ASN:O	1:B:574:THR:HG23	2.01	0.60
1:B:697:ALA:O	1:B:699:LEU:N	2.35	0.60
1:A:149:ILE:HD13	1:A:149:ILE:H	1.67	0.59
1:A:144:ALA:HB2	1:A:180:SER:O	2.02	0.59
1:A:102:GLY:HA3	1:A:197:GLY:O	2.03	0.59
1:A:502:THR:C	1:A:504:SER:H	2.11	0.59
1:B:527:VAL:HG21	1:B:577:ALA:HB2	1.84	0.59
1:A:440:THR:OG1	1:A:441:ARG:N	2.35	0.59
1:B:172:ALA:HB3	1:B:176:GLN:HB2	1.84	0.59
1:A:302:GLN:HB3	1:A:339:LEU:HB3	1.85	0.59
1:B:730:PRO:O	1:B:731:ARG:C	2.46	0.59
1:A:307:GLU:HA	1:A:334:TRP:HA	1.86	0.58
1:B:175:GLY:HA3	1:B:520:TYR:CZ	2.38	0.58
1:A:268:ARG:HG2	1:A:268:ARG:HH11	1.69	0.58
1:B:163:LEU:HA	1:B:169:VAL:HG23	1.84	0.58
1:B:559:LEU:HD23	1:B:560:ILE:N	2.17	0.58
1:A:473:SER:O	1:A:486:VAL:HG22	2.03	0.58
1:B:102:GLY:HA3	1:B:197:GLY:O	2.03	0.58
1:B:463:THR:CB	1:B:496:ASN:HB2	2.30	0.58
1:B:498:LEU:HD11	1:B:506:ASN:CB	2.24	0.58
1:A:162:VAL:HG11	1:A:179:LEU:HD11	1.84	0.58
1:B:201:VAL:O	1:B:450:TYR:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASP:OD2	1:A:217:ARG:HA	2.03	0.58
1:A:201:VAL:O	1:A:450:TYR:HB2	2.03	0.58
1:B:98:PHE:HA	1:B:545:ARG:CD	2.34	0.58
1:B:462:ILE:HD13	1:B:497:VAL:HG23	1.85	0.58
1:A:380:ARG:NH2	2:A:742:FLC:HA1	2.18	0.58
1:B:220:PRO:HB2	1:B:251:GLY:O	2.03	0.58
1:B:690:TYR:HB3	1:B:692:PHE:CE2	2.39	0.58
1:B:696:MET:C	1:B:697:ALA:CA	2.77	0.58
1:A:123:VAL:HG11	1:A:192:ILE:HD12	1.85	0.58
1:A:391:TYR:CE1	1:A:393:GLN:HB2	2.39	0.58
1:B:223:PHE:CE2	1:B:225:ILE:HG13	2.39	0.58
1:A:163:LEU:HD23	1:A:168:PRO:HA	1.85	0.57
1:A:670:SER:O	1:A:671:ALA:CB	2.52	0.57
1:A:176:GLN:NE2	1:A:176:GLN:HA	2.19	0.57
1:B:714:PHE:C	1:B:714:PHE:CD1	2.82	0.57
1:A:239:GLN:HE22	1:A:270:SER:HB2	1.70	0.57
1:A:346:PHE:CZ	1:A:348:PRO:HD3	2.39	0.57
1:A:454:LYS:HA	1:A:463:THR:HG23	1.85	0.57
1:A:112:PHE:CE2	1:A:186:LEU:HD11	2.40	0.57
1:B:511:THR:OG1	1:B:538:ARG:HD2	2.04	0.57
1:A:172:ALA:O	1:A:173:PRO:C	2.48	0.57
1:A:334:TRP:CZ3	1:A:367:GLY:HA2	2.40	0.57
1:B:559:LEU:HG	1:B:584:THR:HG22	1.87	0.57
1:A:492:LEU:CD2	1:A:513:GLY:C	2.78	0.57
1:A:693:GLY:C	1:A:695:GLN:N	2.62	0.57
1:A:710:ASP:HB2	1:A:731:ARG:HB2	1.86	0.57
1:B:162:VAL:HG11	1:B:179:LEU:HD11	1.85	0.57
1:B:220:PRO:CB	1:B:251:GLY:O	2.53	0.57
1:A:715:ILE:CD1	1:A:726:TYR:HB2	2.35	0.57
1:B:698:ASP:O	1:B:739:LEU:HA	2.05	0.57
1:A:118:THR:HG21	1:A:232:GLN:HE22	1.70	0.57
1:A:170:PRO:HG3	1:A:179:LEU:HD21	1.85	0.57
1:B:419:ARG:NH2	1:B:438:ARG:NH2	2.47	0.57
1:A:571:THR:CG2	1:A:723:LYS:NZ	2.65	0.56
1:A:120:MET:CE	1:A:184:VAL:HG22	2.35	0.56
1:A:395:PHE:O	1:A:395:PHE:HD1	1.87	0.56
1:A:457:ILE:HG23	1:A:460:TRP:HB2	1.88	0.56
1:B:120:MET:CE	1:B:184:VAL:HG22	2.35	0.56
1:B:239:GLN:HE21	1:B:270:SER:HB3	1.69	0.56
1:A:149:ILE:HD11	1:A:209:GLY:HA2	1.86	0.56
1:B:174:TYR:HD2	1:B:517:THR:HG21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ARG:HH21	1:A:587:GLU:CD	2.12	0.56
1:B:558:PHE:HZ	1:B:613:VAL:HG22	1.69	0.56
1:A:270:SER:HB3	1:A:276:SER:OG	2.05	0.56
1:A:657:SER:O	1:A:680:GLY:HA2	2.05	0.56
1:B:356:ILE:HD13	1:B:356:ILE:C	2.31	0.56
1:A:130:VAL:HG13	1:A:147:PHE:CE1	2.41	0.56
1:B:402:HIS:CD2	1:B:455:ILE:HG23	2.40	0.56
1:B:582:ARG:HH12	1:B:618:ARG:HD2	1.71	0.56
1:A:156:LEU:HD23	1:A:178:GLN:HB3	1.86	0.56
1:A:287:SER:HB2	1:A:299:SER:OG	2.05	0.56
1:A:315:SER:HA	1:A:672:ASP:O	2.06	0.56
1:A:519:GLN:HB2	1:A:522:GLN:HE21	1.69	0.56
1:B:109:ARG:HA	1:B:112:PHE:CE2	2.41	0.56
1:B:223:PHE:HZ	1:B:225:ILE:HG12	1.71	0.56
1:A:314:LEU:H	1:A:725:ILE:H	1.54	0.56
1:A:570:GLN:HA	1:A:570:GLN:NE2	2.20	0.56
1:A:285:LEU:HD23	1:A:301:LEU:HD12	1.87	0.55
1:B:717:SER:HB3	1:B:723:LYS:HA	1.87	0.55
1:A:492:LEU:HD22	1:A:513:GLY:C	2.31	0.55
1:B:299:SER:HA	1:B:341:SER:O	2.06	0.55
1:A:650:ASN:O	1:A:686:ALA:HA	2.06	0.55
1:B:528:GLN:NE2	1:B:529:SER:N	2.54	0.55
1:A:122:GLU:OE2	1:A:706:LYS:NZ	2.32	0.55
1:A:418:MET:HA	1:A:438:ARG:O	2.06	0.55
1:B:198:GLY:N	1:B:512:GLU:OE2	2.40	0.55
1:A:127:ILE:CD1	1:A:194:VAL:HG21	2.36	0.55
1:A:162:VAL:HA	1:A:212:VAL:O	2.07	0.55
1:A:314:LEU:H	1:A:725:ILE:N	2.05	0.55
1:A:473:SER:HB2	1:A:486:VAL:CG2	2.37	0.55
1:A:660:PHE:CE2	1:A:665:ASN:O	2.60	0.55
1:A:362:GLN:HE21	1:A:383:TRP:NE1	2.04	0.55
1:B:586:LEU:HD23	1:B:587:GLU:N	2.22	0.55
1:B:591:ARG:HH12	1:B:607:TYR:HD2	1.54	0.55
1:A:123:VAL:CG1	1:A:192:ILE:HD12	2.36	0.55
1:B:176:GLN:HE21	1:B:176:GLN:CA	2.06	0.55
1:B:469:GLU:HB3	1:B:471:ILE:CD1	2.35	0.55
1:A:565:GLN:OE1	1:A:578:ARG:NH1	2.40	0.54
1:A:699:LEU:HD22	1:A:738:SER:O	2.07	0.54
1:B:380:ARG:HH22	2:B:742:FLC:HA1	1.71	0.54
1:B:488:TYR:OH	1:B:518:VAL:HB	2.07	0.54
1:A:211:VAL:O	1:A:211:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TYR:CE1	1:A:479:ILE:HD11	2.43	0.54
1:A:198:GLY:HA2	1:A:496:ASN:HD21	1.71	0.54
1:A:366:SER:HB2	1:A:379:PRO:HA	1.86	0.54
1:A:152:LEU:HD21	1:A:562:PHE:CE2	2.43	0.54
1:A:174:TYR:CE2	1:A:471:ILE:HD12	2.43	0.54
1:A:362:GLN:NE2	1:A:383:TRP:NE1	2.49	0.54
1:A:655:PHE:HA	1:A:681:PHE:O	2.07	0.54
1:B:629:PRO:HB3	1:B:661:ALA:O	2.06	0.54
1:A:328:ARG:HH12	1:A:370:GLU:HB3	1.73	0.54
1:A:233:LEU:O	1:A:732:THR:HG23	2.07	0.54
1:B:112:PHE:HE1	1:B:123:VAL:HG11	1.72	0.54
1:B:339:LEU:HD23	1:B:339:LEU:C	2.34	0.54
1:A:104:ARG:HG3	1:A:195:VAL:HG22	1.89	0.53
1:B:297:PHE:N	1:B:297:PHE:CD1	2.76	0.53
1:A:696:MET:CG	1:A:697:ALA:H	2.16	0.53
1:B:380:ARG:HG2	1:B:417:GLU:HB2	1.90	0.53
1:A:397:ILE:HG22	1:A:400:SER:OG	2.09	0.53
1:A:552:THR:CG2	1:A:591:ARG:HB3	2.38	0.53
1:A:628:VAL:HG12	1:A:629:PRO:CD	2.38	0.53
1:A:205:PRO:HD3	1:A:469:GLU:OE2	2.07	0.53
1:A:533:GLU:CB	1:A:534:PRO:CA	2.86	0.53
1:A:637:THR:HG22	1:A:654:ASP:HA	1.90	0.53
1:A:376:THR:HG22	1:A:421:TYR:HB3	1.90	0.53
1:A:504:SER:O	1:A:546:TYR:CD2	2.60	0.53
1:A:569:ASN:HA	1:A:719:ASP:HB3	1.91	0.53
1:B:155:ARG:CZ	1:B:156:LEU:HD23	2.39	0.53
1:B:263:LEU:HB2	1:B:284:MET:HB2	1.90	0.53
1:B:690:TYR:HD2	1:B:692:PHE:CD2	2.27	0.53
1:A:294:VAL:HG13	1:A:347:GLN:C	2.34	0.53
1:B:411:LEU:HD23	1:B:412:ASN:N	2.24	0.53
1:A:594:LEU:HD11	1:A:606:ILE:HD13	1.91	0.53
1:A:660:PHE:HE2	1:A:665:ASN:O	1.92	0.53
1:A:273:ARG:HH22	1:A:726:TYR:HB3	1.74	0.53
1:A:331:ASP:CG	1:A:369:LEU:HD12	2.33	0.53
1:A:397:ILE:HG22	1:A:397:ILE:O	2.08	0.53
1:A:167:ILE:HD12	1:A:167:ILE:H	1.73	0.53
1:A:693:GLY:C	1:A:695:GLN:H	2.16	0.53
1:B:134:GLU:O	1:B:135:ASN:C	2.52	0.53
1:B:402:HIS:NE2	1:B:455:ILE:HG23	2.23	0.53
1:B:596:THR:HG23	1:B:596:THR:O	2.09	0.53
1:B:522:GLN:HB2	1:B:532:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:SER:O	1:B:640:VAL:HG23	2.09	0.53
1:A:322:ASP:O	1:A:325:GLN:HG2	2.09	0.52
1:B:164:MET:HG3	1:B:189:MET:HE1	1.91	0.52
1:A:619:GLU:HG3	1:A:620:LYS:N	2.11	0.52
1:B:154:PRO:O	1:B:155:ARG:C	2.50	0.52
1:B:322:ASP:O	1:B:325:GLN:HG2	2.08	0.52
1:A:603:ASN:O	1:A:642:TYR:HD1	1.93	0.52
1:B:106:VAL:O	1:B:107:ILE:HD13	2.09	0.52
1:B:192:ILE:HD13	1:B:214:PHE:HD1	1.75	0.52
1:B:569:ASN:C	1:B:569:ASN:ND2	2.68	0.52
1:A:254:ALA:HB3	1:A:256:ASN:OD1	2.09	0.52
1:A:294:VAL:HB	1:A:295:HIS:ND1	2.24	0.52
1:B:136:ASN:HA	1:B:726:TYR:CD2	2.44	0.52
1:A:366:SER:HA	1:A:378:SER:O	2.10	0.52
1:B:474:TYR:CD1	1:B:474:TYR:C	2.87	0.52
1:B:558:PHE:CD1	1:B:558:PHE:C	2.87	0.52
1:B:596:THR:O	1:B:596:THR:CG2	2.57	0.52
1:A:380:ARG:HG2	1:A:417:GLU:CB	2.40	0.52
1:B:685:GLY:HA2	1:B:708:ILE:HD13	1.90	0.52
1:A:730:PRO:O	1:A:731:ARG:C	2.53	0.52
1:B:462:ILE:CD1	1:B:497:VAL:HG23	2.40	0.52
1:B:598:THR:HG23	1:B:601:LEU:H	1.75	0.52
1:B:607:TYR:CD1	1:B:607:TYR:C	2.88	0.52
1:A:190:ASP:CG	1:A:217:ARG:HA	2.35	0.52
1:A:455:ILE:O	1:A:461:THR:HA	2.09	0.52
1:A:696:MET:HG2	1:A:697:ALA:N	2.14	0.52
1:A:735:MET:HE3	1:A:736:GLN:C	2.34	0.52
1:B:118:THR:HG22	1:B:122:GLU:OE1	2.10	0.52
1:B:364:LEU:HD22	1:B:365:ARG:N	2.25	0.52
1:B:364:LEU:HD23	1:B:381:ASN:ND2	2.26	0.51
1:A:306:GLY:O	1:A:335:GLY:N	2.36	0.51
1:B:143:LEU:HD11	1:B:280:ILE:HD11	1.89	0.51
1:B:377:LEU:C	1:B:379:PRO:HD3	2.35	0.51
1:A:715:ILE:HD11	1:A:726:TYR:HB2	1.93	0.51
1:B:539:THR:HG23	1:B:560:ILE:HG12	1.92	0.51
1:B:551:LEU:HD13	1:B:551:LEU:C	2.36	0.51
1:B:653:SER:HA	1:B:683:LEU:O	2.10	0.51
1:A:512:GLU:OE1	1:A:512:GLU:N	2.44	0.51
1:A:592:TYR:CD2	1:A:594:LEU:HD23	2.45	0.51
1:A:594:LEU:O	1:A:601:LEU:HB2	2.09	0.51
1:A:397:ILE:O	1:A:400:SER:OG	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:HD22	1:A:513:GLY:O	2.11	0.51
1:A:714:PHE:CD1	1:A:714:PHE:C	2.88	0.51
1:B:118:THR:HG23	1:B:119:THR:CG2	2.39	0.51
1:B:164:MET:SD	1:B:189:MET:HE1	2.51	0.51
1:A:539:THR:HA	1:A:559:LEU:O	2.10	0.51
1:A:566:TYR:N	1:A:566:TYR:CD1	2.78	0.51
1:B:206:GLN:HG2	1:B:516:GLY:HA2	1.92	0.51
1:A:228:GLY:HA2	1:A:737:GLY:O	2.11	0.51
1:B:287:SER:HB2	1:B:299:SER:OG	2.10	0.51
1:B:444:THR:HG22	1:B:445:GLU:N	2.26	0.51
1:B:678:ILE:N	1:B:678:ILE:HD12	2.26	0.51
1:A:352:HIS:N	1:A:352:HIS:HD1	2.08	0.51
1:A:419:ARG:HB2	1:A:438:ARG:HB3	1.93	0.51
1:B:161:THR:O	1:B:211:VAL:HG23	2.11	0.51
1:A:380:ARG:HH12	2:A:742:FLC:HG1	1.75	0.51
1:B:353:LYS:NZ	1:B:353:LYS:HB3	2.26	0.51
1:B:471:ILE:HD12	1:B:471:ILE:N	2.25	0.51
1:B:515:PHE:CD1	1:B:515:PHE:O	2.64	0.51
1:B:693:GLY:O	1:B:695:GLN:O	2.29	0.51
1:A:195:VAL:HB	1:A:211:VAL:HG12	1.91	0.51
1:A:511:THR:HA	1:A:539:THR:O	2.11	0.51
1:B:143:LEU:HD21	1:B:306:GLY:C	2.35	0.51
1:B:239:GLN:NE2	1:B:270:SER:CB	2.73	0.51
1:A:118:THR:HG23	1:A:119:THR:CG2	2.39	0.50
1:A:137:GLY:HA2	1:A:722:ASN:OD1	2.12	0.50
1:B:309:ASP:OD1	1:B:332:ARG:NH1	2.38	0.50
1:A:165:ASP:O	1:A:167:ILE:HD12	2.10	0.50
1:B:522:GLN:CB	1:B:532:VAL:HG11	2.41	0.50
1:A:143:LEU:HD12	1:A:280:ILE:HD11	1.92	0.50
1:A:316:ARG:CD	1:A:669:GLU:OE1	2.49	0.50
1:A:352:HIS:N	1:A:352:HIS:ND1	2.58	0.50
1:A:364:LEU:C	1:A:364:LEU:HD13	2.37	0.50
1:A:394:ILE:HG12	1:A:403:GLU:HG3	1.94	0.50
1:A:706:LYS:HB2	1:A:732:THR:HB	1.92	0.50
1:B:120:MET:HE3	1:B:184:VAL:CG2	2.42	0.50
1:B:653:SER:HB2	1:B:684:TRP:CE3	2.45	0.50
1:B:705:VAL:HB	1:B:708:ILE:HD11	1.93	0.50
1:A:448:ALA:CB	1:A:469:GLU:HG2	2.41	0.50
1:B:101:ALA:HB3	1:B:496:ASN:HD22	1.76	0.50
1:A:442:SER:HB3	1:A:520:TYR:CD1	2.47	0.50
1:B:207:SER:OG	1:B:514:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:ASP:C	1:A:595:GLY:H	2.19	0.50
1:B:501:LEU:HD21	1:B:507:LEU:HD13	1.94	0.50
1:A:229:VAL:HG23	1:A:245:THR:O	2.12	0.50
1:A:388:GLU:HG3	1:A:408:TYR:O	2.12	0.50
1:B:169:VAL:N	1:B:170:PRO:CD	2.75	0.50
1:B:201:VAL:O	1:B:450:TYR:CB	2.60	0.50
1:B:239:GLN:C	1:B:239:GLN:OE1	2.55	0.50
1:A:253:THR:HG22	1:A:258:PHE:O	2.11	0.50
1:A:380:ARG:HG2	1:A:417:GLU:HB2	1.93	0.50
1:B:389:PRO:HD2	1:B:408:TYR:O	2.12	0.50
1:B:692:PHE:O	1:B:693:GLY:O	2.30	0.50
1:A:334:TRP:CZ2	1:A:366:SER:OG	2.65	0.49
1:A:693:GLY:O	1:A:695:GLN:N	2.45	0.49
1:B:459:ASN:HB3	1:B:499:TYR:CE1	2.46	0.49
1:B:613:VAL:O	1:B:613:VAL:HG12	2.11	0.49
1:A:328:ARG:CZ	1:A:370:GLU:HB3	2.41	0.49
1:B:109:ARG:NH2	1:B:187:GLY:O	2.45	0.49
1:B:196:ARG:NH2	1:B:587:GLU:CD	2.63	0.49
1:B:420:TYR:CD2	1:B:432:GLY:HA2	2.47	0.49
1:B:508:TYR:CD1	1:B:508:TYR:C	2.90	0.49
1:B:330:TYR:CE2	1:B:375:ILE:HD11	2.47	0.49
1:B:672:ASP:OD1	1:B:672:ASP:C	2.55	0.49
1:A:339:LEU:HG	1:A:361:THR:HG22	1.94	0.49
1:B:332:ARG:N	1:B:368:TYR:O	2.45	0.49
1:B:706:LYS:HB2	1:B:732:THR:HB	1.93	0.49
1:A:462:ILE:HG22	1:A:464:PRO:HD3	1.94	0.49
1:B:330:TYR:CD2	1:B:375:ILE:HD11	2.47	0.49
1:A:364:LEU:HD22	1:A:365:ARG:H	1.76	0.49
1:A:522:GLN:HB3	1:A:532:VAL:HG11	1.93	0.49
1:A:557:LEU:HD21	1:A:586:LEU:HD12	1.95	0.49
1:B:121:ARG:HD2	1:B:133:PRO:O	2.13	0.49
1:A:592:TYR:HD2	1:A:594:LEU:HD23	1.78	0.49
1:A:640:VAL:HG13	1:A:651:LEU:HB3	1.95	0.49
1:A:642:TYR:CD1	1:A:644:PRO:HD3	2.48	0.49
1:A:109:ARG:C	1:A:111:ASP:N	2.69	0.48
1:B:113:ALA:O	1:B:114:LYS:C	2.55	0.48
1:B:442:SER:HB3	1:B:474:TYR:O	2.13	0.48
1:B:594:LEU:HD12	1:B:604:VAL:CG1	2.43	0.48
1:A:371:GLN:NE2	1:A:376:THR:OG1	2.38	0.48
1:A:692:PHE:O	1:A:693:GLY:O	2.31	0.48
1:A:697:ALA:C	1:A:699:LEU:N	2.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:PHE:CD1	1:B:515:PHE:C	2.91	0.48
1:B:522:GLN:HA	1:B:525:LYS:CG	2.43	0.48
1:B:569:ASN:ND2	1:B:571:THR:OG1	2.36	0.48
1:B:675:THR:HG1	1:B:718:TYR:HE1	1.61	0.48
1:B:699:LEU:C	1:B:699:LEU:HD13	2.38	0.48
1:B:538:ARG:HG3	1:B:540:TRP:NE1	2.27	0.48
1:A:391:TYR:CD1	1:A:391:TYR:C	2.91	0.48
1:B:262:LEU:HD21	1:B:283:LEU:HD11	1.95	0.48
1:A:715:ILE:HD13	1:A:726:TYR:O	2.13	0.48
1:A:150:ARG:NH2	1:A:587:GLU:OE1	2.37	0.48
1:B:112:PHE:CE1	1:B:123:VAL:HG11	2.49	0.48
1:B:152:LEU:HD23	1:B:583:HIS:CE1	2.48	0.48
1:B:197:GLY:HA3	1:B:541:GLU:CD	2.38	0.48
1:B:223:PHE:CD1	1:B:251:GLY:O	2.67	0.48
1:B:669:GLU:HG3	1:B:716:ARG:NH2	2.29	0.48
1:A:237:SER:HA	1:A:324:TRP:CE2	2.49	0.48
1:B:157:ALA:HB3	1:B:179:LEU:HD12	1.96	0.48
1:B:528:GLN:NE2	1:B:529:SER:H	2.11	0.48
1:A:141:HIS:ND1	1:A:143:LEU:HB2	2.29	0.48
1:A:615:ALA:C	1:A:628:VAL:HG23	2.38	0.48
1:A:617:ILE:HG12	1:A:626:ASN:O	2.14	0.48
1:B:200:ALA:HB1	1:B:202:ARG:HB3	1.95	0.48
1:B:459:ASN:O	1:B:499:TYR:CD1	2.67	0.48
1:A:229:VAL:CG2	1:A:230:GLU:N	2.77	0.48
1:A:654:ASP:O	1:A:682:MET:HA	2.13	0.48
1:A:176:GLN:N	1:A:177:PRO:HD3	2.29	0.47
1:A:244:GLU:OE1	1:A:246:HIS:ND1	2.40	0.47
1:A:537:ALA:HA	1:A:561:ASN:O	2.14	0.47
1:A:715:ILE:N	1:A:715:ILE:CD1	2.77	0.47
1:B:498:LEU:CD1	1:B:506:ASN:HB3	2.26	0.47
1:A:176:GLN:CA	1:A:176:GLN:HE21	2.27	0.47
1:A:344:TYR:CD1	1:A:345:GLN:N	2.82	0.47
1:A:107:ILE:N	1:A:107:ILE:CD1	2.73	0.47
1:A:175:GLY:HA3	1:A:520:TYR:CE2	2.49	0.47
1:A:631:SER:O	1:A:632:PRO:C	2.56	0.47
1:A:677:ARG:HH11	1:A:677:ARG:HG2	1.79	0.47
1:B:262:LEU:CD2	1:B:283:LEU:HD11	2.44	0.47
1:B:339:LEU:HG	1:B:361:THR:HG22	1.94	0.47
1:A:253:THR:HG23	1:A:259:GLY:CA	2.44	0.47
1:A:276:SER:HA	1:A:309:ASP:O	2.14	0.47
1:B:509:ALA:HA	1:B:541:GLU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:HA	1:A:726:TYR:CE2	2.49	0.47
1:A:502:THR:C	1:A:504:SER:N	2.69	0.47
1:A:344:TYR:OH	1:A:346:PHE:HB2	2.15	0.47
1:A:603:ASN:HD22	1:A:603:ASN:HA	1.53	0.47
1:A:705:VAL:CG1	1:A:708:ILE:HD13	2.45	0.47
1:B:453:ASP:OD2	1:B:455:ILE:HG12	2.15	0.47
1:B:501:LEU:CD2	1:B:501:LEU:N	2.77	0.47
1:B:617:ILE:HG21	1:B:623:THR:OG1	2.14	0.47
1:B:655:PHE:HA	1:B:681:PHE:O	2.14	0.47
1:A:251:GLY:HA3	1:A:261:ALA:HA	1.97	0.47
1:B:522:GLN:HA	1:B:525:LYS:CD	2.44	0.47
1:A:279:ARG:NH1	1:A:305:ASP:OD1	2.44	0.47
1:A:356:ILE:O	1:A:356:ILE:HG23	2.15	0.47
1:A:109:ARG:HH22	1:A:187:GLY:HA2	1.79	0.47
1:A:119:THR:O	1:A:120:MET:C	2.57	0.47
1:B:216:THR:HG22	1:B:284:MET:HE1	1.97	0.47
1:B:420:TYR:CE2	1:B:432:GLY:HA2	2.50	0.47
1:B:484:GLU:HB3	1:B:523:ILE:CG2	2.45	0.47
1:B:643:LYS:CE	1:B:648:THR:HG23	2.44	0.47
1:A:175:GLY:HA3	1:A:520:TYR:CZ	2.51	0.46
1:A:377:LEU:HB3	1:A:420:TYR:HB2	1.97	0.46
1:A:448:ALA:HB2	1:A:469:GLU:HG2	1.96	0.46
1:A:453:ASP:CG	1:A:455:ILE:HD11	2.40	0.46
1:B:98:PHE:HE1	1:B:545:ARG:O	1.98	0.46
1:B:199:GLY:C	1:B:201:VAL:H	2.21	0.46
1:B:251:GLY:HA3	1:B:261:ALA:CB	2.45	0.46
1:B:697:ALA:N	1:B:697:ALA:HB3	2.26	0.46
1:A:548:ASP:OD1	1:A:551:LEU:HB3	2.15	0.46
1:B:135:ASN:OD1	1:B:135:ASN:N	2.30	0.46
1:B:444:THR:CG2	1:B:445:GLU:N	2.78	0.46
1:B:650:ASN:O	1:B:686:ALA:HA	2.15	0.46
1:A:439:ASP:OD1	1:A:439:ASP:C	2.59	0.46
1:B:239:GLN:O	1:B:239:GLN:CG	2.61	0.46
1:A:454:LYS:CA	1:A:463:THR:HG23	2.46	0.46
1:A:518:VAL:HG22	1:A:533:GLU:CB	2.45	0.46
1:B:642:TYR:CD1	1:B:644:PRO:HD3	2.50	0.46
1:A:184:VAL:HG23	1:A:189:MET:HE3	1.97	0.46
1:A:268:ARG:HG2	1:A:268:ARG:NH1	2.31	0.46
1:A:699:LEU:HD13	1:A:699:LEU:C	2.41	0.46
1:B:190:ASP:CG	1:B:217:ARG:HA	2.40	0.46
1:A:169:VAL:HB	1:A:170:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:PHE:O	1:A:395:PHE:CD1	2.68	0.46
1:A:653:SER:HA	1:A:683:LEU:O	2.16	0.46
1:A:734:TYR:CD1	1:A:734:TYR:C	2.93	0.46
1:B:149:ILE:HD12	1:B:196:ARG:HG2	1.97	0.46
1:B:205:PRO:HB3	1:B:469:GLU:OE2	2.16	0.46
1:B:610:TYR:CG	1:B:611:ALA:N	2.83	0.46
1:A:599:PRO:O	1:A:602:ASP:N	2.41	0.46
1:B:594:LEU:HD12	1:B:604:VAL:HG12	1.96	0.46
1:A:202:ARG:HA	1:A:450:TYR:CD2	2.51	0.46
1:A:397:ILE:O	1:A:397:ILE:CG2	2.63	0.46
1:A:419:ARG:NH1	1:A:437:ASP:OD2	2.49	0.46
1:A:697:ALA:O	1:A:699:LEU:N	2.49	0.46
1:B:161:THR:HB	1:B:211:VAL:CB	2.46	0.46
1:B:226:GLU:O	1:B:227:ALA:HB2	2.14	0.46
1:B:275:HIS:O	1:B:275:HIS:CD2	2.69	0.46
1:B:413:GLU:OE2	1:B:520:TYR:OH	2.29	0.46
1:B:422:THR:HG23	1:B:430:PRO:HB3	1.97	0.46
1:B:284:MET:HA	1:B:301:LEU:O	2.15	0.45
1:B:418:MET:HA	1:B:438:ARG:O	2.15	0.45
1:A:134:GLU:O	1:A:135:ASN:C	2.58	0.45
1:A:273:ARG:NH1	1:A:726:TYR:HB3	2.30	0.45
1:A:120:MET:O	1:A:121:ARG:C	2.59	0.45
1:B:181:LEU:C	1:B:183:PRO:HD3	2.35	0.45
1:B:687:ARG:HG2	1:B:688:VAL:N	2.31	0.45
1:B:695:GLN:HE21	1:B:695:GLN:HB3	1.55	0.45
1:B:697:ALA:O	1:B:699:LEU:HB2	2.17	0.45
1:A:331:ASP:OD1	1:A:369:LEU:HD12	2.16	0.45
1:A:202:ARG:HA	1:A:450:TYR:CE2	2.51	0.45
1:A:711:GLN:NE2	1:A:711:GLN:C	2.74	0.45
1:B:239:GLN:HG2	1:B:271:ASP:O	2.15	0.45
1:B:316:ARG:O	1:B:319:TYR:N	2.50	0.45
1:B:403:GLU:O	1:B:453:ASP:HA	2.16	0.45
1:A:143:LEU:CD1	1:A:280:ILE:HD11	2.46	0.45
1:B:337:ARG:HD2	1:B:339:LEU:HB2	1.99	0.45
1:B:364:LEU:HD13	1:B:364:LEU:C	2.41	0.45
1:B:586:LEU:HD23	1:B:586:LEU:C	2.41	0.45
1:B:664:ALA:O	1:B:665:ASN:HB2	2.16	0.45
1:A:419:ARG:CB	1:A:438:ARG:HB3	2.47	0.45
1:A:689:ALA:HB2	1:A:702:ALA:HB2	1.99	0.45
1:B:219:ILE:HD11	1:B:286:LYS:HB3	1.98	0.45
1:A:579:GLY:HA3	1:A:619:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ILE:CD1	1:B:214:PHE:HD1	2.29	0.45
1:B:285:LEU:HB3	1:B:301:LEU:HB2	1.98	0.45
1:B:453:ASP:O	1:B:464:PRO:HD2	2.17	0.45
1:B:646:ASN:HB2	1:B:690:TYR:CE1	2.51	0.45
1:A:200:ALA:HB3	1:A:202:ARG:HB3	1.99	0.45
1:B:228:GLY:HA2	1:B:737:GLY:O	2.17	0.45
1:B:322:ASP:OD1	1:B:324:TRP:N	2.50	0.45
1:B:365:ARG:HE	1:B:365:ARG:C	2.25	0.45
1:B:400:SER:HB3	1:B:457:ILE:HB	1.99	0.45
1:A:558:PHE:C	1:A:558:PHE:CD1	2.95	0.45
1:B:432:GLY:O	1:B:433:SER:OG	2.27	0.45
1:A:488:TYR:HB2	1:A:515:PHE:HZ	1.83	0.44
1:B:220:PRO:CD	1:B:251:GLY:O	2.65	0.44
1:B:314:LEU:H	1:B:725:ILE:H	1.66	0.44
1:B:339:LEU:HD23	1:B:340:ALA:N	2.32	0.44
1:A:471:ILE:HG21	1:A:517:THR:HG21	1.98	0.44
1:A:586:LEU:HD23	1:A:586:LEU:C	2.42	0.44
1:B:141:HIS:HD2	1:B:310:MET:HE3	1.82	0.44
1:B:149:ILE:CD1	1:B:196:ARG:HG2	2.47	0.44
1:B:202:ARG:HA	1:B:450:TYR:CD2	2.52	0.44
1:B:618:ARG:HA	1:B:618:ARG:NE	2.32	0.44
1:A:200:ALA:CB	1:A:202:ARG:HB3	2.48	0.44
1:A:510:ASN:OD1	1:A:541:GLU:HG3	2.18	0.44
1:A:558:PHE:HZ	1:A:613:VAL:HG13	1.82	0.44
1:B:201:VAL:O	1:B:201:VAL:HG12	2.17	0.44
1:A:689:ALA:CB	1:A:702:ALA:HB2	2.47	0.44
1:B:714:PHE:C	1:B:715:ILE:CG2	2.91	0.44
1:A:705:VAL:CB	1:A:708:ILE:HD13	2.47	0.44
1:B:251:GLY:HA3	1:B:261:ALA:HB2	2.00	0.44
1:B:297:PHE:N	1:B:297:PHE:HD1	2.14	0.44
1:B:617:ILE:N	1:B:617:ILE:HD12	2.33	0.44
1:A:100:HIS:CD2	1:A:104:ARG:HB2	2.52	0.44
1:A:205:PRO:O	1:A:207:SER:N	2.43	0.44
1:A:283:LEU:HB3	1:A:303:TYR:HB3	1.99	0.44
1:A:411:LEU:HD23	1:A:411:LEU:C	2.43	0.44
1:A:418:MET:HG2	1:A:439:ASP:HA	1.99	0.44
1:A:693:GLY:O	1:A:695:GLN:O	2.35	0.44
1:B:532:VAL:HG12	1:B:533:GLU:N	2.33	0.44
1:A:488:TYR:HB2	1:A:515:PHE:CZ	2.53	0.44
1:A:601:LEU:O	1:A:604:VAL:HB	2.18	0.44
1:B:162:VAL:HA	1:B:212:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PRO:HD2	1:B:251:GLY:O	2.18	0.44
1:B:420:TYR:HD2	1:B:434:SER:O	2.01	0.44
1:B:471:ILE:O	1:B:487:SER:HA	2.17	0.44
1:B:643:LYS:HE2	1:B:648:THR:HG23	2.00	0.44
1:A:121:ARG:HD2	1:A:133:PRO:O	2.17	0.44
1:B:316:ARG:O	1:B:317:ALA:C	2.60	0.44
1:A:657:SER:OG	1:A:658:SER:N	2.49	0.44
1:B:143:LEU:HD12	1:B:280:ILE:HD11	1.99	0.44
1:B:260:THR:CG2	1:B:261:ALA:N	2.80	0.44
1:A:432:GLY:O	1:A:433:SER:OG	2.31	0.43
1:A:667:VAL:O	1:A:667:VAL:CG1	2.63	0.43
1:B:167:ILE:HD12	1:B:167:ILE:H	1.82	0.43
1:B:689:ALA:HB2	1:B:702:ALA:HB2	1.99	0.43
1:B:693:GLY:O	1:B:695:GLN:N	2.50	0.43
1:A:113:ALA:HB1	1:A:687:ARG:HH12	1.82	0.43
1:A:201:VAL:HG13	1:A:467:ARG:CB	2.35	0.43
1:A:201:VAL:O	1:A:201:VAL:HG12	2.18	0.43
1:A:572:ASN:ND2	1:A:574:THR:CG2	2.81	0.43
1:A:669:GLU:HG3	1:A:716:ARG:NH2	2.33	0.43
1:B:225:ILE:HG12	1:B:250:VAL:HG22	2.01	0.43
1:A:97:VAL:HB	1:A:104:ARG:HD3	2.00	0.43
1:A:109:ARG:NH2	1:A:187:GLY:HA2	2.33	0.43
1:A:244:GLU:OE2	1:A:246:HIS:ND1	2.50	0.43
1:A:359:PHE:CD1	1:A:359:PHE:C	2.96	0.43
1:A:97:VAL:O	1:A:98:PHE:C	2.62	0.43
1:A:615:ALA:O	1:A:627:LEU:HA	2.18	0.43
1:A:579:GLY:HA3	1:A:619:GLU:HB2	2.01	0.43
1:B:638:LEU:C	1:B:638:LEU:CD1	2.91	0.43
1:B:705:VAL:HG12	1:B:708:ILE:HD12	2.01	0.43
1:A:113:ALA:HB1	1:A:687:ARG:NH1	2.34	0.43
1:A:188:ASN:HB3	1:A:284:MET:HE2	2.01	0.43
1:A:552:THR:HG23	1:A:552:THR:O	2.18	0.43
1:B:125:ASN:ND2	1:B:132:ALA:O	2.51	0.43
1:B:171:PHE:CD1	1:B:171:PHE:C	2.97	0.43
1:A:402:HIS:CD2	1:A:455:ILE:HD12	2.54	0.43
1:B:675:THR:OG1	1:B:718:TYR:HE1	2.02	0.43
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.84	0.43
1:B:162:VAL:HG22	1:B:169:VAL:CG2	2.49	0.43
1:B:200:ALA:O	1:B:201:VAL:HB	2.19	0.43
1:B:345:GLN:OE1	1:B:355:ASN:ND2	2.52	0.43
1:B:570:GLN:CA	1:B:570:GLN:NE2	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG21	1:A:232:GLN:NE2	2.33	0.43
1:A:217:ARG:O	1:A:286:LYS:NZ	2.46	0.43
1:B:276:SER:O	1:B:277:ALA:C	2.62	0.43
1:B:328:ARG:HB3	1:B:331:ASP:CG	2.44	0.43
1:A:116:GLY:HA3	1:A:734:TYR:CZ	2.54	0.42
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.83	0.42
1:A:697:ALA:O	1:A:698:ASP:C	2.62	0.42
1:B:175:GLY:HA3	1:B:520:TYR:CD2	2.53	0.42
1:B:178:GLN:HG2	2:B:743:FLC:HG2	2.01	0.42
1:B:249:MET:C	1:B:250:VAL:HG23	2.44	0.42
1:B:497:VAL:HG12	1:B:509:ALA:O	2.19	0.42
1:A:124:LEU:HA	1:A:127:ILE:HD12	1.99	0.42
1:A:402:HIS:NE2	1:A:455:ILE:HD12	2.34	0.42
1:A:457:ILE:HG23	1:A:457:ILE:O	2.19	0.42
1:A:467:ARG:O	1:A:492:LEU:HB2	2.18	0.42
1:B:603:ASN:HD22	1:B:603:ASN:HA	1.70	0.42
1:B:638:LEU:HD12	1:B:638:LEU:O	2.19	0.42
1:A:98:PHE:CE2	1:A:506:ASN:ND2	2.87	0.42
1:A:398:GLY:C	1:A:400:SER:H	2.26	0.42
1:B:201:VAL:HG13	1:B:467:ARG:CB	2.35	0.42
1:A:172:ALA:O	1:A:174:TYR:N	2.52	0.42
1:A:200:ALA:CB	1:A:200:ALA:H	2.23	0.42
1:A:239:GLN:HE22	1:A:270:SER:CB	2.31	0.42
1:A:296:THR:O	1:A:344:TYR:HD1	2.03	0.42
1:A:508:TYR:CD1	1:A:508:TYR:C	2.97	0.42
1:A:519:GLN:CB	1:A:522:GLN:HE21	2.32	0.42
1:A:522:GLN:OE1	1:A:532:VAL:HG11	2.19	0.42
1:B:528:GLN:HE21	1:B:529:SER:H	1.67	0.42
1:A:99:GLU:OE2	1:A:506:ASN:ND2	2.52	0.42
1:A:118:THR:CG2	1:A:119:THR:HG23	2.44	0.42
1:A:453:ASP:O	1:A:455:ILE:HG12	2.20	0.42
1:A:672:ASP:OD1	1:A:673:GLY:N	2.52	0.42
1:B:167:ILE:N	1:B:167:ILE:CD1	2.83	0.42
1:B:171:PHE:O	1:B:382:TYR:HB3	2.19	0.42
1:B:205:PRO:HB3	1:B:469:GLU:CD	2.45	0.42
1:A:201:VAL:O	1:A:450:TYR:CB	2.66	0.42
1:A:346:PHE:CE2	1:A:348:PRO:HD3	2.55	0.42
1:A:397:ILE:O	1:A:398:GLY:C	2.63	0.42
1:A:680:GLY:O	1:A:681:PHE:HB3	2.19	0.42
1:A:706:LYS:O	1:A:731:ARG:HA	2.20	0.42
1:B:607:TYR:C	1:B:607:TYR:HD1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLN:HE21	1:A:570:GLN:CA	2.27	0.42
1:B:263:LEU:HD23	1:B:263:LEU:HA	1.88	0.42
1:B:356:ILE:O	1:B:356:ILE:CG2	2.68	0.42
1:B:408:TYR:HA	1:B:448:ALA:O	2.19	0.42
1:B:501:LEU:HD22	1:B:501:LEU:N	2.35	0.42
1:A:594:LEU:HD23	1:A:594:LEU:HA	1.74	0.42
1:B:579:GLY:HA3	1:B:619:GLU:HG2	2.01	0.42
1:A:272:TRP:HE1	1:A:273:ARG:HE	1.66	0.42
1:A:356:ILE:HD12	1:A:389:PRO:HB3	2.02	0.42
1:A:677:ARG:HG2	1:A:677:ARG:NH1	2.34	0.42
1:A:696:MET:CG	1:A:697:ALA:N	2.80	0.42
1:B:124:LEU:CD1	1:B:192:ILE:HG21	2.49	0.42
1:A:199:GLY:C	1:A:201:VAL:H	2.27	0.42
1:A:551:LEU:HD23	1:A:592:TYR:CD1	2.55	0.42
1:A:642:TYR:CZ	1:A:644:PRO:HB3	2.55	0.42
1:B:438:ARG:HH12	2:B:742:FLC:HA2	1.85	0.42
1:B:719:ASP:O	1:B:720:ASP:C	2.63	0.42
1:A:440:THR:OG1	1:A:475:GLN:NE2	2.53	0.41
1:A:564:ASN:HA	1:A:579:GLY:O	2.19	0.41
1:A:670:SER:HB3	1:A:675:THR:CB	2.48	0.41
1:B:522:GLN:O	1:B:523:ILE:C	2.63	0.41
1:A:152:LEU:O	1:A:154:PRO:HD3	2.20	0.41
1:A:566:TYR:HB3	1:A:575:VAL:HG12	2.02	0.41
1:B:413:GLU:CG	1:B:444:THR:HB	2.49	0.41
1:B:735:MET:HE2	1:B:736:GLN:CA	2.51	0.41
1:A:169:VAL:N	1:A:170:PRO:CD	2.83	0.41
1:A:178:GLN:HE22	1:A:519:GLN:CD	2.27	0.41
1:A:612:TYR:HA	1:A:633:LYS:O	2.20	0.41
1:A:695:GLN:O	1:A:696:MET:C	2.63	0.41
1:A:700:ASN:HB2	1:A:738:SER:HB3	2.01	0.41
1:A:710:ASP:HB2	1:A:731:ARG:CZ	2.50	0.41
1:B:102:GLY:CA	1:B:510:ASN:ND2	2.83	0.41
1:B:183:PRO:HA	1:B:304:TYR:CD2	2.55	0.41
1:B:490:ALA:HA	1:B:491:PRO:HD2	1.97	0.41
1:A:112:PHE:CD2	1:A:186:LEU:HD11	2.55	0.41
1:A:368:TYR:CE1	1:A:377:LEU:HD13	2.55	0.41
1:B:177:PRO:HD3	1:B:519:GLN:HG2	2.01	0.41
1:B:643:LYS:NZ	1:B:648:THR:CG2	2.84	0.41
1:B:668:LYS:HD2	1:B:668:LYS:HA	1.68	0.41
1:A:159:ARG:O	1:A:209:GLY:CA	2.65	0.41
1:A:740:LYS:O	1:A:741:PHE:HD2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ASP:HB2	1:B:272:TRP:CE3	2.56	0.41
1:A:628:VAL:CG1	1:A:629:PRO:CD	2.99	0.41
1:B:172:ALA:O	1:B:173:PRO:C	2.62	0.41
1:A:501:LEU:HB2	1:A:505:TRP:O	2.20	0.41
1:B:275:HIS:O	1:B:275:HIS:CG	2.73	0.41
1:B:579:GLY:HA3	1:B:619:GLU:CB	2.50	0.41
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.88	0.41
1:A:594:LEU:HB3	1:A:601:LEU:HD13	2.02	0.41
1:B:304:TYR:CD1	1:B:304:TYR:C	2.98	0.41
1:B:330:TYR:O	1:B:331:ASP:CB	2.68	0.41
1:B:351:GLN:O	1:B:393:GLN:HA	2.20	0.41
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.59	0.41
1:A:167:ILE:HD12	1:A:167:ILE:N	2.34	0.41
1:A:339:LEU:C	1:A:339:LEU:HD23	2.46	0.41
1:A:407:GLY:HA3	1:A:450:TYR:CE2	2.56	0.41
1:A:606:ILE:HG22	1:A:640:VAL:HB	2.03	0.41
1:B:143:LEU:CG	1:B:280:ILE:HD11	2.50	0.41
1:B:143:LEU:HG	1:B:280:ILE:HD11	2.03	0.41
1:B:270:SER:OG	1:B:277:ALA:HA	2.20	0.41
1:B:313:GLY:CA	1:B:726:TYR:CE1	3.03	0.41
1:B:380:ARG:HG2	1:B:417:GLU:CB	2.49	0.41
1:B:421:TYR:HE2	1:B:437:ASP:HB3	1.86	0.41
1:B:606:ILE:O	1:B:606:ILE:HG13	2.20	0.41
1:B:716:ARG:HH11	1:B:716:ARG:HG2	1.85	0.41
1:A:366:SER:HB2	1:A:379:PRO:CA	2.50	0.41
1:B:102:GLY:HA3	1:B:510:ASN:ND2	2.35	0.41
1:A:188:ASN:HB3	1:A:284:MET:CE	2.51	0.40
1:A:236:THR:O	1:A:324:TRP:CZ2	2.73	0.40
1:B:388:GLU:OE2	1:B:409:ARG:HB2	2.20	0.40
1:B:558:PHE:CZ	1:B:585:GLY:HA3	2.56	0.40
1:A:105:ASP:OD2	1:A:196:ARG:NH1	2.50	0.40
1:A:471:ILE:HG21	1:A:517:THR:CB	2.51	0.40
1:A:490:ALA:HA	1:A:491:PRO:HD2	1.88	0.40
1:A:528:GLN:NE2	1:A:529:SER:N	2.69	0.40
1:B:223:PHE:HD1	1:B:251:GLY:O	2.00	0.40
1:B:432:GLY:O	1:B:433:SER:CB	2.70	0.40
1:B:536:LYS:O	1:B:563:ASN:OD1	2.40	0.40
1:A:104:ARG:HG2	1:A:105:ASP:N	2.35	0.40
1:A:453:ASP:OD2	1:A:455:ILE:CD1	2.60	0.40
1:B:174:TYR:CE2	1:B:205:PRO:HG3	2.56	0.40
1:A:223:PHE:CD2	1:A:223:PHE:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:THR:OG1	1:B:500:HIS:HE1	2.04	0.40
1:B:103:ALA:O	1:B:196:ARG:N	2.53	0.40
1:B:296:THR:CG2	1:B:345:GLN:HB3	2.51	0.40
1:B:404:VAL:HA	1:B:452:ASP:O	2.22	0.40
1:B:414:SER:C	1:B:415:THR:CG2	2.95	0.40
1:B:706:LYS:O	1:B:731:ARG:HA	2.20	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	645/751 (86%)	552 (86%)	73 (11%)	20 (3%)	3	18
1	B	643/751 (86%)	556 (86%)	72 (11%)	15 (2%)	5	23
All	All	1288/1502 (86%)	1108 (86%)	145 (11%)	35 (3%)	4	20

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	VAL
1	A	110	GLU
1	A	619	GLU
1	A	620	LYS
1	B	200	ALA
1	B	331	ASP
1	B	533	GLU
1	A	206	GLN
1	A	221	GLN
1	A	372	GLY
1	A	533	GLU
1	A	693	GLY

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Mol	Chain	Res	Type
1	B	180	SER
1	B	505	TRP
1	B	568	SER
1	B	693	GLY
1	B	696	MET
1	B	698	ASP
1	A	236	THR
1	A	578	ARG
1	A	671	ALA
1	A	692	PHE
1	B	223	PHE
1	A	222	ASP
1	A	622	ASP
1	A	657	SER
1	A	698	ASP
1	B	227	ALA
1	B	679	PRO
1	A	457	ILE
1	A	577	ALA
1	B	101	ALA
1	B	437	ASP
1	B	523	ILE
1	A	183	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	517/617 (84%)	479 (93%)	38 (7%)	13	38
1	B	513/617 (83%)	461 (90%)	52 (10%)	7	25
All	All	1030/1234 (84%)	940 (91%)	90 (9%)	9	32

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	VAL
1	A	108	ARG
1	A	110	GLU
1	A	149	ILE
1	A	162	VAL
1	A	180	SER
1	A	202	ARG
1	A	236	THR
1	A	244	GLU
1	A	253	THR
1	A	296	THR
1	A	342	LEU
1	A	352	HIS
1	A	353	LYS
1	A	364	LEU
1	A	395	PHE
1	A	397	ILE
1	A	414	SER
1	A	415	THR
1	A	417	GLU
1	A	419	ARG
1	A	440	THR
1	A	466	MET
1	A	475	GLN
1	A	484	GLU
1	A	488	TYR
1	A	497	VAL
1	A	517	THR
1	A	525	LYS
1	A	528	GLN
1	A	536	LYS
1	A	559	LEU
1	A	566	TYR
1	A	603	ASN
1	A	640	VAL
1	A	711	GLN
1	A	715	ILE
1	A	735	MET
1	B	97	VAL
1	B	108	ARG
1	B	124	LEU
1	B	127	ILE
1	B	135	ASN

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Mol	Chain	Res	Type
1	B	149	ILE
1	B	156	LEU
1	B	162	VAL
1	B	167	ILE
1	B	176	GLN
1	B	177	PRO
1	B	180	SER
1	B	190	ASP
1	B	202	ARG
1	B	211	VAL
1	B	244	GLU
1	B	260	THR
1	B	297	PHE
1	B	315	SER
1	B	336	ARG
1	B	342	LEU
1	B	350	SER
1	B	353	LYS
1	B	356	ILE
1	B	364	LEU
1	B	417	GLU
1	B	453	ASP
1	B	463	THR
1	B	484	GLU
1	B	488	TYR
1	B	502	THR
1	B	503	ASP
1	B	514	SER
1	B	515	PHE
1	B	517	THR
1	B	522	GLN
1	B	528	GLN
1	B	536	LYS
1	B	570	GLN
1	B	596	THR
1	B	603	ASN
1	B	622	ASP
1	B	640	VAL
1	B	679	PRO
1	B	695	GLN
1	B	699	LEU
1	B	700	ASN

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Mol	Chain	Res	Type
1	B	711	GLN
1	B	715	ILE
1	B	723	LYS
1	B	735	MET
1	B	738	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	176	GLN
1	A	232	GLN
1	A	239	GLN
1	A	240	ASN
1	A	362	GLN
1	A	371	GLN
1	A	402	HIS
1	A	416	HIS
1	A	475	GLN
1	A	496	ASN
1	A	522	GLN
1	A	528	GLN
1	A	569	ASN
1	A	589	GLN
1	A	603	ASN
1	A	614	ASN
1	A	646	ASN
1	A	665	ASN
1	A	700	ASN
1	A	711	GLN
1	B	125	ASN
1	B	136	ASN
1	B	176	GLN
1	B	206	GLN
1	B	240	ASN
1	B	275	HIS
1	B	325	GLN
1	B	345	GLN
1	B	355	ASN
1	B	381	ASN
1	B	393	GLN
1	B	416	HIS

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Mol	Chain	Res	Type
1	B	475	GLN
1	B	500	HIS
1	B	528	GLN
1	B	569	ASN
1	B	589	GLN
1	B	603	ASN
1	B	646	ASN
1	B	652	ASN
1	B	656	GLN
1	B	695	GLN
1	B	711	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	FLC	A	742	3	12,12,12	3.60	3 (25%)	17,17,17	6.86	8 (47%)
2	FLC	B	743	3	12,12,12	3.87	7 (58%)	17,17,17	6.30	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FLC	B	742	3	12,12,12	5.55	7 (58%)	17,17,17	6.73	7 (41%)
2	FLC	A	743	3	12,12,12	4.68	6 (50%)	17,17,17	6.44	8 (47%)

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	FLC	A	742	3	-	10/16/16/16	-
2	FLC	B	743	3	-	4/16/16/16	-
2	FLC	B	742	3	-	3/16/16/16	-
2	FLC	A	743	3	-	10/16/16/16	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	742	FLC	CA-CB	11.23	1.67	1.54
2	B	742	FLC	CB-CBC	10.93	1.64	1.53
2	A	743	FLC	CG-CB	10.11	1.66	1.54
2	B	743	FLC	CA-CB	9.94	1.66	1.54
2	B	742	FLC	CG-CB	9.67	1.65	1.54
2	A	743	FLC	CA-CB	9.63	1.65	1.54
2	A	742	FLC	CG-CB	7.35	1.63	1.54
2	A	742	FLC	CA-CB	7.32	1.63	1.54
2	A	742	FLC	CB-CBC	6.02	1.59	1.53
2	B	743	FLC	CG-CB	5.92	1.61	1.54
2	A	743	FLC	CB-CBC	5.52	1.59	1.53
2	B	743	FLC	CB-CBC	4.09	1.57	1.53
2	B	743	FLC	CA-CAC	3.57	1.61	1.50
2	A	743	FLC	CG-CGC	3.39	1.61	1.50
2	A	743	FLC	CA-CAC	3.38	1.61	1.50
2	B	742	FLC	CA-CAC	2.94	1.59	1.50
2	B	742	FLC	CG-CGC	2.74	1.59	1.50
2	B	742	FLC	OB2-CBC	-2.74	1.20	1.30
2	B	743	FLC	CG-CGC	2.42	1.58	1.50
2	A	743	FLC	OA2-CAC	-2.36	1.23	1.30
2	B	743	FLC	OA2-CAC	-2.13	1.23	1.30
2	B	742	FLC	OG2-CGC	-2.03	1.24	1.30
2	B	743	FLC	OG2-CGC	-2.01	1.24	1.30

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	742	FLC	OHB-CB-CBC	-22.22	77.45	108.96
2	B	742	FLC	OHB-CB-CBC	-19.83	80.83	108.96
2	A	743	FLC	OHB-CB-CBC	-19.62	81.13	108.96
2	B	743	FLC	OHB-CB-CBC	-17.56	84.06	108.96
2	B	743	FLC	OHB-CB-CG	-13.45	78.71	109.38
2	A	743	FLC	OHB-CB-CG	-13.25	79.16	109.38
2	A	742	FLC	OHB-CB-CG	-12.27	81.39	109.38
2	B	742	FLC	OHB-CB-CG	-12.03	81.93	109.38
2	B	742	FLC	OHB-CB-CA	-10.75	84.87	109.38
2	B	743	FLC	OHB-CB-CA	-10.73	84.91	109.38
2	A	743	FLC	OHB-CB-CA	-8.66	89.63	109.38
2	A	742	FLC	OHB-CB-CA	-7.96	91.22	109.38
2	B	742	FLC	CA-CB-CBC	6.76	124.98	110.03
2	A	742	FLC	CG-CB-CBC	5.71	122.67	110.03
2	A	742	FLC	CA-CB-CBC	5.71	122.66	110.03
2	B	743	FLC	CA-CB-CBC	4.88	120.83	110.03
2	A	743	FLC	CG-CB-CBC	4.60	120.21	110.03
2	B	742	FLC	CB-CA-CAC	4.47	126.14	113.92
2	A	743	FLC	CA-CB-CBC	4.25	119.44	110.03
2	B	742	FLC	CB-CG-CGC	4.25	125.54	113.92
2	B	742	FLC	CG-CB-CBC	4.21	119.36	110.03
2	B	743	FLC	CG-CB-CA	3.86	119.22	109.31
2	A	743	FLC	CB-CA-CAC	3.03	122.22	113.92
2	A	742	FLC	CB-CG-CGC	2.93	121.94	113.92
2	A	742	FLC	CB-CA-CAC	2.93	121.93	113.92
2	B	743	FLC	CB-CA-CAC	2.80	121.58	113.92
2	A	743	FLC	CB-CG-CGC	2.71	121.33	113.92
2	A	743	FLC	CG-CB-CA	2.71	116.25	109.31
2	B	743	FLC	OB2-CBC-CB	2.63	118.19	113.14
2	B	743	FLC	CG-CB-CBC	2.27	115.05	110.03
2	A	742	FLC	OG1-CGC-CG	-2.10	117.01	122.95
2	B	743	FLC	OG1-CGC-CG	-2.07	117.09	122.95

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	742	FLC	CG-CB-CBC-OB1
2	A	742	FLC	CG-CB-CBC-OB2
2	A	742	FLC	OHB-CB-CBC-OB1
2	A	742	FLC	OHB-CB-CBC-OB2

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Mol	Chain	Res	Type	Atoms
2	A	743	FLC	CG-CB-CBC-OB1
2	A	743	FLC	CG-CB-CBC-OB2
2	A	743	FLC	OHB-CB-CBC-OB1
2	A	743	FLC	OHB-CB-CBC-OB2
2	A	742	FLC	CAC-CA-CB-CBC
2	A	743	FLC	CAC-CA-CB-CBC
2	B	742	FLC	CAC-CA-CB-CBC
2	B	742	FLC	CBC-CB-CG-CGC
2	B	743	FLC	CAC-CA-CB-CBC
2	B	743	FLC	CBC-CB-CG-CGC
2	A	743	FLC	CBC-CB-CG-CGC
2	A	743	FLC	OHB-CB-CG-CGC
2	B	743	FLC	OHB-CB-CG-CGC
2	A	742	FLC	CBC-CB-CG-CGC
2	B	743	FLC	OHB-CB-CBC-OB2
2	B	742	FLC	OHB-CB-CG-CGC
2	A	742	FLC	CA-CB-CBC-OB1
2	A	742	FLC	CA-CB-CBC-OB2
2	A	743	FLC	CA-CB-CBC-OB1
2	A	743	FLC	CA-CB-CBC-OB2
2	A	742	FLC	OHB-CB-CG-CGC
2	A	742	FLC	CAC-CA-CB-OHB
2	A	743	FLC	CAC-CA-CB-OHB

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	742	FLC	5	0
2	B	743	FLC	1	0
2	B	742	FLC	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	696:MET	C	697:ALA	N	1.72
1	B	533:GLU	C	534:PRO	N	1.13

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	647/751 (86%)	0.03	13 (2%) 65 49	9, 49, 87, 117	0
1	B	645/751 (85%)	0.15	15 (2%) 61 46	15, 60, 99, 128	0
All	All	1292/1502 (86%)	0.09	28 (2%) 62 47	9, 54, 96, 128	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	694	PRO	5.4
1	B	223	PHE	4.8
1	B	696	MET	4.8
1	B	694	PRO	4.2
1	A	693	GLY	4.0
1	A	696	MET	3.8
1	A	273	ARG	3.4
1	B	436	TYR	3.3
1	A	503	ASP	3.3
1	B	556	GLY	3.0
1	A	623	THR	3.0
1	A	582	ARG	2.7
1	B	697	ALA	2.7
1	A	555	MET	2.6
1	A	496	ASN	2.5
1	A	618	ARG	2.4
1	A	200	ALA	2.3
1	B	676	GLY	2.3
1	B	600	THR	2.2
1	B	488	TYR	2.2
1	A	396	MET	2.2
1	B	222	ASP	2.2
1	B	418	MET	2.1
1	A	325	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	346	PHE	2.1
1	B	693	GLY	2.0
1	B	622	ASP	2.0
1	B	501	LEU	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	FLC	A	742	13/13	0.89	0.16	56,56,56,56	0
2	FLC	B	743	13/13	0.89	0.12	56,56,56,56	0
2	FLC	B	742	13/13	0.90	0.11	56,56,56,56	0
2	FLC	A	743	13/13	0.91	0.12	56,56,56,56	0
3	FE	B	745	1/1	0.95	0.04	73,73,73,73	0
3	FE	A	745	1/1	0.98	0.07	44,44,44,44	0
3	FE	A	744	1/1	0.98	0.04	40,40,40,40	0
3	FE	B	744	1/1	0.99	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.