Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:23 AM GMT

PDB ID	:	3ALX
Title	:	Crystal structure of the measles virus hemagglutinin bound to its cellular receptor SLAM (MV-H(L482R)-SLAM(N102H/R108Y) fusion)
Authors	:	Hashiguchi, T.; Ose, T.; Kubota, M.; Maita, N.; Kamishikiryo, J.; Maenaka, K.; Yanagi, Y.
Deposited on	:	2010-08-09
Resolution	:	3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

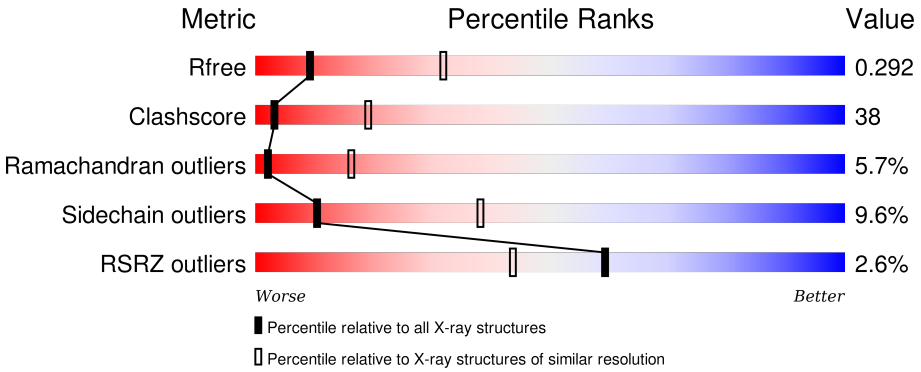
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	559	41% 40% 11% • 8%
1	B	559	4% 44% 44% 6% • 6%
1	C	559	2% 35% 46% 10% • 8%
1	D	559	2% 31% 51% 8% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16313 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 Hemagglutinin, CDw150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4053	2598	677	750	28			
1	B	526	Total	C	N	O	S	0	0	0
			4141	2651	695	767	28			
1	C	514	Total	C	N	O	S	0	0	0
			4051	2599	676	748	28			
1	D	504	Total	C	N	O	S	0	0	0
			3984	2562	663	732	27			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
A	182	THR	-	EXPRESSION TAG	UNP E2RZS2
A	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
A	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
A	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
A	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3
A	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
A	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
A	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
A	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
B	182	THR	-	EXPRESSION TAG	UNP E2RZS2
B	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
B	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
B	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
B	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3

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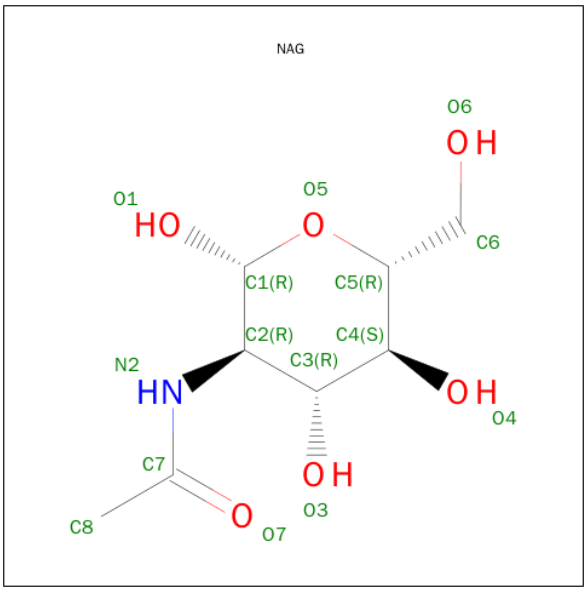
Chain	Residue	Modelled	Actual	Comment	Reference
B	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
B	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
B	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
B	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
C	182	THR	-	EXPRESSION TAG	UNP E2RZS2
C	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
C	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
C	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
C	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3
C	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
C	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
C	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
C	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
D	182	THR	-	EXPRESSION TAG	UNP E2RZS2
D	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
D	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
D	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
D	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3
D	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
D	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
D	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
D	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



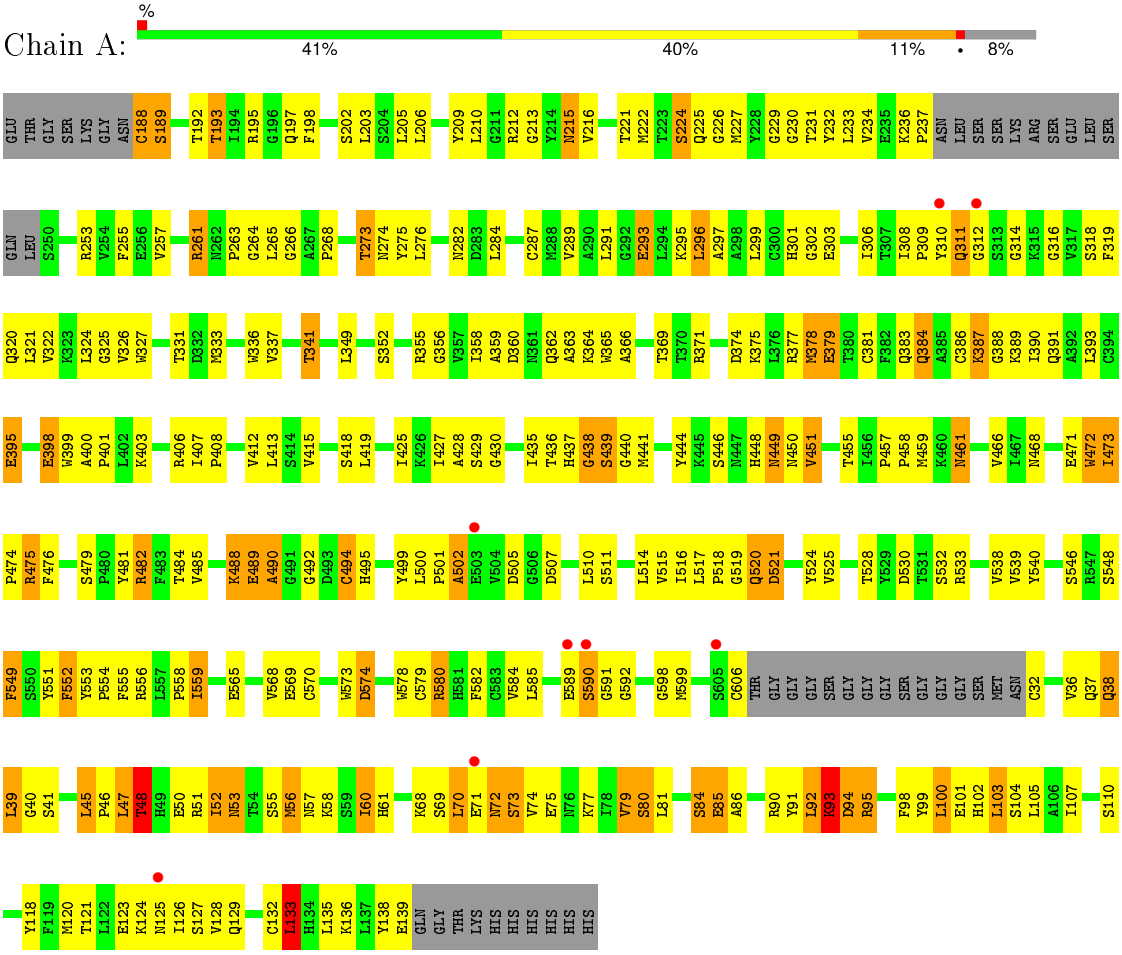
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

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

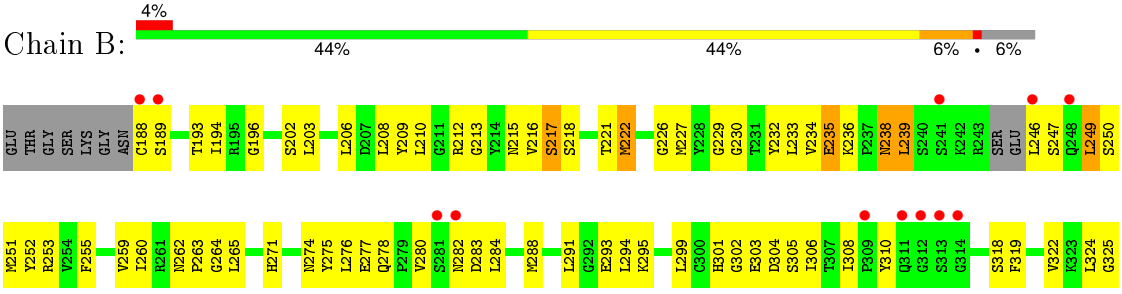
- Molecule 1: Hemagglutinin, CDw150

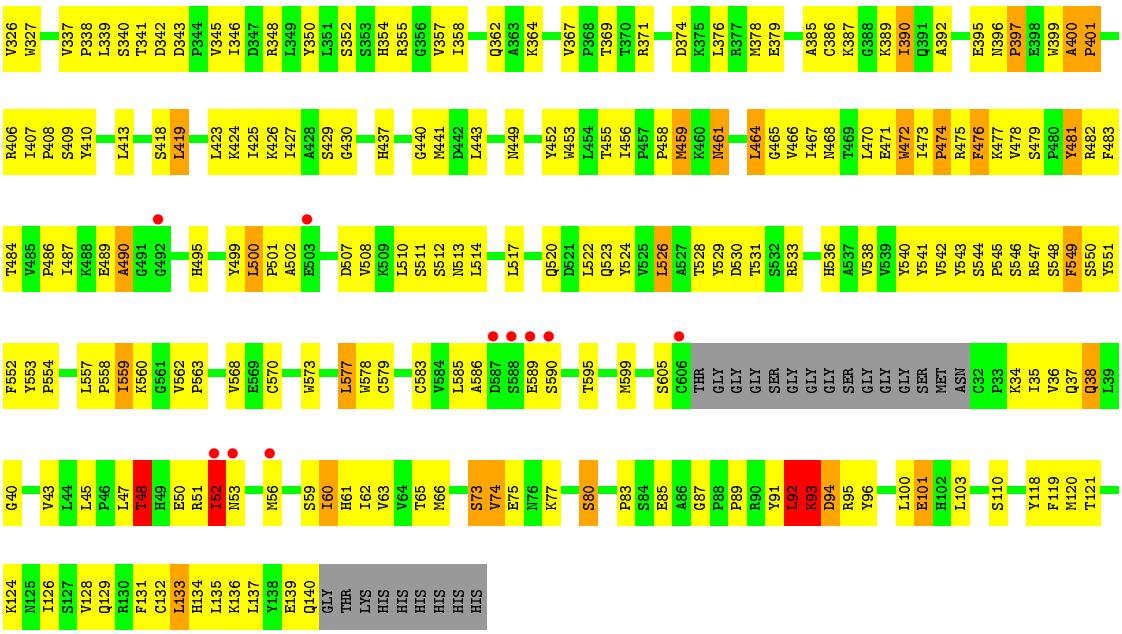
Chain A:



- Molecule 1: Hemagglutinin, CDw150

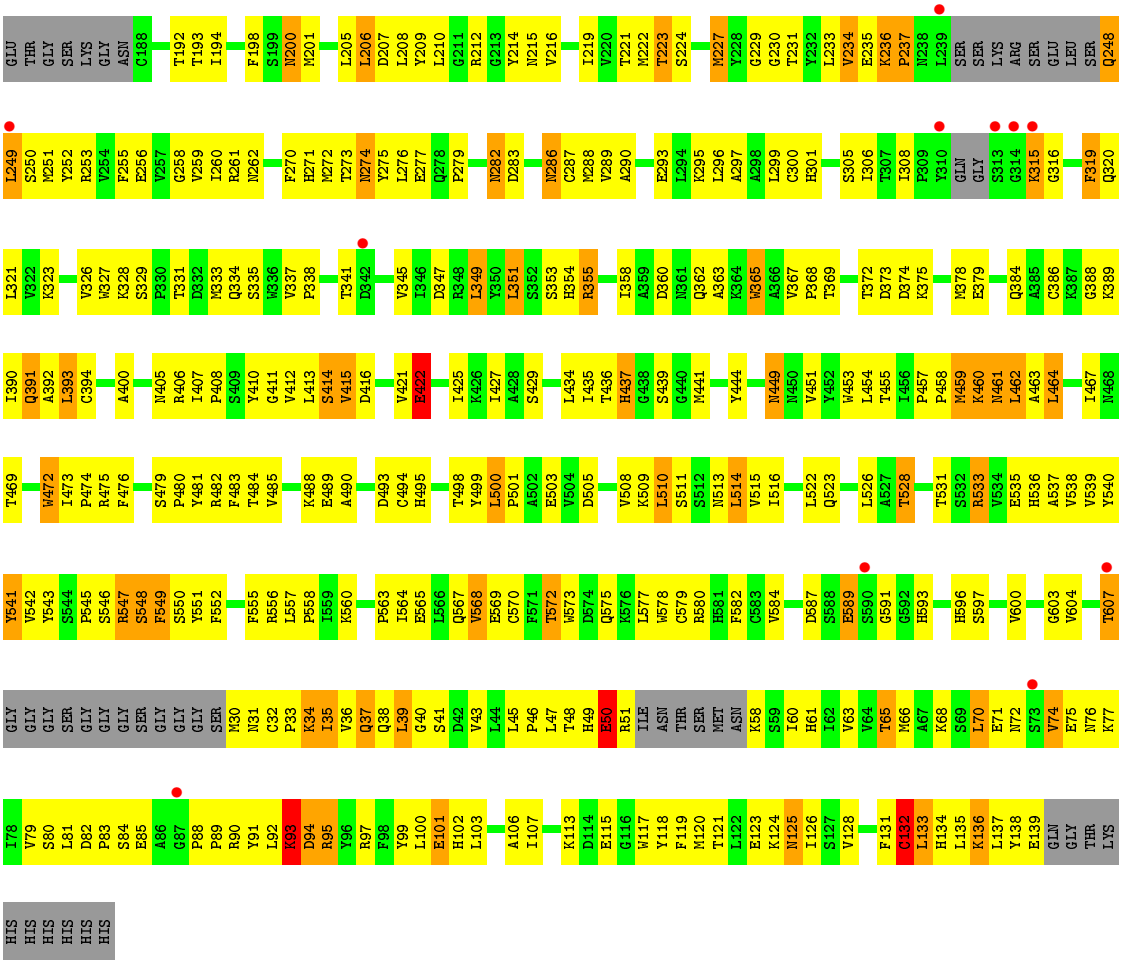
Chain B:





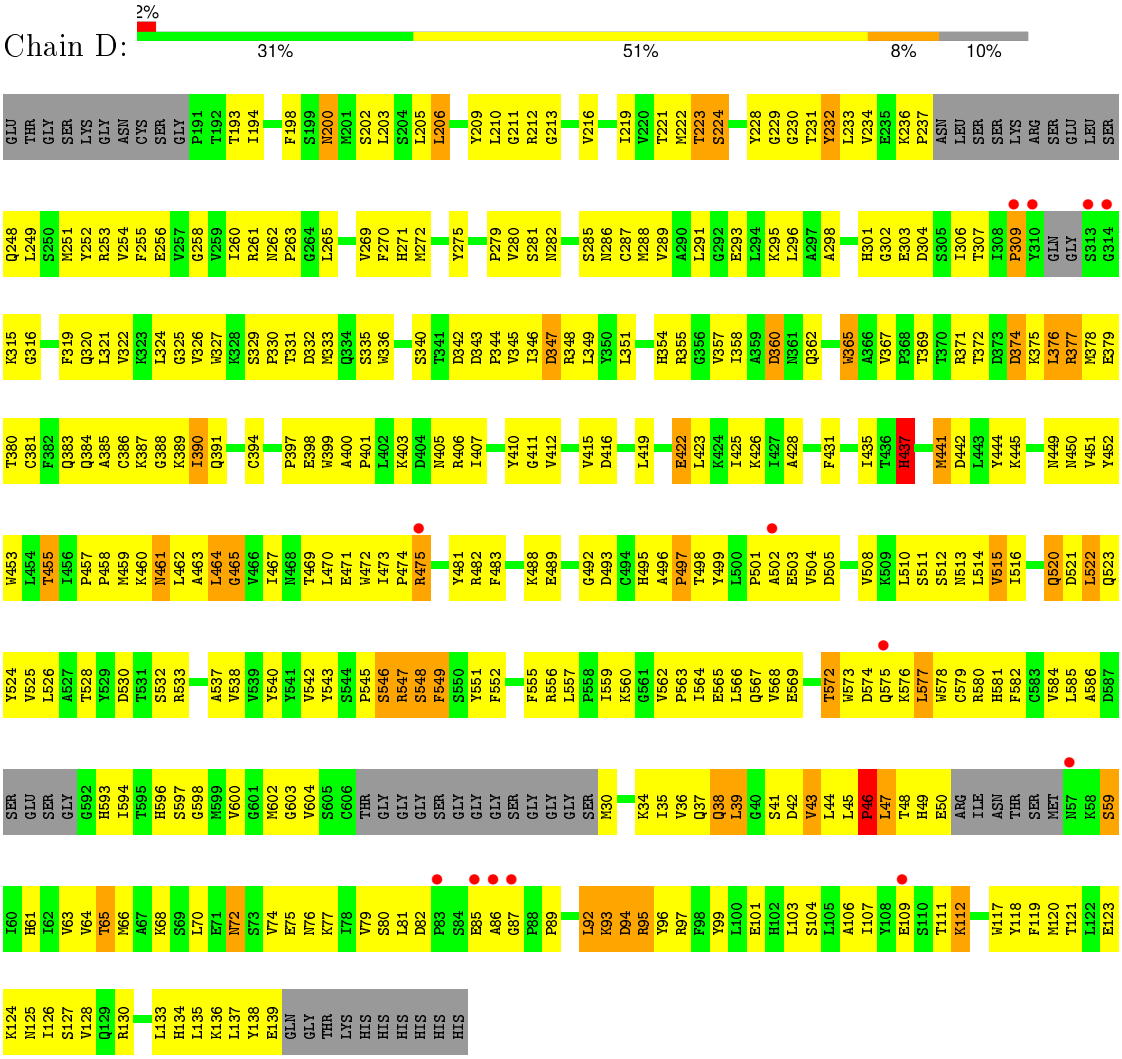
• Molecule 1: Hemagglutinin, CDw150

Chain C:



• Molecule 1: Hemagglutinin, CDw150

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	187.71Å 170.07Å 110.68Å 90.00° 117.28° 90.00°	Depositor
Resolution (Å)	19.97 – 3.15 19.96 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.97-3.15) 99.2 (19.96-3.16)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 3.15Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.231 , 0.292 0.232 , 0.292	Depositor DCC
R_{free} test set	2644 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 52452 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16313	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.49	0/4155	0.74	2/5646 (0.0%)
1	B	0.44	0/4243	0.71	2/5763 (0.0%)
1	C	0.46	0/4151	0.71	1/5638 (0.0%)
1	D	0.41	0/4083	0.66	0/5545
All	All	0.45	0/16632	0.70	5/22592 (0.0%)

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	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	48	THR	N-CA-C	-6.29	94.02	111.00
1	C	132	CYS	CA-CB-SG	-6.03	103.15	114.00
1	A	48	THR	N-CA-C	-5.52	96.09	111.00
1	B	92	LEU	N-CA-C	-5.35	96.54	111.00
1	A	92	LEU	N-CA-C	-5.34	96.58	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	541	TYR	Sidechain

5.2 Too-close contacts (i)

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	4053	0	4023	288	0
1	B	4141	0	4119	297	0
1	C	4051	0	4024	313	0
1	D	3984	0	3964	350	0
2	A	14	0	13	0	0
2	B	28	0	26	0	0
2	C	28	0	26	1	0
2	D	14	0	13	1	0
All	All	16313	0	16208	1224	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 38.

All (1224) 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:85:GLU:HG2	1:A:86:ALA:H	1.09	1.16
1:A:236:LYS:HB3	1:A:237:PRO:HD2	1.30	1.14
1:D:503:GLU:HB2	1:D:76:ASN:HD22	1.05	1.09
1:A:60:ILE:HG22	1:A:61:HIS:H	1.13	1.08
1:A:540:TYR:HE1	1:A:568:VAL:HG21	1.22	1.04
1:C:546:SER:HB3	1:C:547:ARG:HH21	1.15	1.04
1:B:483:PHE:HZ	1:B:524:TYR:HH	1.04	0.99
1:C:194:ILE:HG13	1:C:604:VAL:HG12	1.44	0.98
1:D:37:GLN:HE22	1:D:43:VAL:HA	1.28	0.97
1:D:457:PRO:HB3	1:D:513:ASN:HA	1.49	0.95
1:D:503:GLU:HB2	1:D:76:ASN:ND2	1.82	0.94
1:A:589:GLU:HG3	1:A:590:SER:H	1.34	0.93
1:D:37:GLN:NE2	1:D:43:VAL:HA	1.84	0.92
1:C:546:SER:HB3	1:C:547:ARG:NH2	1.84	0.91
1:B:74:VAL:HG13	1:B:75:GLU:H	1.33	0.90
1:B:558:PRO:HG2	1:B:559:ILE:HG23	1.52	0.90
1:D:194:ILE:HG13	1:D:604:VAL:HG12	1.55	0.89
1:C:306:ILE:HD13	1:C:351:LEU:HD21	1.55	0.89
1:C:237:PRO:HG2	1:C:249:LEU:HA	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:TRP:H	1:B:472:TRP:HE3	1.19	0.88
1:B:473:ILE:HB	1:B:474:PRO:HD3	1.55	0.88
1:D:47:LEU:HD13	1:D:120:MET:HB2	1.56	0.87
1:B:472:TRP:HA	1:B:476:PHE:HA	1.57	0.86
1:C:81:LEU:HD23	1:C:89:PRO:HB3	1.56	0.85
1:D:520:GLN:NE2	1:D:520:GLN:H	1.73	0.85
1:D:458:PRO:HG2	1:D:511:SER:HB3	1.58	0.85
1:D:437:HIS:HB3	1:D:459:MET:HG2	1.58	0.85
1:B:430:GLY:HA3	1:B:476:PHE:HE2	1.42	0.84
1:B:475:ARG:NH1	1:B:477:LYS:HD3	1.91	0.84
1:C:457:PRO:HB3	1:C:513:ASN:HA	1.58	0.84
1:A:85:GLU:HG2	1:A:86:ALA:N	1.92	0.84
1:A:540:TYR:CE1	1:A:568:VAL:HG21	2.12	0.83
1:B:562:VAL:HB	1:B:586:ALA:HB3	1.60	0.83
1:D:93:LYS:NZ	1:D:93:LYS:HA	1.93	0.83
1:D:222:MET:HE2	1:D:291:LEU:HB2	1.60	0.82
1:D:121:THR:HG23	1:D:128:VAL:HG13	1.59	0.82
1:B:400:ALA:HB3	1:B:401:PRO:HD3	1.60	0.82
1:B:216:VAL:HG22	1:B:234:VAL:HG12	1.61	0.82
1:A:236:LYS:HB3	1:A:237:PRO:CD	2.10	0.82
1:C:135:LEU:HD23	1:C:136:LYS:N	1.95	0.82
1:B:464:LEU:HG	1:B:465:GLY:H	1.45	0.81
1:D:286:ASN:ND2	1:D:304:ASP:HB3	1.95	0.81
1:A:60:ILE:HG22	1:A:61:HIS:N	1.95	0.81
1:C:36:VAL:HG12	1:C:136:LYS:HB3	1.63	0.81
1:A:450:ASN:HA	1:A:472:TRP:CH2	2.16	0.80
1:B:89:PRO:HG2	1:B:91:TYR:CE2	2.17	0.80
1:D:261:ARG:HB2	1:D:261:ARG:NH1	1.97	0.80
1:C:390:ILE:HG23	1:C:393:LEU:HB2	1.64	0.80
1:B:93:LYS:HD2	1:B:94:ASP:C	2.01	0.79
1:C:531:THR:HG22	1:C:536:HIS:CD2	2.17	0.79
1:C:47:LEU:HD13	1:C:120:MET:HB2	1.65	0.79
1:C:378:MET:HB2	1:C:407:ILE:HG21	1.64	0.78
1:D:123:GLU:HB3	1:D:128:VAL:HG22	1.63	0.78
1:C:252:TYR:CE1	1:C:279:PRO:HG3	2.17	0.78
1:C:296:LEU:HD23	1:C:296:LEU:O	1.83	0.78
1:A:93:LYS:HD2	1:A:94:ASP:H	1.48	0.78
1:D:537:ALA:HA	1:D:557:LEU:HD22	1.64	0.78
1:C:545:PRO:HB3	1:C:71:GLU:HA	1.64	0.78
1:D:503:GLU:CB	1:D:76:ASN:HD22	1.91	0.77
1:C:93:LYS:HD2	1:C:94:ASP:N	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:PRO:HD2	1:C:132:CYS:SG	2.25	0.77
1:A:378:MET:HB3	1:A:407:ILE:HG21	1.68	0.77
1:D:38:GLN:HB3	1:D:41:SER:OG	1.85	0.76
1:B:236:LYS:HE3	1:B:238:ASN:HB3	1.65	0.76
1:A:374:ASP:HB2	1:A:407:ILE:HB	1.65	0.76
1:C:68:LYS:HD2	1:C:115:GLU:O	1.86	0.76
1:A:36:VAL:HA	1:A:136:LYS:O	1.84	0.76
1:A:71:GLU:O	1:A:72:ASN:HB2	1.85	0.76
1:A:84:SER:O	1:A:85:GLU:HB2	1.85	0.76
1:A:461:ASN:H	1:A:461:ASN:ND2	1.83	0.76
1:D:525:VAL:HG12	1:D:542:VAL:HA	1.67	0.76
1:B:77:LYS:HB3	1:B:92:LEU:HD11	1.68	0.76
1:D:464:LEU:HG	1:D:465:GLY:H	1.50	0.75
1:A:274:ASN:HD22	1:A:324:LEU:HB3	1.51	0.75
1:D:35:ILE:HD11	1:D:45:LEU:HG	1.68	0.75
1:C:384:GLN:HE22	1:C:490:ALA:HA	1.51	0.75
1:C:194:ILE:CG1	1:C:604:VAL:HG12	2.17	0.75
1:A:461:ASN:H	1:A:461:ASN:HD22	1.34	0.75
1:A:473:ILE:HG22	1:A:474:PRO:N	2.02	0.74
1:B:95:ARG:HH11	1:B:95:ARG:HG3	1.51	0.74
1:D:309:PRO:HG3	1:D:316:GLY:HA2	1.69	0.74
1:D:343:ASP:OD1	1:D:345:VAL:HG12	1.86	0.74
1:D:237:PRO:HA	1:D:249:LEU:HD23	1.69	0.74
1:D:540:TYR:HE1	1:D:568:VAL:HG21	1.53	0.74
1:A:231:THR:HG21	1:A:287:CYS:HB2	1.69	0.74
1:B:139:GLU:O	1:B:140:GLN:HB2	1.87	0.73
1:A:556:ARG:HH12	1:A:125:ASN:HA	1.53	0.73
1:B:140:GLN:HG3	1:C:421:VAL:HA	1.68	0.73
1:A:93:LYS:HD2	1:A:94:ASP:N	2.03	0.73
1:B:570:CYS:HB3	1:B:577:LEU:HD21	1.71	0.73
1:D:354:HIS:CE1	1:D:367:VAL:HG12	2.24	0.73
1:B:93:LYS:HD2	1:B:94:ASP:H	1.53	0.73
1:C:378:MET:CB	1:C:407:ILE:HG21	2.19	0.73
1:A:40:GLY:HA2	1:A:110:SER:O	1.88	0.73
1:A:580:ARG:HG3	1:A:580:ARG:HH11	1.53	0.73
1:A:222:MET:HB3	1:A:355:ARG:HD3	1.71	0.72
1:D:72:ASN:N	1:D:72:ASN:HD22	1.86	0.72
1:B:481:TYR:O	1:B:482:ARG:HG2	1.90	0.72
1:D:93:LYS:HG3	1:D:94:ASP:H	1.54	0.72
1:B:464:LEU:HG	1:B:465:GLY:N	2.04	0.72
1:A:326:VAL:HG23	1:A:327:TRP:CD1	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LYS:HD2	1:A:94:ASP:C	2.09	0.72
1:D:303:GLU:HG3	1:D:304:ASP:H	1.54	0.72
1:B:91:TYR:HB3	1:B:93:LYS:HB3	1.70	0.72
1:B:35:ILE:O	1:B:35:ILE:HG13	1.89	0.72
1:C:77:LYS:HD2	1:C:80:SER:OG	1.89	0.72
1:A:60:ILE:CG2	1:A:61:HIS:H	1.97	0.72
1:D:65:THR:HG23	1:D:119:PHE:HB2	1.71	0.72
1:C:45:LEU:HD21	1:C:135:LEU:HD12	1.70	0.72
1:C:216:VAL:HG22	1:C:234:VAL:HG13	1.71	0.72
1:B:340:SER:HB3	1:B:426:LYS:HA	1.72	0.72
1:B:461:ASN:H	1:B:461:ASN:HD22	1.35	0.72
1:B:378:MET:CB	1:B:407:ILE:HG21	2.19	0.71
1:A:552:PHE:HE1	1:A:121:THR:HG1	1.37	0.71
1:C:528:THR:HG22	1:C:539:VAL:HB	1.71	0.71
1:A:580:ARG:HB3	1:A:599:MET:HE2	1.73	0.71
1:C:308:ILE:HD11	1:C:349:LEU:HD12	1.71	0.71
1:D:219:ILE:H	1:D:219:ILE:HD12	1.56	0.71
1:B:288:MET:HE3	1:B:299:LEU:HB3	1.73	0.71
1:A:540:TYR:O	1:A:552:PHE:HA	1.91	0.71
1:B:529:TYR:CD1	1:B:563:PRO:HG3	2.26	0.71
1:A:585:LEU:HD23	1:A:585:LEU:H	1.55	0.71
1:A:556:ARG:NH1	1:A:125:ASN:HA	2.06	0.71
1:B:337:VAL:HG12	1:B:423:LEU:HB3	1.72	0.71
1:D:378:MET:HB3	1:D:407:ILE:HG21	1.72	0.71
1:D:37:GLN:CD	1:D:43:VAL:HG23	2.10	0.70
1:B:74:VAL:HG13	1:B:75:GLU:N	2.03	0.70
1:A:398:GLU:O	1:A:403:LYS:HE3	1.91	0.70
1:D:97:ARG:HB3	1:D:106:ALA:HB3	1.71	0.70
1:B:458:PRO:HG3	1:B:465:GLY:H	1.54	0.70
1:A:70:LEU:HD22	1:A:70:LEU:H	1.56	0.70
1:D:253:ARG:HH21	1:D:285:SER:HB2	1.56	0.70
1:C:216:VAL:HG22	1:C:234:VAL:CG1	2.21	0.70
1:C:587:ASP:O	1:C:591:GLY:HA2	1.92	0.69
1:B:399:TRP:CD1	1:B:401:PRO:HD2	2.27	0.69
1:C:222:MET:HB3	1:C:355:ARG:HD3	1.74	0.69
1:B:346:ILE:HG23	1:B:369:THR:HG21	1.73	0.69
1:D:306:ILE:HD12	1:D:306:ILE:N	2.08	0.69
1:B:544:SER:HB2	1:B:549:PHE:HB3	1.73	0.69
1:D:415:VAL:HG12	1:D:425:ILE:HA	1.75	0.68
1:D:194:ILE:HG12	1:D:551:TYR:CD2	2.28	0.68
1:C:464:LEU:CD2	1:C:498:THR:HB	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:564:ILE:O	1:D:564:ILE:HD12	1.93	0.68
1:C:89:PRO:HG2	1:C:91:TYR:CE2	2.27	0.68
1:D:216:VAL:HG22	1:D:234:VAL:HG22	1.75	0.68
1:C:406:ARG:O	1:C:408:PRO:HD3	1.92	0.68
1:C:261:ARG:HH11	1:C:271:HIS:HB3	1.59	0.67
1:C:389:LYS:HE3	1:C:500:LEU:H	1.58	0.67
1:B:348:ARG:HD3	1:B:350:TYR:OH	1.94	0.67
1:C:43:VAL:CG2	1:C:107:ILE:HB	2.24	0.67
1:B:475:ARG:O	1:B:476:PHE:HB3	1.95	0.67
1:D:194:ILE:HD12	1:D:194:ILE:N	2.09	0.67
1:B:62:ILE:HD13	1:B:83:PRO:HD3	1.75	0.67
1:A:236:LYS:CB	1:A:237:PRO:HD2	2.16	0.67
1:A:461:ASN:N	1:A:461:ASN:HD22	1.88	0.67
1:D:458:PRO:HG2	1:D:511:SER:CB	2.25	0.67
1:B:74:VAL:O	1:B:75:GLU:HB3	1.94	0.67
1:D:288:MET:HB3	1:D:365:TRP:NE1	2.10	0.67
1:D:384:GLN:HA	1:D:387:LYS:HE3	1.77	0.66
1:C:37:GLN:HG2	1:C:43:VAL:HG12	1.77	0.66
1:D:545:PRO:C	1:D:547:ARG:H	1.99	0.66
1:B:549:PHE:O	1:B:549:PHE:HD1	1.78	0.66
1:A:224:SER:O	1:A:225:GLN:HB2	1.95	0.66
1:D:261:ARG:HH11	1:D:261:ARG:CB	2.09	0.66
1:C:546:SER:CB	1:C:547:ARG:HH21	2.02	0.66
1:C:326:VAL:HG13	1:C:327:TRP:H	1.61	0.66
1:A:52:ILE:HD13	1:D:282:ASN:HD21	1.60	0.66
1:D:512:SER:HA	1:D:566:LEU:O	1.96	0.66
1:C:353:SER:OG	1:C:567:GLN:NE2	2.29	0.66
1:B:499:TYR:CD2	1:B:501:PRO:HD3	2.30	0.66
1:D:205:LEU:HB2	1:D:272:MET:HE1	1.78	0.65
1:D:77:LYS:HD2	1:D:80:SER:OG	1.96	0.65
1:A:448:HIS:HB2	1:A:451:VAL:CG1	2.26	0.65
1:A:91:TYR:HB3	1:A:93:LYS:HB3	1.77	0.65
1:B:430:GLY:CA	1:B:476:PHE:HE2	2.09	0.65
1:B:461:ASN:H	1:B:461:ASN:ND2	1.92	0.65
1:C:82:ASP:OD2	1:C:84:SER:HB3	1.96	0.65
1:A:585:LEU:HD23	1:A:585:LEU:N	2.12	0.65
1:D:43:VAL:HG13	1:D:107:ILE:HB	1.79	0.65
1:D:521:ASP:HB2	1:D:546:SER:HB2	1.79	0.65
1:D:514:LEU:CD1	1:D:526:LEU:HD23	2.26	0.65
1:B:140:GLN:HE21	1:C:421:VAL:HA	1.62	0.65
1:D:289:VAL:HG13	1:D:296:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASN:HD22	1:B:461:ASN:N	1.91	0.65
1:A:499:TYR:CD2	1:A:501:PRO:HD3	2.32	0.65
1:A:51:ARG:HH12	1:A:102:HIS:HB3	1.62	0.65
1:C:273:THR:O	1:C:274:ASN:HB2	1.97	0.65
1:C:439:SER:HB2	1:C:457:PRO:HG2	1.78	0.64
1:B:369:THR:O	1:B:409:SER:HB3	1.97	0.64
1:D:211:GLY:C	1:D:213:GLY:H	2.01	0.64
1:A:430:GLY:HA3	1:A:476:PHE:CE2	2.33	0.64
1:B:101:GLU:CD	1:B:101:GLU:H	2.00	0.64
1:B:216:VAL:HA	1:B:233:LEU:O	1.97	0.64
1:B:467:ILE:O	1:B:481:TYR:HB3	1.96	0.64
1:B:583:CYS:O	1:B:595:THR:HA	1.96	0.64
1:A:52:ILE:CD1	1:D:282:ASN:HD21	2.10	0.64
1:A:520:GLN:HG3	1:A:520:GLN:O	1.97	0.64
1:A:589:GLU:CG	1:A:590:SER:H	2.07	0.64
1:B:61:HIS:CE1	1:B:63:VAL:HG22	2.33	0.64
1:B:215:ASN:CB	1:B:235:GLU:HB2	2.27	0.64
1:B:343:ASP:OD2	1:B:346:ILE:HG13	1.97	0.64
1:B:93:LYS:CG	1:B:94:ASP:N	2.60	0.64
1:B:378:MET:HB2	1:B:407:ILE:HG21	1.79	0.64
1:D:377:ARG:HG3	1:D:377:ARG:HH11	1.63	0.64
1:C:305:SER:C	1:C:306:ILE:HD12	2.19	0.64
1:C:107:ILE:HD11	1:C:118:TYR:CE2	2.32	0.64
1:B:533:ARG:HG2	1:B:61:HIS:CD2	2.32	0.64
1:D:547:ARG:HG3	1:D:548:SER:H	1.63	0.64
1:D:206:LEU:HG	1:D:232:TYR:CE2	2.33	0.64
1:A:337:VAL:CG1	1:A:425:ILE:HG13	2.28	0.64
1:C:410:TYR:CE1	1:C:435:ILE:HD11	2.32	0.63
1:C:65:THR:HG21	1:C:75:GLU:HB3	1.81	0.63
1:C:473:ILE:HG22	1:C:474:PRO:HD3	1.80	0.63
1:B:557:LEU:HD23	1:B:559:ILE:HD11	1.79	0.63
1:A:56:MET:HG2	1:A:57:ASN:H	1.62	0.63
1:D:533:ARG:HB3	1:D:61:HIS:CD2	2.34	0.63
1:A:580:ARG:HH11	1:A:580:ARG:CG	2.12	0.63
1:D:467:ILE:O	1:D:481:TYR:HB3	1.98	0.63
1:A:309:PRO:HG3	1:A:316:GLY:HA3	1.80	0.63
1:B:352:SER:N	1:B:354:HIS:NE2	2.46	0.63
1:B:188:CYS:O	1:B:189:SER:HB3	1.99	0.63
1:C:461:ASN:HD22	1:C:461:ASN:C	2.01	0.63
1:A:358:ILE:HA	1:A:362:GLN:O	1.98	0.63
1:B:386:CYS:HA	1:B:390:ILE:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:GLN:HB3	1:D:41:SER:CB	2.29	0.63
1:A:189:SER:HB2	1:D:252:TYR:OH	1.98	0.63
1:C:505:ASP:HB3	1:C:508:VAL:HG12	1.80	0.62
1:A:559:ILE:HD13	1:A:559:ILE:H	1.64	0.62
1:A:448:HIS:HB2	1:A:451:VAL:HG12	1.81	0.62
1:B:74:VAL:CG1	1:B:75:GLU:H	2.11	0.62
1:D:449:ASN:O	1:D:450:ASN:HB2	2.00	0.62
1:A:517:LEU:HD11	1:A:525:VAL:CG2	2.28	0.62
1:A:375:LYS:O	1:A:379:GLU:HB2	1.99	0.62
1:B:93:LYS:HD2	1:B:95:ARG:N	2.15	0.62
1:D:124:LYS:HE3	1:D:125:ASN:OD1	1.99	0.62
1:B:36:VAL:HA	1:B:136:LYS:O	1.99	0.62
1:B:357:VAL:HG21	1:B:452:TYR:HE1	1.64	0.62
1:B:103:LEU:HD13	1:B:120:MET:HE3	1.81	0.62
1:C:293:GLU:CB	1:C:295:LYS:HE2	2.30	0.62
1:A:309:PRO:HB2	1:A:341:THR:HG21	1.82	0.62
1:B:229:GLY:N	1:B:291:LEU:HD11	2.14	0.62
1:C:251:MET:CE	1:C:283:ASP:HB3	2.30	0.62
1:A:70:LEU:HD22	1:A:70:LEU:N	2.14	0.61
1:D:295:LYS:NZ	1:D:358:ILE:HG21	2.15	0.61
1:C:345:VAL:HG13	1:C:372:THR:OG1	2.00	0.61
1:B:208:LEU:O	1:B:212:ARG:HG2	2.00	0.61
1:A:530:ASP:OD1	1:A:532:SER:HB3	2.00	0.61
1:D:261:ARG:HH12	1:D:271:HIS:HB3	1.65	0.61
1:C:390:ILE:HG22	1:C:394:CYS:SG	2.40	0.61
1:C:259:VAL:HB	1:C:261:ARG:HH12	1.65	0.61
1:C:205:LEU:HB2	1:C:272:MET:HE1	1.81	0.61
1:C:193:THR:OG1	1:C:607:THR:HG22	1.99	0.61
1:D:349:LEU:HD23	1:D:369:THR:HG23	1.82	0.61
1:A:301:HIS:HB2	1:A:319:PHE:CD2	2.34	0.61
1:D:451:VAL:HA	1:D:470:LEU:O	1.99	0.61
1:B:400:ALA:HB3	1:B:401:PRO:CD	2.30	0.61
1:B:288:MET:CE	1:B:299:LEU:HD23	2.30	0.61
1:C:389:LYS:HG2	1:C:485:VAL:HG21	1.81	0.61
1:C:297:ALA:H	1:C:358:ILE:HD11	1.65	0.61
1:A:349:LEU:HD23	1:A:369:THR:HG22	1.81	0.61
1:D:263:PRO:HG2	1:D:265:LEU:CD1	2.31	0.61
1:D:93:LYS:HA	1:D:93:LYS:HZ1	1.63	0.61
1:B:62:ILE:HD12	1:B:62:ILE:N	2.16	0.61
1:C:210:LEU:HD11	1:C:582:PHE:HE2	1.65	0.61
1:C:546:SER:CB	1:C:547:ARG:HE	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LEU:O	1:D:104:SER:HA	2.01	0.61
1:A:450:ASN:O	1:A:451:VAL:HB	1.99	0.61
1:C:546:SER:HB3	1:C:547:ARG:HE	1.64	0.61
1:A:77:LYS:O	1:A:92:LEU:HD12	2.00	0.61
1:A:95:ARG:HB2	1:A:95:ARG:NH1	2.16	0.61
1:D:557:LEU:HD12	1:D:596:HIS:CE1	2.36	0.61
1:A:303:GLU:HB2	1:A:306:ILE:CD1	2.31	0.61
1:C:548:SER:O	1:C:550:SER:N	2.33	0.61
1:B:121:THR:HG23	1:B:128:VAL:HG13	1.82	0.61
1:D:293:GLU:CD	1:D:360:ASP:H	2.04	0.61
1:D:70:LEU:HD13	1:D:117:TRP:CZ2	2.36	0.61
1:B:531:THR:HG22	1:B:536:HIS:CD2	2.35	0.61
1:C:48:THR:HG21	1:C:103:LEU:HD12	1.82	0.61
1:B:60:ILE:O	1:B:83:PRO:HD2	2.01	0.61
1:D:263:PRO:HG2	1:D:265:LEU:HD12	1.83	0.61
1:D:87:GLY:O	1:D:89:PRO:HD3	2.01	0.61
1:A:472:TRP:CE3	1:A:473:ILE:HG12	2.37	0.60
1:C:538:VAL:HG23	1:C:557:LEU:HD11	1.82	0.60
1:B:396:ASN:N	1:B:397:PRO:HD3	2.15	0.60
1:B:93:LYS:CD	1:B:94:ASP:H	2.13	0.60
1:D:514:LEU:HD12	1:D:526:LEU:HB3	1.83	0.60
1:C:210:LEU:HD13	1:C:597:SER:CB	2.31	0.60
1:D:303:GLU:HG3	1:D:304:ASP:N	2.17	0.60
1:A:93:LYS:CD	1:A:94:ASP:H	2.15	0.60
1:A:95:ARG:CZ	1:A:95:ARG:HB2	2.32	0.60
1:B:455:THR:HB	1:B:514:LEU:HD22	1.84	0.60
1:D:222:MET:CE	1:D:291:LEU:HB2	2.28	0.60
1:D:377:ARG:HG3	1:D:377:ARG:NH1	2.16	0.60
1:A:212:ARG:HD3	1:C:201:MET:SD	2.42	0.60
1:D:261:ARG:CB	1:D:261:ARG:NH1	2.65	0.60
1:C:388:GLY:O	1:C:391:GLN:HB3	2.01	0.60
1:C:252:TYR:HE1	1:C:279:PRO:HG3	1.66	0.60
1:C:358:ILE:HA	1:C:362:GLN:O	2.01	0.60
1:A:188:CYS:SG	1:A:549:PHE:HZ	2.25	0.60
1:D:505:ASP:HB3	1:D:508:VAL:HG23	1.84	0.60
1:C:236:LYS:HB2	1:C:237:PRO:CD	2.32	0.60
1:C:43:VAL:HG22	1:C:107:ILE:HB	1.83	0.60
1:C:384:GLN:HE22	1:C:490:ALA:CA	2.14	0.60
1:B:549:PHE:O	1:B:549:PHE:CD1	2.55	0.60
1:D:378:MET:CB	1:D:407:ILE:HG21	2.32	0.59
1:B:202:SER:O	1:B:203:LEU:HD23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:MET:HG2	1:A:57:ASN:N	2.17	0.59
1:C:81:LEU:CD2	1:C:89:PRO:HB3	2.30	0.59
1:A:261:ARG:O	1:A:263:PRO:HD3	2.02	0.59
1:A:46:PRO:O	1:A:48:THR:O	2.21	0.59
1:C:546:SER:HB3	1:C:547:ARG:CZ	2.33	0.59
1:B:121:THR:CG2	1:B:128:VAL:HG13	2.33	0.59
1:D:498:THR:HG22	1:D:499:TYR:N	2.17	0.59
1:D:520:GLN:HE21	1:D:520:GLN:H	1.51	0.59
1:D:514:LEU:CD1	1:D:526:LEU:HB3	2.33	0.59
1:A:507:ASP:HB3	1:A:532:SER:N	2.17	0.59
1:C:413:LEU:HD23	1:C:427:ILE:HB	1.83	0.59
1:A:488:LYS:O	1:A:489:GLU:HB2	2.03	0.59
1:C:542:VAL:HG21	1:C:551:TYR:CZ	2.38	0.59
1:D:121:THR:HG23	1:D:128:VAL:CG1	2.31	0.59
1:B:346:ILE:HG23	1:B:369:THR:CG2	2.33	0.59
1:C:537:ALA:HA	1:C:557:LEU:HG	1.84	0.59
1:A:38:GLN:HE21	1:D:422:GLU:HB3	1.68	0.58
1:C:369:THR:CG2	1:C:411:GLY:HA3	2.32	0.58
1:D:286:ASN:HD21	1:D:304:ASP:HB3	1.67	0.58
1:C:251:MET:HE3	1:C:283:ASP:HB3	1.84	0.58
1:A:521:ASP:CG	1:A:546:SER:HB2	2.23	0.58
1:B:288:MET:HE1	1:B:299:LEU:HD23	1.84	0.58
1:B:570:CYS:HB3	1:B:577:LEU:CD2	2.33	0.58
1:D:398:GLU:O	1:D:403:LYS:HE3	2.03	0.58
1:A:293:GLU:O	1:A:295:LYS:HG2	2.03	0.58
1:B:93:LYS:CG	1:B:94:ASP:H	2.16	0.58
1:C:132:CYS:SG	1:C:133:LEU:N	2.72	0.58
1:D:483:PHE:HZ	1:D:524:TYR:OH	1.87	0.58
1:D:580:ARG:HA	1:D:598:GLY:O	2.03	0.58
1:B:541:TYR:HB3	1:B:543:TYR:HE2	1.68	0.58
1:B:472:TRP:CZ3	1:B:473:ILE:HG13	2.39	0.58
1:A:91:TYR:HB2	1:A:93:LYS:HG2	1.86	0.58
1:D:124:LYS:HG2	1:D:127:SER:HB2	1.83	0.58
1:C:61:HIS:HB3	1:C:123:GLU:HB2	1.85	0.58
1:B:140:GLN:HE22	1:C:422:GLU:HG2	1.68	0.58
1:A:224:SER:O	1:A:227:MET:HG2	2.04	0.58
1:D:472:TRP:CZ3	1:D:473:ILE:HB	2.39	0.58
1:C:540:TYR:HE1	1:C:568:VAL:CG2	2.17	0.58
1:B:430:GLY:HA3	1:B:476:PHE:CE2	2.32	0.57
1:B:472:TRP:HE3	1:B:472:TRP:N	1.96	0.57
1:C:439:SER:CB	1:C:457:PRO:HG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LYS:HD2	1:B:94:ASP:N	2.19	0.57
1:D:540:TYR:CE1	1:D:568:VAL:HG21	2.38	0.57
1:A:41:SER:O	1:A:110:SER:OG	2.19	0.57
1:A:299:LEU:HD21	1:A:425:ILE:HD13	1.85	0.57
1:D:461:ASN:N	1:D:461:ASN:HD22	2.00	0.57
1:A:437:HIS:CE1	1:A:459:MET:HB2	2.38	0.57
1:C:526:LEU:C	1:C:526:LEU:HD12	2.24	0.57
1:C:368:PRO:HD3	1:C:441:MET:HE3	1.86	0.57
1:D:526:LEU:HD12	1:D:526:LEU:C	2.25	0.57
1:B:56:MET:HB3	1:B:101:GLU:HA	1.86	0.57
1:D:520:GLN:HG2	1:D:521:ASP:N	2.19	0.57
1:A:378:MET:CB	1:A:407:ILE:HG21	2.34	0.57
1:B:340:SER:CB	1:B:426:LYS:HA	2.34	0.57
1:A:540:TYR:HE1	1:A:568:VAL:CG2	2.08	0.57
1:B:215:ASN:HB2	1:B:235:GLU:HB2	1.86	0.57
1:C:323:LYS:HB3	1:C:333:MET:HG2	1.87	0.57
1:D:499:TYR:CD2	1:D:501:PRO:HD3	2.40	0.57
1:A:320:GLN:HG3	1:A:336:TRP:CZ2	2.39	0.57
1:D:520:GLN:HG2	1:D:521:ASP:OD2	2.05	0.57
1:B:318:SER:HB3	1:B:337:VAL:O	2.04	0.57
1:D:124:LYS:HE2	1:D:127:SER:CB	2.34	0.57
1:D:298:ALA:O	1:D:321:LEU:HD12	2.04	0.57
1:B:103:LEU:HD13	1:B:120:MET:CE	2.34	0.57
1:B:325:GLY:C	1:B:327:TRP:H	2.08	0.57
1:D:236:LYS:HD3	1:D:252:TYR:CD2	2.40	0.57
1:D:101:GLU:CD	1:D:101:GLU:H	2.08	0.57
1:D:542:VAL:HG21	1:D:551:TYR:CZ	2.40	0.57
1:C:390:ILE:CG2	1:C:393:LEU:HB2	2.34	0.57
1:C:235:GLU:HA	1:C:250:SER:O	2.05	0.57
1:C:38:GLN:HG3	1:C:138:TYR:CE2	2.40	0.57
1:B:303:GLU:O	1:B:306:ILE:HD11	2.04	0.57
1:A:84:SER:O	1:A:85:GLU:CB	2.52	0.57
1:C:319:PHE:HB2	1:C:425:ILE:CD1	2.35	0.57
1:D:552:PHE:HE1	1:D:121:THR:HG1	1.52	0.57
1:A:326:VAL:HG23	1:A:327:TRP:NE1	2.19	0.57
1:A:210:LEU:O	1:A:213:GLY:N	2.32	0.57
1:A:274:ASN:ND2	1:A:324:LEU:HB3	2.17	0.57
1:A:216:VAL:HA	1:A:233:LEU:O	2.05	0.57
1:B:357:VAL:HG21	1:B:452:TYR:CE1	2.39	0.57
1:D:293:GLU:OE1	1:D:360:ASP:N	2.38	0.57
1:B:326:VAL:HG13	1:B:327:TRP:CD1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LEU:HB3	1:B:559:ILE:HD13	1.85	0.56
1:C:540:TYR:HE1	1:C:568:VAL:HG21	1.70	0.56
1:C:81:LEU:HD22	1:C:82:ASP:H	1.70	0.56
1:C:259:VAL:HB	1:C:261:ARG:NH1	2.20	0.56
1:C:537:ALA:HB2	1:C:556:ARG:HA	1.87	0.56
1:C:326:VAL:HG13	1:C:327:TRP:N	2.19	0.56
1:D:514:LEU:HD11	1:D:526:LEU:HD23	1.88	0.56
1:C:248:GLN:N	1:C:248:GLN:OE1	2.39	0.56
1:A:399:TRP:CZ3	1:A:435:ILE:HG22	2.41	0.56
1:B:458:PRO:HB2	1:B:511:SER:OG	2.05	0.56
1:B:89:PRO:HG2	1:B:91:TYR:HE2	1.69	0.56
1:D:124:LYS:HE2	1:D:127:SER:HB2	1.87	0.56
1:C:262:ASN:HB2	1:C:573:TRP:HZ2	1.71	0.56
1:B:134:HIS:CE1	1:B:136:LYS:NZ	2.74	0.56
1:B:541:TYR:HB3	1:B:543:TYR:CE2	2.39	0.56
1:C:349:LEU:HD23	1:C:369:THR:HG22	1.87	0.56
1:D:229:GLY:HA2	1:D:256:GLU:O	2.06	0.56
1:D:342:ASP:O	1:D:344:PRO:HD3	2.05	0.56
1:B:100:LEU:O	1:B:100:LEU:HD13	2.06	0.56
1:D:34:LYS:HE3	1:D:134:HIS:HD2	1.70	0.56
1:B:378:MET:HB2	1:B:407:ILE:HD13	1.88	0.56
1:B:418:SER:O	1:B:419:LEU:HD12	2.06	0.56
1:D:565:GLU:HB3	1:D:584:VAL:HB	1.87	0.56
1:C:349:LEU:CD2	1:C:369:THR:HG22	2.36	0.55
1:D:253:ARG:HH21	1:D:285:SER:CB	2.18	0.55
1:C:375:LYS:O	1:C:379:GLU:HB3	2.06	0.55
1:C:546:SER:HB3	1:C:547:ARG:NE	2.21	0.55
1:B:61:HIS:HE1	1:B:63:VAL:HG22	1.68	0.55
1:A:358:ILE:HG12	1:A:363:ALA:HB2	1.89	0.55
1:A:301:HIS:ND1	1:A:302:GLY:N	2.55	0.55
1:D:355:ARG:HB2	1:D:442:ASP:HB3	1.87	0.55
1:A:39:LEU:HB2	1:A:138:TYR:O	2.06	0.55
1:D:559:ILE:HG12	1:D:560:LYS:N	2.21	0.55
1:C:36:VAL:HA	1:C:136:LYS:O	2.06	0.55
1:B:140:GLN:HE21	1:C:422:GLU:H	1.55	0.55
1:D:493:ASP:HB2	1:D:495:HIS:NE2	2.21	0.55
1:D:444:TYR:HB2	1:D:453:TRP:HB2	1.89	0.55
1:A:202:SER:OG	1:A:203:LEU:N	2.39	0.55
1:D:200:ASN:HD22	1:D:200:ASN:H	1.52	0.55
1:C:464:LEU:HD22	1:C:498:THR:HB	1.88	0.55
1:A:337:VAL:HG12	1:A:425:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LEU:HD23	1:D:82:ASP:N	2.22	0.55
1:C:139:GLU:N	1:C:139:GLU:OE2	2.40	0.55
1:C:410:TYR:O	1:C:429:SER:HA	2.07	0.55
1:D:461:ASN:O	1:D:504:VAL:HG21	2.06	0.55
1:C:34:LYS:N	1:C:34:LYS:HD2	2.22	0.55
1:D:515:VAL:HG13	1:D:525:VAL:HG23	1.89	0.55
1:B:475:ARG:O	1:B:476:PHE:CB	2.54	0.55
1:C:392:ALA:C	1:C:394:CYS:H	2.11	0.55
1:D:450:ASN:O	1:D:471:GLU:HA	2.07	0.55
1:A:481:TYR:C	1:A:482:ARG:HG2	2.26	0.55
1:D:64:VAL:HB	1:D:79:VAL:HG13	1.88	0.55
1:D:200:ASN:H	1:D:200:ASN:ND2	2.05	0.55
1:D:503:GLU:HG2	1:D:93:LYS:CD	2.37	0.55
1:B:472:TRP:CE3	1:B:472:TRP:N	2.75	0.55
1:B:389:LYS:HG3	1:B:390:ILE:N	2.21	0.55
1:D:289:VAL:HG13	1:D:296:LEU:CD1	2.38	0.54
1:D:206:LEU:HD22	1:D:210:LEU:HD11	1.89	0.54
1:D:124:LYS:HE2	1:D:127:SER:OG	2.06	0.54
1:B:517:LEU:HB2	1:B:523:GLN:HG3	1.89	0.54
1:A:378:MET:HB3	1:A:407:ILE:HD13	1.89	0.54
1:C:410:TYR:HD2	1:C:454:LEU:HD11	1.73	0.54
1:A:437:HIS:ND1	1:A:459:MET:HB2	2.21	0.54
1:C:321:LEU:N	1:C:335:SER:O	2.31	0.54
1:B:540:TYR:HE1	1:B:568:VAL:HG21	1.72	0.54
1:A:446:SER:OG	1:A:451:VAL:HG13	2.07	0.54
1:D:383:GLN:HA	1:D:386:CYS:HB2	1.89	0.54
1:C:288:MET:HB2	1:C:365:TRP:NE1	2.23	0.54
1:D:376:LEU:HD23	1:D:376:LEU:O	2.08	0.54
1:B:589:GLU:HG2	1:B:590:SER:H	1.72	0.54
1:D:219:ILE:HD12	1:D:219:ILE:N	2.21	0.54
1:A:299:LEU:HD21	1:A:425:ILE:CD1	2.38	0.54
1:A:459:MET:CE	1:A:459:MET:HA	2.38	0.54
1:C:198:PHE:CE1	1:C:600:VAL:HB	2.43	0.54
1:B:542:VAL:O	1:B:550:SER:HA	2.07	0.54
1:B:40:GLY:HA2	1:B:110:SER:O	2.08	0.54
1:B:217:SER:O	1:B:218:SER:HB2	2.06	0.54
1:D:44:LEU:HD11	1:D:104:SER:HB2	1.88	0.54
1:C:461:ASN:HB3	1:C:508:VAL:HG13	1.89	0.54
1:C:215:ASN:O	1:C:234:VAL:HA	2.08	0.54
1:D:483:PHE:HZ	1:D:524:TYR:HH	1.55	0.54
1:C:485:VAL:O	1:C:485:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:CYS:SG	1:B:133:LEU:N	2.81	0.54
1:B:255:PHE:HD1	1:B:276:LEU:HD22	1.73	0.54
1:D:93:LYS:HZ2	1:D:93:LYS:HA	1.73	0.54
1:A:121:THR:HG23	1:A:128:VAL:HG13	1.89	0.54
1:A:322:VAL:HG12	1:A:324:LEU:CD1	2.37	0.54
1:D:345:VAL:HG23	1:D:372:THR:OG1	2.08	0.54
1:D:394:CYS:O	1:D:397:PRO:HD3	2.08	0.54
1:C:91:TYR:C	1:C:93:LYS:H	2.07	0.54
1:C:93:LYS:HD2	1:C:94:ASP:H	1.69	0.54
1:D:530:ASP:OD2	1:D:533:ARG:NH1	2.40	0.54
1:A:558:PRO:HG2	1:A:559:ILE:HG23	1.89	0.54
1:D:496:ALA:HB1	1:D:497:PRO:HD2	1.89	0.54
1:A:68:LYS:H	1:A:68:LYS:HD2	1.72	0.54
1:B:208:LEU:HD12	1:B:212:ARG:HD3	1.89	0.54
1:D:537:ALA:HB2	1:D:556:ARG:HA	1.89	0.53
1:B:499:TYR:CZ	1:B:501:PRO:HB3	2.43	0.53
1:C:125:ASN:OD1	1:C:126:ILE:HG13	2.07	0.53
1:D:92:LEU:HD23	1:D:92:LEU:H	1.72	0.53
1:B:73:SER:OG	1:B:74:VAL:N	2.41	0.53
1:B:65:THR:HB	1:B:75:GLU:HG3	1.89	0.53
1:C:341:THR:HA	1:C:427:ILE:HG23	1.89	0.53
1:B:385:ALA:HB2	1:B:487:ILE:HG13	1.91	0.53
1:D:219:ILE:O	1:D:567:GLN:HG3	2.09	0.53
1:D:377:ARG:HD3	1:D:377:ARG:O	2.09	0.53
1:B:140:GLN:NE2	1:C:422:GLU:HG2	2.22	0.53
1:A:47:LEU:HA	1:A:133:LEU:HD12	1.91	0.53
1:C:464:LEU:HD21	1:C:498:THR:HB	1.90	0.53
1:D:265:LEU:HD12	1:D:269:VAL:HG21	1.89	0.53
1:A:438:GLY:O	1:A:440:GLY:N	2.42	0.53
1:D:329:SER:HB2	1:D:330:PRO:HD2	1.90	0.53
1:B:471:GLU:O	1:B:476:PHE:HA	2.09	0.53
1:A:580:ARG:HB3	1:A:599:MET:CE	2.38	0.53
1:D:580:ARG:NH1	1:D:597:SER:OG	2.42	0.53
1:B:464:LEU:HD11	1:B:526:LEU:HD21	1.90	0.53
1:A:519:GLY:O	1:B:520:GLN:HG2	2.08	0.53
1:A:455:THR:CG2	1:A:516:ILE:HD11	2.38	0.53
1:B:308:ILE:HG23	1:B:341:THR:HG22	1.91	0.53
1:D:64:VAL:HB	1:D:79:VAL:CG1	2.39	0.53
1:B:437:HIS:CD2	1:B:459:MET:HB2	2.44	0.53
1:A:268:PRO:HD3	1:A:573:TRP:CE3	2.44	0.53
1:B:36:VAL:O	1:B:37:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLY:C	1:B:327:TRP:N	2.61	0.53
1:B:526:LEU:C	1:B:526:LEU:HD12	2.29	0.52
1:C:219:ILE:HG21	1:C:582:PHE:CG	2.44	0.52
1:D:461:ASN:O	1:D:462:LEU:HD23	2.08	0.52
1:B:255:PHE:CZ	1:B:322:VAL:HG21	2.44	0.52
1:B:262:ASN:HB2	1:B:573:TRP:HZ2	1.74	0.52
1:B:507:ASP:O	1:B:530:ASP:HA	2.10	0.52
1:A:533:ARG:NH1	1:A:554:PRO:HB3	2.24	0.52
1:C:93:LYS:HD2	1:C:94:ASP:C	2.30	0.52
1:D:231:THR:HG22	1:D:289:VAL:CG2	2.39	0.52
1:D:488:LYS:HG3	1:D:489:GLU:HG2	1.92	0.52
1:D:537:ALA:CB	1:D:556:ARG:HA	2.40	0.52
1:B:277:GLU:O	1:B:278:GLN:HG3	2.09	0.52
1:C:200:ASN:N	1:C:200:ASN:OD1	2.41	0.52
1:D:437:HIS:O	1:D:459:MET:SD	2.68	0.52
1:A:384:GLN:HG3	1:A:490:ALA:HB2	1.90	0.52
1:C:91:TYR:HB3	1:C:93:LYS:HB3	1.90	0.52
1:D:280:VAL:HG12	1:D:282:ASN:H	1.73	0.52
1:A:222:MET:SD	1:A:355:ARG:HG2	2.50	0.52
1:D:472:TRP:CE3	1:D:473:ILE:HB	2.44	0.52
1:A:123:GLU:HG2	1:A:128:VAL:HG22	1.91	0.52
1:B:410:TYR:CD1	1:B:478:VAL:HG11	2.45	0.52
1:A:52:ILE:O	1:A:53:ASN:HB3	2.10	0.52
1:B:262:ASN:HB2	1:B:573:TRP:CZ2	2.45	0.52
1:B:140:GLN:NE2	1:C:422:GLU:H	2.08	0.52
1:C:454:LEU:HD23	1:C:454:LEU:C	2.29	0.52
1:B:389:LYS:HG3	1:B:390:ILE:HG23	1.91	0.52
1:A:215:ASN:O	1:A:234:VAL:HA	2.08	0.52
1:D:93:LYS:HG3	1:D:94:ASP:N	2.25	0.52
1:C:229:GLY:HA3	1:C:296:LEU:HD12	1.92	0.52
1:A:94:ASP:HB3	1:A:95:ARG:HH11	1.75	0.52
1:A:273:THR:HB	1:A:326:VAL:O	2.10	0.52
1:A:430:GLY:HA3	1:A:476:PHE:HE2	1.73	0.52
1:A:132:CYS:O	1:A:133:LEU:HB2	2.09	0.52
1:B:413:LEU:HD12	1:B:427:ILE:CD1	2.40	0.52
1:B:251:MET:SD	1:B:283:ASP:HB3	2.50	0.52
1:B:210:LEU:O	1:B:213:GLY:N	2.36	0.52
1:A:188:CYS:SG	1:A:549:PHE:CZ	3.04	0.52
1:A:393:LEU:HD21	1:A:436:THR:CB	2.40	0.52
1:C:363:ALA:O	1:C:414:SER:HA	2.09	0.52
1:A:38:GLN:OE1	1:A:38:GLN:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:PHE:HB2	1:D:425:ILE:CD1	2.39	0.51
1:B:514:LEU:HD23	1:B:514:LEU:O	2.10	0.51
1:B:459:MET:C	1:B:459:MET:SD	2.89	0.51
1:A:551:TYR:CD2	1:A:552:PHE:N	2.78	0.51
1:B:294:LEU:HB3	1:B:326:VAL:HG12	1.91	0.51
1:D:95:ARG:H	1:D:95:ARG:HE	1.58	0.51
1:A:71:GLU:O	1:A:72:ASN:CB	2.57	0.51
1:D:206:LEU:HD22	1:D:210:LEU:CD1	2.40	0.51
1:C:210:LEU:HD13	1:C:597:SER:HB3	1.92	0.51
1:C:49:HIS:O	1:C:50:GLU:HG3	2.11	0.51
1:A:388:GLY:O	1:A:391:GLN:HB2	2.11	0.51
1:A:193:THR:HG22	1:A:129:GLN:HG3	1.91	0.51
1:B:475:ARG:HH12	1:B:477:LYS:HD3	1.72	0.51
1:D:206:LEU:CD2	1:D:210:LEU:HG	2.40	0.51
1:C:301:HIS:CG	1:C:306:ILE:HD11	2.46	0.51
1:B:238:ASN:O	1:B:239:LEU:HB2	2.10	0.51
1:A:556:ARG:NH2	1:A:125:ASN:O	2.44	0.51
1:C:461:ASN:ND2	1:C:462:LEU:HD23	2.26	0.51
1:D:112:LYS:HB2	1:D:112:LYS:NZ	2.25	0.51
1:B:458:PRO:HG3	1:B:465:GLY:N	2.23	0.51
1:A:378:MET:HE2	1:A:378:MET:HA	1.92	0.51
1:A:461:ASN:N	1:A:461:ASN:ND2	2.47	0.51
1:B:378:MET:CB	1:B:407:ILE:HD13	2.40	0.51
1:A:318:SER:HB3	1:A:337:VAL:O	2.11	0.51
1:C:121:THR:HG22	1:C:128:VAL:CG2	2.41	0.51
1:D:221:THR:HG22	1:D:230:GLY:HA3	1.93	0.51
1:A:79:VAL:HG13	1:A:79:VAL:O	2.11	0.51
1:D:261:ARG:HH12	1:D:271:HIS:CB	2.23	0.51
1:D:38:GLN:HB3	1:D:41:SER:HB3	1.93	0.51
1:B:37:GLN:O	1:B:137:LEU:HA	2.11	0.51
1:C:541:TYR:CE1	1:C:552:PHE:CB	2.94	0.51
1:A:500:LEU:C	1:A:502:ALA:H	2.15	0.51
1:A:533:ARG:NH1	1:A:123:GLU:OE1	2.44	0.51
1:C:391:GLN:HG2	1:C:392:ALA:N	2.25	0.51
1:A:580:ARG:NH1	1:A:580:ARG:CG	2.74	0.51
1:C:472:TRP:CZ3	1:C:473:ILE:HD13	2.46	0.51
1:B:134:HIS:CE1	1:B:136:LYS:HZ2	2.29	0.51
1:C:293:GLU:HB2	1:C:295:LYS:HE2	1.92	0.51
1:D:577:LEU:HD22	1:D:578:TRP:N	2.25	0.51
1:C:451:VAL:CG1	1:C:469:THR:HB	2.41	0.51
1:B:585:LEU:HD12	1:B:585:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ILE:HA	1:C:603:GLY:O	2.11	0.50
1:D:510:LEU:HD12	1:D:511:SER:H	1.76	0.50
1:B:299:LEU:HD21	1:B:425:ILE:HD13	1.93	0.50
1:B:319:PHE:HB2	1:B:425:ILE:HD11	1.93	0.50
1:C:589:GLU:O	1:C:591:GLY:N	2.43	0.50
1:C:437:HIS:ND1	1:C:459:MET:HG2	2.26	0.50
1:D:233:LEU:HD13	1:D:251:MET:HE3	1.94	0.50
1:B:354:HIS:ND1	1:B:367:VAL:HG12	2.26	0.50
1:C:293:GLU:HB3	1:C:295:LYS:HE2	1.93	0.50
1:B:221:THR:HG22	1:B:230:GLY:HA3	1.93	0.50
1:B:259:VAL:HG12	1:B:260:ILE:N	2.26	0.50
1:D:48:THR:HG21	1:D:103:LEU:HD13	1.93	0.50
1:A:437:HIS:O	1:A:439:SER:N	2.45	0.50
1:A:565:GLU:HB3	1:A:584:VAL:HB	1.94	0.50
1:A:449:ASN:O	1:A:472:TRP:HH2	1.94	0.50
1:C:369:THR:HG23	1:C:411:GLY:HA3	1.91	0.50
1:C:236:LYS:CB	1:C:237:PRO:CD	2.90	0.50
1:C:82:ASP:CG	1:C:84:SER:HB3	2.31	0.50
1:D:219:ILE:HG21	1:D:582:PHE:CD1	2.47	0.50
1:D:378:MET:HG3	1:D:431:PHE:CE2	2.47	0.50
1:A:371:ARG:HD2	1:A:429:SER:HB2	1.93	0.50
1:C:453:TRP:HB3	1:C:516:ILE:HD12	1.93	0.50
1:D:464:LEU:CG	1:D:465:GLY:H	2.23	0.50
1:B:299:LEU:HD11	1:B:425:ILE:HD11	1.94	0.50
1:B:60:ILE:HD12	1:B:124:LYS:HA	1.92	0.50
1:A:50:GLU:HG2	1:A:52:ILE:CG2	2.41	0.50
1:A:499:TYR:CZ	1:A:501:PRO:HB3	2.45	0.50
1:B:500:LEU:CD2	1:B:502:ALA:HB3	2.42	0.50
1:B:337:VAL:CG1	1:B:423:LEU:HB3	2.42	0.50
1:D:441:MET:HA	1:D:455:THR:O	2.12	0.50
1:A:458:PRO:HB2	1:A:511:SER:CB	2.41	0.50
1:B:282:ASN:OD1	1:B:284:LEU:HB2	2.12	0.50
1:A:485:VAL:O	1:A:495:HIS:HB3	2.12	0.50
1:A:93:LYS:HD2	1:A:94:ASP:CA	2.43	0.49
1:D:306:ILE:CD1	1:D:306:ILE:N	2.75	0.49
1:B:47:LEU:HD13	1:B:120:MET:HB2	1.93	0.49
1:D:326:VAL:HG13	1:D:327:TRP:N	2.28	0.49
1:B:51:ARG:O	1:B:53:ASN:N	2.45	0.49
1:D:457:PRO:O	1:D:459:MET:HE2	2.10	0.49
1:D:415:VAL:CG1	1:D:425:ILE:HA	2.42	0.49
1:B:453:TRP:CE2	1:B:522:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:MET:CE	1:A:378:MET:HA	2.43	0.49
1:D:354:HIS:ND1	1:D:367:VAL:HG12	2.26	0.49
1:D:547:ARG:HG3	1:D:549:PHE:H	1.76	0.49
1:C:205:LEU:HB2	1:C:272:MET:CE	2.43	0.49
1:B:326:VAL:HG22	1:B:326:VAL:O	2.12	0.49
1:A:466:VAL:CG1	1:A:468:ASN:HD21	2.26	0.49
1:C:459:MET:SD	1:C:460:LYS:HB2	2.53	0.49
1:D:579:CYS:SG	1:D:602:MET:HE1	2.53	0.49
1:D:481:TYR:CD2	1:D:482:ARG:HG2	2.47	0.49
1:C:367:VAL:HG13	1:C:368:PRO:HD2	1.93	0.49
1:B:308:ILE:N	1:B:308:ILE:HD12	2.27	0.49
1:A:320:GLN:HB2	1:A:336:TRP:CH2	2.47	0.49
1:B:85:GLU:HG3	1:B:87:GLY:H	1.77	0.49
1:D:458:PRO:HB3	1:D:465:GLY:N	2.28	0.49
1:A:233:LEU:HD23	1:A:253:ARG:HA	1.95	0.49
1:D:135:LEU:HD12	1:D:136:LYS:H	1.76	0.49
1:B:514:LEU:HD23	1:B:514:LEU:C	2.33	0.49
1:B:540:TYR:HE1	1:B:568:VAL:CG2	2.25	0.49
1:D:503:GLU:HG2	1:D:93:LYS:HD2	1.93	0.49
1:D:523:GLN:O	1:D:524:TYR:HB3	2.12	0.49
1:D:72:ASN:N	1:D:72:ASN:ND2	2.59	0.49
1:D:295:LYS:HA	1:D:325:GLY:HA2	1.94	0.49
1:B:280:VAL:HG12	1:B:282:ASN:H	1.77	0.49
1:C:287:CYS:HA	1:C:299:LEU:O	2.13	0.49
1:B:293:GLU:O	1:B:295:LYS:HG2	2.13	0.49
1:C:509:LYS:HB2	1:C:563:PRO:HG3	1.94	0.49
1:D:231:THR:HG21	1:D:287:CYS:HB2	1.95	0.49
1:C:472:TRP:N	1:C:472:TRP:CD1	2.81	0.49
1:C:541:TYR:CE1	1:C:552:PHE:HB3	2.48	0.49
1:D:559:ILE:CG1	1:D:560:LYS:N	2.76	0.49
1:C:227:MET:HB2	1:C:258:GLY:O	2.13	0.49
1:B:559:ILE:HG12	1:B:560:LYS:N	2.28	0.48
1:D:464:LEU:HG	1:D:465:GLY:N	2.23	0.48
1:C:206:LEU:CD2	1:C:210:LEU:HG	2.42	0.48
1:A:261:ARG:C	1:A:263:PRO:HD3	2.33	0.48
1:A:192:THR:HG22	1:A:606:CYS:SG	2.53	0.48
1:C:255:PHE:O	1:C:275:TYR:HB2	2.13	0.48
1:D:545:PRO:C	1:D:547:ARG:N	2.67	0.48
1:D:547:ARG:CG	1:D:548:SER:H	2.26	0.48
1:B:306:ILE:HD12	1:B:306:ILE:N	2.27	0.48
1:C:99:TYR:HB3	1:C:101:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:VAL:CB	1:B:586:ALA:HB3	2.39	0.48
1:C:68:LYS:HD3	1:C:113:LYS:O	2.12	0.48
1:A:257:VAL:HG13	1:A:274:ASN:HB3	1.94	0.48
1:A:337:VAL:HG11	1:A:425:ILE:HG13	1.94	0.48
1:D:399:TRP:O	1:D:403:LYS:HG3	2.14	0.48
1:D:75:GLU:OE2	1:D:130:ARG:NH2	2.41	0.48
1:C:230:GLY:HA2	1:C:289:VAL:HG11	1.95	0.48
1:B:95:ARG:NH1	1:B:95:ARG:HG3	2.22	0.48
1:A:52:ILE:HG12	1:A:52:ILE:O	2.13	0.48
1:B:513:ASN:OD1	1:B:568:VAL:HG12	2.13	0.48
1:B:540:TYR:O	1:B:552:PHE:HA	2.14	0.48
1:A:466:VAL:CG1	1:A:468:ASN:ND2	2.76	0.48
1:D:332:ASP:O	1:D:333:MET:HB3	2.13	0.48
1:C:236:LYS:C	1:C:249:LEU:HB3	2.34	0.48
1:C:82:ASP:C	1:C:84:SER:H	2.17	0.48
1:A:222:MET:HB3	1:A:355:ARG:CD	2.41	0.48
1:D:253:ARG:HG3	1:D:253:ARG:HH11	1.78	0.48
1:C:548:SER:O	1:C:549:PHE:C	2.51	0.48
1:C:541:TYR:CD1	1:C:552:PHE:HB3	2.49	0.48
1:B:227:MET:HE2	1:B:294:LEU:HD13	1.96	0.48
1:D:307:THR:HA	1:D:348:ARG:HG2	1.95	0.48
1:A:95:ARG:H	1:A:95:ARG:HH11	1.62	0.48
1:A:580:ARG:HB2	1:A:580:ARG:CZ	2.44	0.48
1:D:321:LEU:N	1:D:335:SER:O	2.36	0.48
1:A:520:GLN:CG	1:A:520:GLN:O	2.61	0.48
1:B:206:LEU:HD13	1:B:232:TYR:CD1	2.49	0.48
1:C:480:PRO:HB2	1:C:484:THR:HG21	1.95	0.48
1:C:249:LEU:HD22	1:C:249:LEU:H	1.78	0.48
1:C:37:GLN:CA	1:C:37:GLN:HE21	2.27	0.48
1:C:374:ASP:HB2	1:C:407:ILE:HB	1.95	0.48
1:B:38:GLN:HG3	1:C:422:GLU:HB3	1.96	0.48
1:C:210:LEU:HD11	1:C:582:PHE:CE2	2.48	0.48
1:B:263:PRO:HB2	1:B:265:LEU:HD13	1.96	0.48
1:C:363:ALA:HB3	1:C:415:VAL:HG23	1.94	0.48
1:B:441:MET:HE2	1:B:456:ILE:HD11	1.96	0.48
1:D:194:ILE:CD1	1:D:194:ILE:N	2.77	0.48
1:A:399:TRP:CD1	1:A:401:PRO:HD2	2.49	0.48
1:B:43:VAL:HG21	1:B:135:LEU:HD21	1.95	0.48
1:A:91:TYR:CB	1:A:93:LYS:HB3	2.42	0.48
1:A:135:LEU:HG	1:A:136:LYS:N	2.28	0.48
1:B:374:ASP:HB2	1:B:407:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:ARG:HG3	1:B:533:ARG:HH11	1.79	0.48
1:D:280:VAL:HG12	1:D:281:SER:N	2.29	0.48
1:A:303:GLU:HB2	1:A:306:ILE:HD13	1.95	0.48
1:D:198:PHE:CE1	1:D:600:VAL:HB	2.49	0.48
1:D:255:PHE:O	1:D:275:TYR:HA	2.14	0.48
1:B:301:HIS:ND1	1:B:302:GLY:N	2.62	0.48
1:B:399:TRP:NE1	1:B:401:PRO:HD2	2.28	0.48
1:B:93:LYS:HB2	1:B:96:TYR:HD1	1.78	0.48
1:D:482:ARG:HD2	1:D:72:ASN:HD21	1.79	0.48
1:A:55:SER:HB3	1:A:57:ASN:HD21	1.79	0.48
1:A:515:VAL:HG12	1:A:525:VAL:HB	1.96	0.48
1:C:48:THR:HG22	1:C:103:LEU:HB2	1.95	0.48
1:D:59:SER:HB2	1:D:123:GLU:O	2.14	0.47
1:B:91:TYR:CB	1:B:93:LYS:HB3	2.41	0.47
1:A:309:PRO:HB2	1:A:341:THR:CG2	2.43	0.47
1:B:392:ALA:HA	1:B:395:GLU:CD	2.35	0.47
1:C:458:PRO:HD2	1:C:511:SER:HB3	1.95	0.47
1:D:467:ILE:HD12	1:D:483:PHE:HE2	1.79	0.47
1:B:308:ILE:HD13	1:B:348:ARG:HA	1.95	0.47
1:C:461:ASN:HD22	1:C:462:LEU:N	2.11	0.47
1:D:514:LEU:HD13	1:D:526:LEU:HD23	1.96	0.47
1:B:37:GLN:HB2	1:B:137:LEU:HD23	1.97	0.47
1:B:47:LEU:HA	1:B:133:LEU:HD12	1.97	0.47
1:A:510:LEU:O	1:A:528:THR:HA	2.14	0.47
1:C:37:GLN:O	1:C:137:LEU:HA	2.15	0.47
1:C:390:ILE:CG2	1:C:394:CYS:SG	3.03	0.47
1:A:80:SER:O	1:A:81:LEU:HB2	2.14	0.47
1:D:552:PHE:HE1	1:D:121:THR:OG1	1.97	0.47
1:D:537:ALA:HA	1:D:557:LEU:CD2	2.41	0.47
1:A:125:ASN:OD1	1:A:126:ILE:N	2.48	0.47
1:C:589:GLU:C	1:C:591:GLY:H	2.17	0.47
1:C:219:ILE:HG21	1:C:582:PHE:CD2	2.50	0.47
1:C:288:MET:HB3	1:C:354:HIS:HB2	1.95	0.47
1:C:480:PRO:CB	1:C:484:THR:HG21	2.44	0.47
1:D:202:SER:O	1:D:203:LEU:HD23	2.14	0.47
1:A:101:GLU:CD	1:A:101:GLU:H	2.18	0.47
1:C:91:TYR:HB3	1:C:93:LYS:HG2	1.95	0.47
1:A:472:TRP:CZ3	1:A:473:ILE:HG12	2.49	0.47
1:D:261:ARG:HB2	1:D:261:ARG:CZ	2.45	0.47
1:C:531:THR:HG22	1:C:536:HIS:CG	2.48	0.47
1:C:384:GLN:HE22	1:C:490:ALA:CB	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:THR:HG21	1:C:411:GLY:HA3	1.96	0.47
1:D:347:ASP:H	1:D:371:ARG:HA	1.80	0.47
1:A:519:GLY:C	1:A:521:ASP:H	2.17	0.47
1:B:294:LEU:N	1:B:294:LEU:HD22	2.29	0.47
1:B:206:LEU:HD13	1:B:232:TYR:CG	2.49	0.47
1:A:139:GLU:N	1:A:139:GLU:OE2	2.47	0.47
1:C:569:GLU:O	1:C:569:GLU:HG3	2.15	0.47
1:A:255:PHE:CZ	1:A:322:VAL:HG21	2.49	0.47
1:B:339:LEU:HD12	1:B:425:ILE:HB	1.95	0.47
1:B:264:GLY:C	1:B:265:LEU:HD12	2.35	0.47
1:D:374:ASP:HB3	1:D:407:ILE:HG12	1.97	0.47
1:D:526:LEU:HD12	1:D:526:LEU:O	2.15	0.47
1:C:522:LEU:HD12	1:C:523:GLN:N	2.29	0.47
1:A:524:TYR:N	1:A:524:TYR:CD2	2.83	0.47
1:B:471:GLU:OE2	1:B:477:LYS:O	2.32	0.47
1:C:81:LEU:HD22	1:C:82:ASP:N	2.30	0.47
1:A:517:LEU:HD11	1:A:525:VAL:HG23	1.97	0.47
1:A:293:GLU:OE2	1:A:359:ALA:HA	2.15	0.47
1:A:459:MET:HE2	1:A:459:MET:HA	1.96	0.47
1:D:577:LEU:C	1:D:577:LEU:HD22	2.35	0.47
1:D:261:ARG:HB3	1:D:261:ARG:HH11	1.80	0.46
1:A:569:GLU:OE2	1:A:582:PHE:HE1	1.97	0.46
1:D:501:PRO:O	1:D:504:VAL:HG12	2.15	0.46
1:D:324:LEU:HD23	1:D:332:ASP:HB3	1.96	0.46
1:D:223:THR:O	1:D:224:SER:HB2	2.15	0.46
1:A:98:PHE:HZ	1:A:103:LEU:HD22	1.79	0.46
1:B:77:LYS:NZ	1:B:80:SER:HB2	2.30	0.46
1:B:92:LEU:HD23	1:B:92:LEU:N	2.31	0.46
1:C:540:TYR:CE1	1:C:568:VAL:HG21	2.50	0.46
1:A:98:PHE:CG	1:A:99:TYR:N	2.83	0.46
1:D:389:LYS:C	1:D:391:GLN:H	2.19	0.46
1:C:329:SER:OG	1:C:331:THR:HG23	2.14	0.46
1:D:228:TYR:CE1	1:D:258:GLY:HA3	2.51	0.46
1:D:43:VAL:HG22	1:D:45:LEU:CD1	2.45	0.46
1:C:35:ILE:HD13	1:C:45:LEU:HD23	1.97	0.46
1:A:299:LEU:CD1	1:A:321:LEU:HD13	2.46	0.46
1:D:293:GLU:O	1:D:295:LYS:HE3	2.14	0.46
1:D:295:LYS:HZ2	1:D:358:ILE:HG21	1.80	0.46
1:D:498:THR:HG22	1:D:499:TYR:H	1.80	0.46
1:D:36:VAL:HG22	1:D:136:LYS:HB3	1.97	0.46
1:D:410:TYR:CE1	1:D:435:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:LEU:HD21	1:D:423:LEU:HD11	1.97	0.46
1:A:38:GLN:NE2	1:D:422:GLU:HB3	2.31	0.46
1:D:514:LEU:HD12	1:D:514:LEU:HA	1.74	0.46
1:D:63:VAL:HG12	1:D:64:VAL:N	2.30	0.46
1:A:437:HIS:C	1:A:439:SER:H	2.18	0.46
1:B:126:ILE:HG13	1:B:126:ILE:O	2.15	0.46
1:D:569:GLU:O	1:D:569:GLU:HG3	2.15	0.46
1:C:135:LEU:HD23	1:C:135:LEU:C	2.35	0.46
1:D:538:VAL:HG21	1:D:581:HIS:CD2	2.50	0.46
1:D:556:ARG:HH21	1:D:556:ARG:HG3	1.81	0.46
1:A:231:THR:OG1	1:A:253:ARG:HD2	2.16	0.46
1:A:38:GLN:HG3	1:D:422:GLU:HB3	1.98	0.46
1:D:205:LEU:HB2	1:D:272:MET:CE	2.46	0.46
1:A:507:ASP:OD1	1:A:90:ARG:NH1	2.47	0.46
1:C:50:GLU:O	1:C:51:ARG:C	2.54	0.46
1:D:461:ASN:ND2	1:D:461:ASN:N	2.62	0.46
1:B:52:ILE:HD13	1:C:282:ASN:OD1	2.16	0.46
1:D:39:LEU:HB2	1:D:138:TYR:O	2.16	0.46
1:D:521:ASP:HB2	1:D:546:SER:CB	2.44	0.46
1:C:107:ILE:HD11	1:C:118:TYR:HE2	1.78	0.46
1:A:95:ARG:N	1:A:95:ARG:HH11	2.14	0.46
1:A:415:VAL:CG1	1:A:425:ILE:HG12	2.46	0.46
1:A:47:LEU:HD21	1:A:105:LEU:HB2	1.98	0.46
1:B:51:ARG:C	1:B:53:ASN:H	2.19	0.46
1:B:222:MET:HB3	1:B:355:ARG:HD3	1.98	0.46
1:A:377:ARG:HH11	1:A:377:ARG:HG2	1.80	0.46
1:A:230:GLY:HA2	1:A:289:VAL:HG11	1.98	0.46
1:D:35:ILE:HG12	1:D:133:LEU:HD22	1.97	0.46
1:B:374:ASP:C	1:B:376:LEU:H	2.19	0.46
1:D:504:VAL:O	1:D:504:VAL:HG13	2.16	0.46
1:C:121:THR:HG22	1:C:128:VAL:HG22	1.98	0.46
1:A:45:LEU:HD13	1:A:133:LEU:HD13	1.98	0.46
1:B:473:ILE:HB	1:B:474:PRO:CD	2.37	0.46
1:C:421:VAL:O	1:C:422:GLU:C	2.53	0.46
1:D:65:THR:OG1	1:D:66:MET:N	2.49	0.46
1:C:543:TYR:OH	1:C:75:GLU:HB2	2.16	0.46
1:C:236:LYS:HB2	1:C:237:PRO:HD2	1.97	0.46
1:D:464:LEU:CG	1:D:465:GLY:N	2.79	0.46
1:A:93:LYS:HD2	1:A:94:ASP:O	2.15	0.46
1:D:516:ILE:HD13	1:D:524:TYR:HB3	1.98	0.46
1:C:461:ASN:ND2	1:C:461:ASN:C	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:ALA:HB2	1:D:498:THR:O	2.15	0.46
1:C:542:VAL:HG21	1:C:551:TYR:OH	2.16	0.46
1:D:572:THR:HG22	1:D:576:LYS:O	2.16	0.46
1:C:79:VAL:HG23	1:C:90:ARG:O	2.16	0.46
1:D:107:ILE:HD11	1:D:118:TYR:CE2	2.51	0.46
1:D:194:ILE:HA	1:D:603:GLY:O	2.15	0.46
1:B:247:SER:O	1:B:249:LEU:HD13	2.16	0.46
1:B:61:HIS:C	1:B:62:ILE:HD12	2.37	0.46
1:C:233:LEU:HD21	1:C:253:ARG:NH2	2.31	0.46
1:A:264:GLY:O	1:A:265:LEU:HD23	2.16	0.46
1:C:208:LEU:O	1:C:212:ARG:HG2	2.16	0.45
1:C:123:GLU:HG2	1:C:128:VAL:HG23	1.98	0.45
1:C:434:LEU:HD13	1:C:495:HIS:O	2.16	0.45
1:A:395:GLU:O	1:A:395:GLU:OE1	2.34	0.45
1:C:481:TYR:CD2	1:C:482:ARG:HG2	2.51	0.45
1:C:488:LYS:C	1:C:489:GLU:HG2	2.37	0.45
1:A:589:GLU:CG	1:A:590:SER:N	2.78	0.45
1:A:589:GLU:O	1:A:591:GLY:N	2.46	0.45
1:C:236:LYS:NZ	1:C:277:GLU:OE1	2.42	0.45
1:C:36:VAL:C	1:C:37:GLN:HE21	2.19	0.45
1:A:585:LEU:CD2	1:A:585:LEU:N	2.79	0.45
1:A:393:LEU:O	1:A:393:LEU:HD12	2.16	0.45
1:A:282:ASN:OD1	1:A:284:LEU:HB2	2.16	0.45
1:D:593:HIS:HB2	2:D:901:NAG:O7	2.16	0.45
1:D:304:ASP:HB2	1:D:351:LEU:O	2.17	0.45
1:B:215:ASN:HB3	1:B:235:GLU:HB2	1.99	0.45
1:C:219:ILE:HG22	1:C:219:ILE:O	2.16	0.45
1:D:461:ASN:H	1:D:461:ASN:ND2	2.15	0.45
1:B:294:LEU:O	1:B:326:VAL:HG12	2.17	0.45
1:B:522:LEU:O	1:B:545:PRO:HD2	2.17	0.45
1:A:395:GLU:H	1:A:395:GLU:HG3	1.56	0.45
1:A:366:ALA:O	1:A:441:MET:HB3	2.16	0.45
1:A:473:ILE:HG22	1:A:474:PRO:CD	2.46	0.45
1:B:35:ILE:HA	1:C:334:GLN:O	2.16	0.45
1:C:533:ARG:HB3	1:C:61:HIS:CD2	2.51	0.45
1:A:573:TRP:O	1:A:574:ASP:CB	2.62	0.45
1:B:406:ARG:O	1:B:408:PRO:HD3	2.17	0.45
1:D:379:GLU:HG3	1:D:380:THR:H	1.82	0.45
1:C:236:LYS:HD3	1:C:252:TYR:CD2	2.52	0.45
1:D:306:ILE:HD12	1:D:306:ILE:H	1.81	0.45
1:D:206:LEU:HG	1:D:232:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:HG11	1:C:333:MET:SD	2.57	0.45
1:A:301:HIS:HB2	1:A:319:PHE:CE2	2.51	0.45
1:D:200:ASN:N	1:D:200:ASN:HD22	2.10	0.45
1:B:276:LEU:HD23	1:B:277:GLU:N	2.31	0.45
1:B:265:LEU:HD11	1:D:209:TYR:CE2	2.52	0.45
1:C:510:LEU:HD12	1:C:563:PRO:HB2	1.99	0.45
1:C:467:ILE:HD12	1:C:483:PHE:HE2	1.82	0.45
1:C:315:LYS:O	1:C:315:LYS:HG3	2.16	0.45
1:D:499:TYR:CE2	1:D:501:PRO:HD3	2.51	0.45
1:C:123:GLU:HA	1:C:128:VAL:HG23	1.99	0.45
1:C:119:PHE:HA	1:C:131:PHE:O	2.15	0.45
1:C:570:CYS:HA	1:C:578:TRP:O	2.16	0.45
1:D:99:TYR:O	1:D:103:LEU:N	2.50	0.45
1:C:536:HIS:CE1	1:C:560:LYS:HB3	2.51	0.45
1:D:211:GLY:C	1:D:213:GLY:N	2.68	0.45
1:A:559:ILE:CD1	1:A:559:ILE:H	2.28	0.45
1:C:540:TYR:O	1:C:552:PHE:HA	2.17	0.45
1:A:32:CYS:SG	1:A:133:LEU:N	2.90	0.45
1:A:466:VAL:HG12	1:A:468:ASN:ND2	2.32	0.45
1:B:274:ASN:ND2	1:B:324:LEU:HG	2.32	0.45
1:B:473:ILE:CB	1:B:474:PRO:HD3	2.34	0.45
1:A:580:ARG:NH1	1:A:580:ARG:HB2	2.31	0.45
1:D:369:THR:OG1	1:D:411:GLY:HA3	2.17	0.45
1:C:253:ARG:HD3	1:C:287:CYS:SG	2.57	0.45
1:C:223:THR:O	1:C:224:SER:HB2	2.17	0.45
1:B:529:TYR:CE1	1:B:563:PRO:HD3	2.51	0.45
1:C:558:PRO:HD2	1:C:596:HIS:NE2	2.32	0.45
1:A:505:ASP:OD2	1:A:77:LYS:HD3	2.18	0.44
1:C:564:ILE:HD11	1:C:584:VAL:CG1	2.47	0.44
1:B:362:GLN:HB3	1:B:364:LYS:HE2	1.99	0.44
1:B:252:TYR:N	1:B:252:TYR:CD2	2.85	0.44
1:B:194:ILE:HD12	1:B:194:ILE:N	2.32	0.44
1:B:558:PRO:HG2	1:B:559:ILE:N	2.32	0.44
1:C:386:CYS:O	1:C:391:GLN:HA	2.16	0.44
1:A:93:LYS:CD	1:A:94:ASP:N	2.76	0.44
1:A:36:VAL:O	1:A:37:GLN:HG2	2.18	0.44
1:C:367:VAL:O	1:C:369:THR:HG23	2.17	0.44
1:A:52:ILE:HB	1:D:302:GLY:HA3	2.00	0.44
1:D:498:THR:CG2	1:D:499:TYR:N	2.80	0.44
1:A:444:TYR:CD2	1:A:516:ILE:HG12	2.52	0.44
1:D:254:VAL:HG12	1:D:255:PHE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:THR:O	1:B:50:GLU:N	2.48	0.44
1:C:406:ARG:HG3	1:C:406:ARG:HH11	1.82	0.44
1:A:308:ILE:HG23	1:A:309:PRO:HD2	1.98	0.44
1:C:38:GLN:O	1:C:41:SER:OG	2.32	0.44
1:C:565:GLU:HB3	1:C:584:VAL:CG2	2.47	0.44
1:D:96:TYR:CD2	1:D:107:ILE:HG12	2.53	0.44
1:C:306:ILE:HG12	1:C:319:PHE:HE1	1.83	0.44
1:A:93:LYS:CG	1:A:94:ASP:N	2.80	0.44
1:B:386:CYS:SG	1:B:386:CYS:O	2.74	0.44
1:D:453:TRP:CH2	1:D:522:LEU:HD13	2.53	0.44
1:D:572:THR:HA	1:D:577:LEU:HA	1.98	0.44
1:A:100:LEU:O	1:A:103:LEU:HD23	2.17	0.44
1:C:276:LEU:HA	1:C:276:LEU:HD12	1.85	0.44
1:A:310:TYR:O	1:A:312:GLY:N	2.47	0.44
1:D:103:LEU:HD22	1:D:120:MET:SD	2.57	0.44
1:B:458:PRO:HB3	1:B:464:LEU:HA	1.98	0.44
1:D:545:PRO:O	1:D:547:ARG:N	2.51	0.44
1:B:418:SER:O	1:B:419:LEU:HB2	2.18	0.44
1:A:384:GLN:CG	1:A:490:ALA:HB2	2.46	0.44
1:D:135:LEU:HD12	1:D:136:LYS:N	2.31	0.44
1:A:472:TRP:HE3	1:A:473:ILE:HG12	1.81	0.44
1:B:337:VAL:HA	1:B:338:PRO:HD3	1.88	0.44
1:B:533:ARG:HG3	1:B:533:ARG:NH1	2.31	0.44
1:C:48:THR:CG2	1:C:103:LEU:HB2	2.47	0.44
1:A:455:THR:HG22	1:A:516:ILE:HD11	1.98	0.44
1:D:136:LYS:HG2	1:D:137:LEU:N	2.33	0.44
1:C:503:GLU:OE1	1:C:76:ASN:HB3	2.18	0.44
1:D:288:MET:O	1:D:298:ALA:HA	2.18	0.44
1:D:450:ASN:ND2	1:D:473:ILE:CG2	2.81	0.44
1:A:399:TRP:HZ3	1:A:435:ILE:HG22	1.81	0.44
1:D:585:LEU:HD12	1:D:594:ILE:HG22	1.99	0.44
1:D:400:ALA:HB3	1:D:401:PRO:CD	2.48	0.44
1:D:260:ILE:HG12	1:D:270:PHE:CE1	2.52	0.44
1:C:91:TYR:HB3	1:C:93:LYS:CG	2.48	0.44
1:A:38:GLN:HB3	1:A:41:SER:HB3	2.00	0.44
1:A:569:GLU:HG3	1:A:580:ARG:HG2	2.00	0.44
1:D:206:LEU:HD23	1:D:210:LEU:HG	1.99	0.44
1:C:206:LEU:HD22	1:C:210:LEU:CD1	2.48	0.44
1:C:288:MET:HB2	1:C:365:TRP:CD1	2.52	0.44
1:C:569:GLU:O	1:C:579:CYS:HA	2.18	0.44
1:C:131:PHE:N	1:C:131:PHE:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:PRO:O	1:D:48:THR:N	2.51	0.44
1:D:303:GLU:CG	1:D:304:ASP:H	2.29	0.44
1:A:36:VAL:C	1:A:37:GLN:HG2	2.38	0.44
1:B:299:LEU:HD11	1:B:425:ILE:CD1	2.48	0.44
1:B:229:GLY:H	1:B:291:LEU:HD11	1.81	0.44
1:D:574:ASP:O	1:D:576:LYS:N	2.51	0.44
1:D:375:LYS:CA	1:D:379:GLU:HB3	2.47	0.44
1:C:74:VAL:HG12	1:C:74:VAL:O	2.17	0.44
1:D:94:ASP:HB3	1:D:95:ARG:H	1.41	0.43
1:D:585:LEU:HD12	1:D:585:LEU:O	2.18	0.43
1:C:390:ILE:O	1:C:390:ILE:HG22	2.18	0.43
1:D:309:PRO:HG3	1:D:316:GLY:CA	2.44	0.43
1:C:499:TYR:CE2	1:C:501:PRO:HB3	2.53	0.43
1:C:444:TYR:CZ	1:C:515:VAL:HA	2.54	0.43
1:A:570:CYS:HA	1:A:578:TRP:O	2.19	0.43
1:D:538:VAL:HG23	1:D:557:LEU:HD11	2.00	0.43
1:A:580:ARG:HA	1:A:599:MET:HA	2.00	0.43
1:C:505:ASP:OD2	1:C:77:LYS:HE2	2.19	0.43
1:C:77:LYS:HG2	1:C:92:LEU:HD13	2.00	0.43
1:B:352:SER:OG	1:B:440:GLY:HA2	2.18	0.43
1:D:358:ILE:HA	1:D:362:GLN:O	2.18	0.43
1:C:345:VAL:HG11	1:C:373:ASP:OD1	2.18	0.43
1:A:46:PRO:O	1:A:46:PRO:HG2	2.18	0.43
1:D:405:ASN:N	1:D:405:ASN:HD22	2.15	0.43
1:A:310:TYR:C	1:A:312:GLY:H	2.22	0.43
1:B:196:GLY:HA3	1:B:553:TYR:CZ	2.54	0.43
1:C:392:ALA:O	1:C:394:CYS:N	2.43	0.43
1:C:490:ALA:HB3	1:C:494:CYS:HB3	2.00	0.43
1:D:232:TYR:CD1	1:D:232:TYR:N	2.86	0.43
1:A:312:GLY:O	1:A:314:GLY:N	2.44	0.43
1:B:93:LYS:HD3	1:B:96:TYR:N	2.33	0.43
1:D:514:LEU:HD13	1:D:526:LEU:CD2	2.48	0.43
1:D:451:VAL:CG1	1:D:469:THR:HB	2.48	0.43
1:C:70:LEU:HD12	1:C:117:TRP:CE2	2.53	0.43
1:A:206:LEU:HD13	1:A:232:TYR:CD1	2.53	0.43
1:B:551:TYR:N	1:B:551:TYR:CD1	2.87	0.43
1:D:516:ILE:CD1	1:D:524:TYR:HB3	2.48	0.43
1:D:346:ILE:HG23	1:D:369:THR:CG2	2.49	0.43
1:C:514:LEU:HG	1:C:526:LEU:HD23	2.00	0.43
1:B:400:ALA:CB	1:B:401:PRO:HD3	2.42	0.43
1:B:481:TYR:O	1:B:482:ARG:CG	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PRO:HA	1:A:104:SER:HA	2.00	0.43
1:C:39:LEU:HG	1:C:138:TYR:O	2.19	0.43
1:C:117:TRP:NE1	1:C:134:HIS:HB2	2.34	0.43
1:A:296:LEU:HD12	1:A:297:ALA:N	2.34	0.43
1:D:412:VAL:N	1:D:428:ALA:O	2.36	0.43
1:D:139:GLU:OE1	1:D:139:GLU:HA	2.19	0.43
1:A:556:ARG:HH22	1:A:125:ASN:HB2	1.83	0.43
1:C:462:LEU:HB2	1:C:463:ALA:H	1.69	0.43
1:C:39:LEU:C	1:C:41:SER:H	2.22	0.43
1:A:573:TRP:O	1:A:574:ASP:HB3	2.19	0.43
1:B:508:VAL:HG13	1:B:528:THR:HG23	2.00	0.43
1:C:593:HIS:HD2	2:C:901:NAG:H81	1.83	0.43
1:A:58:LYS:HG3	1:A:58:LYS:O	2.18	0.43
1:C:319:PHE:HB2	1:C:425:ILE:HD12	2.01	0.43
1:C:508:VAL:HG23	1:C:528:THR:OG1	2.17	0.43
1:A:69:SER:OG	1:A:70:LEU:N	2.51	0.43
1:A:50:GLU:HG2	1:A:52:ILE:HG23	2.00	0.43
1:C:580:ARG:NH1	1:C:597:SER:OG	2.52	0.43
1:C:39:LEU:O	1:C:41:SER:N	2.51	0.43
1:C:467:ILE:HB	1:C:482:ARG:HB2	2.00	0.43
1:B:48:THR:C	1:B:50:GLU:H	2.20	0.43
1:B:66:MET:HG3	1:B:118:TYR:CZ	2.54	0.43
1:D:74:VAL:O	1:D:74:VAL:HG12	2.19	0.43
1:A:387:LYS:HA	1:A:387:LYS:CE	2.49	0.43
1:C:374:ASP:CG	1:C:406:ARG:HE	2.22	0.43
1:D:482:ARG:HD2	1:D:72:ASN:ND2	2.34	0.43
1:B:533:ARG:NH2	1:B:554:PRO:HB3	2.34	0.43
1:D:473:ILE:N	1:D:474:PRO:HD2	2.34	0.43
1:D:346:ILE:HG23	1:D:369:THR:HG22	2.01	0.43
1:D:346:ILE:HA	1:D:371:ARG:HG2	2.01	0.43
1:A:551:TYR:HD2	1:A:552:PHE:N	2.16	0.42
1:B:538:VAL:HG23	1:B:557:LEU:HD11	2.01	0.42
1:A:473:ILE:HA	1:A:473:ILE:HD13	1.88	0.42
1:A:70:LEU:HA	1:A:73:SER:HB2	2.01	0.42
1:B:343:ASP:OD2	1:B:345:VAL:HB	2.19	0.42
1:D:566:LEU:HG	1:D:566:LEU:O	2.19	0.42
1:B:443:LEU:HD22	1:B:452:TYR:HB3	2.01	0.42
1:D:200:ASN:N	1:D:200:ASN:ND2	2.64	0.42
1:D:388:GLY:O	1:D:391:GLN:HB2	2.18	0.42
1:D:375:LYS:NZ	1:D:405:ASN:HB3	2.33	0.42
1:B:340:SER:HB2	1:B:424:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:TYR:O	1:C:210:LEU:C	2.56	0.42
1:D:461:ASN:O	1:D:504:VAL:CG2	2.67	0.42
1:C:290:ALA:HB2	1:C:365:TRP:CZ2	2.54	0.42
1:C:286:ASN:O	1:C:300:CYS:HA	2.18	0.42
1:B:558:PRO:HG2	1:B:559:ILE:H	1.84	0.42
1:B:559:ILE:H	1:B:559:ILE:CD1	2.32	0.42
1:D:61:HIS:HE1	1:D:63:VAL:CG2	2.32	0.42
1:B:395:GLU:O	1:B:396:ASN:HB2	2.19	0.42
1:B:418:SER:O	1:B:419:LEU:CB	2.67	0.42
1:A:440:GLY:O	1:A:457:PRO:HD2	2.19	0.42
1:A:427:ILE:HG12	1:A:428:ALA:N	2.35	0.42
1:A:539:VAL:HA	1:A:553:TYR:O	2.18	0.42
1:B:470:LEU:HD11	1:B:476:PHE:CE1	2.55	0.42
1:B:400:ALA:CB	1:B:401:PRO:CD	2.95	0.42
1:D:543:TYR:C	1:D:545:PRO:HD3	2.40	0.42
1:B:265:LEU:HD11	1:D:209:TYR:HE2	1.83	0.42
1:D:437:HIS:HB3	1:D:459:MET:CG	2.39	0.42
1:B:233:LEU:HD23	1:B:253:ARG:HA	2.01	0.42
1:A:406:ARG:O	1:A:408:PRO:HD3	2.20	0.42
1:D:301:HIS:CE1	1:D:306:ILE:HG13	2.54	0.42
1:D:252:TYR:CE1	1:D:279:PRO:HB3	2.54	0.42
1:C:99:TYR:O	1:C:100:LEU:C	2.58	0.42
1:C:337:VAL:CG1	1:C:338:PRO:HD2	2.49	0.42
1:D:320:GLN:HB2	1:D:336:TRP:CZ3	2.53	0.42
1:C:229:GLY:HA2	1:C:256:GLU:O	2.20	0.42
1:C:464:LEU:HD22	1:C:498:THR:O	2.19	0.42
1:D:564:ILE:C	1:D:564:ILE:HD12	2.40	0.42
1:B:59:SER:O	1:B:61:HIS:N	2.53	0.42
1:C:537:ALA:CB	1:C:556:ARG:HA	2.50	0.42
1:D:385:ALA:O	1:D:390:ILE:HG12	2.20	0.42
1:D:111:THR:OG1	1:D:112:LYS:N	2.53	0.42
1:D:326:VAL:HG13	1:D:327:TRP:H	1.84	0.42
1:B:371:ARG:HH11	1:B:429:SER:HB3	1.84	0.42
1:B:464:LEU:CG	1:B:465:GLY:N	2.79	0.42
1:A:475:ARG:O	1:A:476:PHE:C	2.58	0.42
1:A:400:ALA:HB3	1:A:401:PRO:CD	2.50	0.42
1:B:487:ILE:HG22	1:B:490:ALA:HB3	2.01	0.42
1:C:453:TRP:CB	1:C:516:ILE:HD12	2.50	0.42
1:D:49:HIS:O	1:D:50:GLU:HG3	2.19	0.42
1:D:262:ASN:HB2	1:D:573:TRP:HZ2	1.84	0.42
1:A:552:PHE:HE1	1:A:121:THR:OG1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:ILE:HG22	1:C:474:PRO:CD	2.49	0.42
1:B:229:GLY:HA3	1:B:291:LEU:HD21	2.02	0.42
1:C:61:HIS:CE1	1:C:63:VAL:CG2	3.03	0.42
1:D:559:ILE:CG1	1:D:560:LYS:H	2.33	0.42
1:D:307:THR:HA	1:D:348:ARG:CG	2.50	0.42
1:A:265:LEU:HD22	1:C:214:TYR:CZ	2.55	0.42
1:A:356:GLY:HA3	1:A:364:LYS:O	2.19	0.42
1:D:340:SER:HB3	1:D:426:LYS:HA	2.01	0.42
1:D:37:GLN:NE2	1:D:43:VAL:CA	2.70	0.42
1:A:38:GLN:CG	1:D:422:GLU:HB3	2.49	0.42
1:C:293:GLU:OE2	1:C:358:ILE:HG22	2.19	0.42
1:B:548:SER:O	1:B:550:SER:N	2.53	0.42
1:D:586:ALA:HB2	1:D:593:HIS:CE1	2.55	0.42
1:A:124:LYS:HB2	1:A:127:SER:HB2	2.02	0.42
1:D:445:LYS:HA	1:D:452:TYR:CD2	2.55	0.42
1:B:470:LEU:HD13	1:B:478:VAL:CG2	2.50	0.41
1:D:516:ILE:HD13	1:D:524:TYR:CB	2.50	0.41
1:D:384:GLN:NE2	1:D:489:GLU:HB2	2.35	0.41
1:D:81:LEU:CD1	1:D:89:PRO:HG2	2.50	0.41
1:D:233:LEU:HD13	1:D:251:MET:CE	2.50	0.41
1:A:81:LEU:C	1:A:81:LEU:HD23	2.39	0.41
1:A:538:VAL:HB	1:A:555:PHE:HB3	2.02	0.41
1:C:97:ARG:HB3	1:C:106:ALA:HB3	2.02	0.41
1:A:365:TRP:O	1:A:412:VAL:HA	2.19	0.41
1:D:222:MET:HE2	1:D:291:LEU:N	2.35	0.41
1:A:222:MET:CE	1:A:291:LEU:HB2	2.50	0.41
1:B:379:GLU:HA	1:B:407:ILE:HD11	2.01	0.41
1:C:205:LEU:N	1:C:272:MET:HE2	2.35	0.41
1:C:205:LEU:O	1:C:208:LEU:HB3	2.20	0.41
1:A:205:LEU:HG	1:A:209:TYR:CE1	2.54	0.41
1:C:95:ARG:HG2	1:C:95:ARG:NH1	2.35	0.41
1:A:533:ARG:NH1	1:A:554:PRO:CB	2.82	0.41
1:B:62:ILE:CD1	1:B:62:ILE:N	2.82	0.41
1:C:293:GLU:OE1	1:C:360:ASP:N	2.48	0.41
1:A:47:LEU:HD13	1:A:47:LEU:N	2.34	0.41
1:A:383:GLN:HA	1:A:386:CYS:HB2	2.02	0.41
1:B:524:TYR:CD2	1:B:524:TYR:N	2.88	0.41
1:C:536:HIS:CD2	1:C:560:LYS:HG2	2.56	0.41
1:A:327:TRP:CZ3	1:C:328:LYS:HD3	2.56	0.41
1:A:318:SER:HB3	1:A:337:VAL:C	2.40	0.41
1:A:379:GLU:HA	1:A:379:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:C	1:B:37:GLN:HG2	2.40	0.41
1:D:357:VAL:HG22	1:D:358:ILE:N	2.35	0.41
1:B:546:SER:OG	1:B:547:ARG:N	2.53	0.41
1:A:325:GLY:C	1:A:327:TRP:N	2.73	0.41
1:D:298:ALA:HB3	1:D:322:VAL:HB	2.01	0.41
1:D:125:ASN:OD1	1:D:126:ILE:N	2.46	0.41
1:B:548:SER:C	1:B:550:SER:N	2.73	0.41
1:C:124:LYS:O	1:C:125:ASN:C	2.59	0.41
1:B:262:ASN:C	1:B:264:GLY:H	2.24	0.41
1:C:233:LEU:HD21	1:C:253:ARG:CZ	2.50	0.41
1:D:248:GLN:HG2	1:D:249:LEU:N	2.36	0.41
1:B:139:GLU:O	1:B:140:GLN:CB	2.63	0.41
1:C:389:LYS:HE3	1:C:500:LEU:N	2.30	0.41
1:B:348:ARG:HD3	1:B:350:TYR:CZ	2.56	0.41
1:C:30:MET:O	1:C:32:CYS:N	2.53	0.41
1:A:198:PHE:CD2	1:A:198:PHE:N	2.89	0.41
1:A:418:SER:O	1:A:419:LEU:HB2	2.21	0.41
1:D:542:VAL:HB	1:D:551:TYR:CE1	2.56	0.41
1:C:406:ARG:HG3	1:C:406:ARG:NH1	2.35	0.41
1:A:455:THR:HG21	1:A:516:ILE:HD11	2.03	0.41
1:B:466:VAL:CG1	1:B:468:ASN:HD21	2.34	0.41
1:A:255:PHE:HB2	1:A:276:LEU:HB3	2.01	0.41
1:A:229:GLY:N	1:A:291:LEU:HD11	2.35	0.41
1:C:261:ARG:NH1	1:C:271:HIS:ND1	2.68	0.41
1:B:208:LEU:O	1:B:209:TYR:C	2.56	0.41
1:D:559:ILE:HG12	1:D:560:LYS:O	2.21	0.41
1:D:386:CYS:HA	1:D:390:ILE:HG13	2.03	0.41
1:D:348:ARG:HH11	1:D:348:ARG:HG2	1.86	0.41
1:C:575:GLN:HB2	1:C:575:GLN:HE21	1.70	0.41
1:B:486:PRO:HA	1:B:495:HIS:ND1	2.36	0.41
1:D:99:TYR:HB2	1:D:104:SER:OG	2.21	0.41
1:D:542:VAL:HG21	1:D:551:TYR:OH	2.21	0.41
1:C:88:PRO:HA	1:C:89:PRO:HD2	1.81	0.41
1:D:520:GLN:CG	1:D:521:ASP:N	2.83	0.41
1:A:378:MET:HB3	1:A:407:ILE:CD1	2.51	0.41
1:A:569:GLU:O	1:A:579:CYS:HA	2.20	0.41
1:A:569:GLU:CG	1:A:580:ARG:HG2	2.50	0.41
1:A:224:SER:C	1:A:226:GLY:H	2.24	0.41
1:A:308:ILE:HA	1:A:309:PRO:HD3	1.94	0.41
1:B:352:SER:H	1:B:354:HIS:CD2	2.38	0.41
1:B:36:VAL:O	1:B:37:GLN:CG	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:TYR:O	1:B:210:LEU:C	2.59	0.41
1:C:48:THR:OG1	1:C:49:HIS:N	2.54	0.41
1:B:392:ALA:HA	1:B:395:GLU:OE1	2.21	0.41
1:B:203:LEU:HB2	1:B:271:HIS:HA	2.03	0.41
1:C:61:HIS:HE1	1:C:63:VAL:CG2	2.34	0.41
1:B:500:LEU:HD22	1:B:502:ALA:HB3	2.02	0.41
1:B:545:PRO:O	1:B:546:SER:C	2.59	0.41
1:A:103:LEU:HD13	1:A:120:MET:SD	2.61	0.41
1:C:260:ILE:HG12	1:C:270:PHE:CE1	2.56	0.41
1:C:572:THR:HA	1:C:577:LEU:HA	2.03	0.41
1:D:30:MET:HG3	1:D:30:MET:O	2.21	0.41
1:C:37:GLN:CG	1:C:43:VAL:HG12	2.47	0.41
1:C:407:ILE:N	1:C:407:ILE:HD12	2.35	0.41
1:C:308:ILE:CD1	1:C:349:LEU:HD12	2.47	0.41
1:D:530:ASP:OD1	1:D:532:SER:HB3	2.21	0.41
1:D:347:ASP:CG	1:D:406:ARG:HH22	2.24	0.41
1:B:129:GLN:HG2	1:B:131:PHE:CE1	2.55	0.41
1:D:37:GLN:OE1	1:D:43:VAL:HG23	2.21	0.40
1:B:562:VAL:HG23	1:B:586:ALA:O	2.21	0.40
1:A:72:ASN:O	1:A:74:VAL:N	2.55	0.40
1:B:570:CYS:HA	1:B:578:TRP:O	2.21	0.40
1:A:580:ARG:HA	1:A:598:GLY:O	2.21	0.40
1:B:337:VAL:O	1:B:337:VAL:HG23	2.19	0.40
1:D:231:THR:OG1	1:D:253:ARG:NH1	2.54	0.40
1:B:540:TYR:CE1	1:B:568:VAL:HG21	2.54	0.40
1:D:574:ASP:C	1:D:576:LYS:H	2.25	0.40
1:C:516:ILE:O	1:C:516:ILE:HG22	2.20	0.40
1:A:387:LYS:HE2	1:A:387:LYS:HA	2.03	0.40
1:A:197:GLN:NE2	1:A:266:GLY:O	2.51	0.40
1:B:65:THR:OG1	1:B:119:PHE:HB2	2.21	0.40
1:B:93:LYS:HB2	1:B:96:TYR:H	1.86	0.40
1:C:473:ILE:N	1:C:474:PRO:CD	2.84	0.40
1:B:392:ALA:HA	1:B:395:GLU:HG2	2.03	0.40
1:A:107:ILE:HD11	1:A:118:TYR:CE2	2.57	0.40
1:C:91:TYR:HB3	1:C:93:LYS:CB	2.51	0.40
1:D:472:TRP:C	1:D:474:PRO:HD2	2.42	0.40
1:D:474:PRO:O	1:D:475:ARG:HB3	2.21	0.40
1:B:395:GLU:O	1:B:395:GLU:HG3	2.21	0.40
1:C:488:LYS:O	1:C:489:GLU:HG2	2.22	0.40
1:A:310:TYR:N	1:A:310:TYR:CD2	2.89	0.40
1:D:562:VAL:HA	1:D:563:PRO:HD2	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:CYS:O	1:B:599:MET:HA	2.20	0.40
1:C:306:ILE:N	1:C:306:ILE:HD12	2.37	0.40
1:D:345:VAL:O	1:D:345:VAL:HG22	2.21	0.40
1:C:508:VAL:O	1:C:508:VAL:HG13	2.20	0.40
1:D:230:GLY:HA2	1:D:289:VAL:HG11	2.02	0.40
1:B:358:ILE:HA	1:B:362:GLN:O	2.21	0.40
1:C:236:LYS:O	1:C:249:LEU:HB3	2.21	0.40
1:B:236:LYS:O	1:B:249:LEU:O	2.39	0.40
1:B:308:ILE:N	1:B:308:ILE:CD1	2.85	0.40
1:C:65:THR:CG2	1:C:75:GLU:HB3	2.48	0.40
1:C:535:GLU:OE2	1:C:556:ARG:HD3	2.22	0.40
1:B:294:LEU:HD12	1:B:326:VAL:HG11	2.03	0.40
1:C:493:ASP:HB2	1:C:495:HIS:NE2	2.36	0.40
1:D:262:ASN:HB2	1:D:573:TRP:CZ2	2.57	0.40
1:C:416:ASP:OD1	1:C:416:ASP:C	2.60	0.40
1:C:412:VAL:CG2	1:C:476:PHE:HE1	2.34	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	509/559 (91%)	416 (82%)	62 (12%)	31 (6%)	2 14
1	B	520/559 (93%)	412 (79%)	86 (16%)	22 (4%)	3 24
1	C	504/559 (90%)	407 (81%)	67 (13%)	30 (6%)	2 14
1	D	492/559 (88%)	389 (79%)	70 (14%)	33 (7%)	1 11
All	All	2025/2236 (91%)	1624 (80%)	285 (14%)	116 (6%)	2 16

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	A	389	LYS
1	A	439	SER
1	A	490	ALA
1	A	494	CYS
1	A	502	ALA
1	A	548	SER
1	A	39	LEU
1	A	60	ILE
1	A	72	ASN
1	A	73	SER
1	A	85	GLU
1	A	93	LYS
1	A	94	ASP
1	B	476	PHE
1	B	512	SER
1	B	60	ILE
1	B	73	SER
1	B	74	VAL
1	B	93	LYS
1	C	236	LYS
1	C	237	PRO
1	C	449	ASN
1	C	549	PHE
1	C	31	ASN
1	C	39	LEU
1	C	93	LYS
1	D	309	PRO
1	D	347	ASP
1	D	376	LEU
1	D	460	LYS
1	D	497	PRO
1	D	547	ARG
1	D	38	GLN
1	D	86	ALA
1	D	94	ASP
1	A	438	GLY
1	A	475	ARG
1	A	574	ASP
1	A	590	SER
1	A	592	GLY
1	A	52	ILE
1	A	79	VAL

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Mol	Chain	Res	Type
1	B	239	LEU
1	B	397	PRO
1	B	474	PRO
1	B	490	ALA
1	B	52	ILE
1	B	94	ASP
1	C	274	ASN
1	C	315	LYS
1	C	347	ASP
1	C	422	GLU
1	C	475	ARG
1	C	548	SER
1	C	50	GLU
1	D	374	ASP
1	D	437	HIS
1	D	465	GLY
1	D	475	ARG
1	D	522	LEU
1	D	546	SER
1	D	548	SER
1	D	575	GLN
1	D	39	LEU
1	D	47	LEU
1	D	59	SER
1	D	109	GLU
1	A	189	SER
1	A	451	VAL
1	A	53	ASN
1	A	133	LEU
1	B	222	MET
1	B	250	SER
1	B	489	GLU
1	C	393	LEU
1	C	40	GLY
1	C	101	GLU
1	D	390	ILE
1	D	92	LEU
1	A	390	ILE
1	B	238	ASN
1	B	481	TYR
1	C	460	LYS
1	C	125	ASN

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Mol	Chain	Res	Type
1	C	133	LEU
1	D	224	SER
1	D	502	ALA
1	D	46	PRO
1	A	352	SER
1	A	75	GLU
1	A	84	SER
1	B	400	ALA
1	B	549	PHE
1	C	400	ALA
1	C	74	VAL
1	D	212	ARG
1	D	381	CYS
1	D	422	GLU
1	D	441	MET
1	D	68	LYS
1	A	473	ILE
1	B	390	ILE
1	C	462	LEU
1	C	46	PRO
1	C	83	PRO
1	C	94	ASP
1	D	492	GLY
1	C	316	GLY
1	C	500	LEU
1	D	43	VAL
1	B	401	PRO
1	C	35	ILE
1	A	492	GLY
1	C	60	ILE
1	B	226	GLY

5.3.2 Protein sidechains (i)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	457/489 (94%)	403 (88%)	54 (12%)	6 28
1	B	468/489 (96%)	433 (92%)	35 (8%)	17 53
1	C	457/489 (94%)	400 (88%)	57 (12%)	6 25
1	D	449/489 (92%)	419 (93%)	30 (7%)	20 58
All	All	1831/1956 (94%)	1655 (90%)	176 (10%)	10 38

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	CYS
1	A	193	THR
1	A	195	ARG
1	A	215	ASN
1	A	221	THR
1	A	224	SER
1	A	261	ARG
1	A	273	THR
1	A	275	TYR
1	A	293	GLU
1	A	296	LEU
1	A	311	GLN
1	A	331	THR
1	A	333	MET
1	A	341	THR
1	A	360	ASP
1	A	378	MET
1	A	379	GLU
1	A	381	CYS
1	A	384	GLN
1	A	387	LYS
1	A	395	GLU
1	A	398	GLU
1	A	413	LEU
1	A	449	ASN
1	A	461	ASN
1	A	471	GLU
1	A	472	TRP
1	A	479	SER
1	A	482	ARG

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Mol	Chain	Res	Type
1	A	484	THR
1	A	488	LYS
1	A	489	GLU
1	A	494	CYS
1	A	514	LEU
1	A	518	PRO
1	A	520	GLN
1	A	521	ASP
1	A	549	PHE
1	A	552	PHE
1	A	559	ILE
1	A	580	ARG
1	A	38	GLN
1	A	45	LEU
1	A	47	LEU
1	A	48	THR
1	A	56	MET
1	A	70	LEU
1	A	80	SER
1	A	93	LYS
1	A	95	ARG
1	A	100	LEU
1	A	103	LEU
1	A	133	LEU
1	B	193	THR
1	B	217	SER
1	B	235	GLU
1	B	246	LEU
1	B	249	LEU
1	B	275	TYR
1	B	304	ASP
1	B	305	SER
1	B	310	TYR
1	B	342	ASP
1	B	387	LYS
1	B	419	LEU
1	B	449	ASN
1	B	459	MET
1	B	461	ASN
1	B	464	LEU
1	B	472	TRP
1	B	479	SER

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Mol	Chain	Res	Type
1	B	484	THR
1	B	500	LEU
1	B	510	LEU
1	B	526	LEU
1	B	559	ILE
1	B	577	LEU
1	B	605	SER
1	B	34	LYS
1	B	38	GLN
1	B	45	LEU
1	B	48	THR
1	B	52	ILE
1	B	80	SER
1	B	92	LEU
1	B	93	LYS
1	B	101	GLU
1	B	133	LEU
1	C	192	THR
1	C	200	ASN
1	C	206	LEU
1	C	207	ASP
1	C	221	THR
1	C	223	THR
1	C	227	MET
1	C	231	THR
1	C	234	VAL
1	C	248	GLN
1	C	249	LEU
1	C	282	ASN
1	C	286	ASN
1	C	319	PHE
1	C	320	GLN
1	C	349	LEU
1	C	351	LEU
1	C	355	ARG
1	C	365	TRP
1	C	391	GLN
1	C	405	ASN
1	C	414	SER
1	C	415	VAL
1	C	422	GLU
1	C	436	THR

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Mol	Chain	Res	Type
1	C	437	HIS
1	C	449	ASN
1	C	455	THR
1	C	459	MET
1	C	461	ASN
1	C	464	LEU
1	C	472	TRP
1	C	479	SER
1	C	510	LEU
1	C	514	LEU
1	C	528	THR
1	C	533	ARG
1	C	547	ARG
1	C	555	PHE
1	C	568	VAL
1	C	572	THR
1	C	589	GLU
1	C	607	THR
1	C	34	LYS
1	C	37	GLN
1	C	50	GLU
1	C	58	LYS
1	C	65	THR
1	C	66	MET
1	C	70	LEU
1	C	72	ASN
1	C	85	GLU
1	C	93	LYS
1	C	95	ARG
1	C	102	HIS
1	C	132	CYS
1	C	136	LYS
1	D	193	THR
1	D	200	ASN
1	D	206	LEU
1	D	223	THR
1	D	232	TYR
1	D	315	LYS
1	D	331	THR
1	D	360	ASP
1	D	365	TRP
1	D	377	ARG

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Mol	Chain	Res	Type
1	D	416	ASP
1	D	437	HIS
1	D	455	THR
1	D	461	ASN
1	D	464	LEU
1	D	515	VAL
1	D	520	GLN
1	D	528	THR
1	D	549	PHE
1	D	555	PHE
1	D	572	THR
1	D	577	LEU
1	D	42	ASP
1	D	46	PRO
1	D	65	THR
1	D	72	ASN
1	D	85	GLU
1	D	93	LYS
1	D	95	ARG
1	D	112	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	A	278	GLN
1	A	320	GLN
1	A	448	HIS
1	A	449	ASN
1	A	461	ASN
1	A	468	ASN
1	A	567	GLN
1	A	581	HIS
1	A	37	GLN
1	A	57	ASN
1	A	76	ASN
1	B	278	GLN
1	B	320	GLN
1	B	334	GLN
1	B	383	GLN
1	B	461	ASN
1	B	468	ASN

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Mol	Chain	Res	Type
1	B	567	GLN
1	B	575	GLN
1	B	37	GLN
1	B	61	HIS
1	B	72	ASN
1	B	125	ASN
1	B	140	GLN
1	C	286	ASN
1	C	334	GLN
1	C	383	GLN
1	C	384	GLN
1	C	461	ASN
1	C	468	ASN
1	C	523	GLN
1	C	567	GLN
1	C	575	GLN
1	C	593	HIS
1	C	37	GLN
1	C	61	HIS
1	D	197	GLN
1	D	200	ASN
1	D	248	GLN
1	D	286	ASN
1	D	320	GLN
1	D	383	GLN
1	D	405	ASN
1	D	461	ASN
1	D	468	ASN
1	D	520	GLN
1	D	523	GLN
1	D	575	GLN
1	D	593	HIS
1	D	37	GLN
1	D	49	HIS
1	D	61	HIS
1	D	72	ASN
1	D	76	ASN
1	D	102	HIS
1	D	129	GLN
1	D	134	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	NAG	A	901	1	14,14,15	0.86	1 (7%)	15,19,21	1.23	2 (13%)
2	NAG	B	801	1	14,14,15	1.05	1 (7%)	15,19,21	0.87	1 (6%)
2	NAG	B	901	1	14,14,15	0.56	0	15,19,21	0.94	1 (6%)
2	NAG	C	801	1	14,14,15	0.81	0	15,19,21	0.59	0
2	NAG	C	901	1	14,14,15	0.72	0	15,19,21	0.78	0
2	NAG	D	901	1	14,14,15	0.93	1 (7%)	15,19,21	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	NAG	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	1/6/23/26	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	901	1	-	0/6/23/26	0/1/1/1
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	NAG	C4-C5	2.13	1.57	1.53
2	D	901	NAG	C1-C2	2.27	1.55	1.52
2	B	801	NAG	C1-C2	3.29	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	NAG	C2-N2-C7	-2.84	119.39	123.04
2	B	901	NAG	C2-N2-C7	-2.66	119.62	123.04
2	B	801	NAG	C3-C4-C5	-2.06	106.61	110.20
2	A	901	NAG	C3-C4-C5	3.09	115.58	110.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	NAG	1	0
2	D	901	NAG	1	0

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, 95^{th} 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	515/559 (92%)	-0.26	8 (1%) 74 61	33, 57, 97, 115	0
1	B	526/559 (94%)	-0.12	22 (4%) 40 24	38, 66, 109, 122	0
1	C	514/559 (91%)	-0.16	11 (2%) 67 50	39, 66, 101, 118	0
1	D	504/559 (90%)	-0.08	13 (2%) 59 44	49, 75, 114, 130	0
All	All	2059/2236 (92%)	-0.16	54 (2%) 59 44	33, 67, 108, 130	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	GLY	5.1
1	B	589	GLU	4.6
1	C	590	SER	4.5
1	B	590	SER	4.2
1	A	310	TYR	3.9
1	C	314	GLY	3.9
1	D	313	SER	3.9
1	B	313	SER	3.7
1	B	309	PRO	3.4
1	B	311	GLN	3.4
1	C	249	LEU	3.3
1	B	246	LEU	3.3
1	B	312	GLY	3.3
1	D	309	PRO	3.2
1	D	502	ALA	3.1
1	C	342	ASP	3.1
1	B	241	SER	2.9
1	B	587	ASP	2.8
1	D	314	GLY	2.8
1	D	87	GLY	2.7
1	B	606	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	575	GLN	2.6
1	B	588	SER	2.6
1	D	83	PRO	2.6
1	A	589	GLU	2.6
1	A	312	GLY	2.4
1	C	313	SER	2.4
1	A	590	SER	2.4
1	A	605	SER	2.4
1	B	189	SER	2.4
1	B	492	GLY	2.3
1	C	239	LEU	2.3
1	D	310	TYR	2.3
1	B	56	MET	2.3
1	B	282	ASN	2.3
1	A	71	GLU	2.3
1	B	188	CYS	2.3
1	C	607	THR	2.3
1	B	503	GLU	2.2
1	A	503	GLU	2.2
1	C	87	GLY	2.2
1	D	85	GLU	2.2
1	A	125	ASN	2.1
1	D	86	ALA	2.1
1	B	281	SER	2.1
1	D	109	GLU	2.1
1	B	52	ILE	2.1
1	B	248	GLN	2.1
1	C	315	LYS	2.1
1	B	53	ASN	2.0
1	D	475	ARG	2.0
1	C	310	TYR	2.0
1	C	73	SER	2.0
1	D	57	ASN	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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	B	901	14/15	0.82	0.28	0.98	100,102,104,104	0
2	NAG	A	901	14/15	0.87	0.26	0.55	88,90,91,91	0
2	NAG	D	901	14/15	0.67	0.46	-	95,98,103,105	0
2	NAG	C	901	14/15	0.77	0.36	-	94,97,99,99	0
2	NAG	C	801	14/15	0.67	0.52	-	90,94,98,98	0
2	NAG	B	801	14/15	0.69	0.47	-	89,91,93,93	0

6.5 Other polymers

There are no such residues in this entry.