



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:37 AM GMT

PDB ID : 2HU4
Title : N1 neuraminidase in complex with oseltamivir 2
Authors : Russell, R.J.; Haire, L.F.; Stevens, D.J.; Collins, P.J.; Lin, Y.P.; Blackburn, G.M.; Hay, A.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2006-07-26
Resolution : 2.50 Å(reported)

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

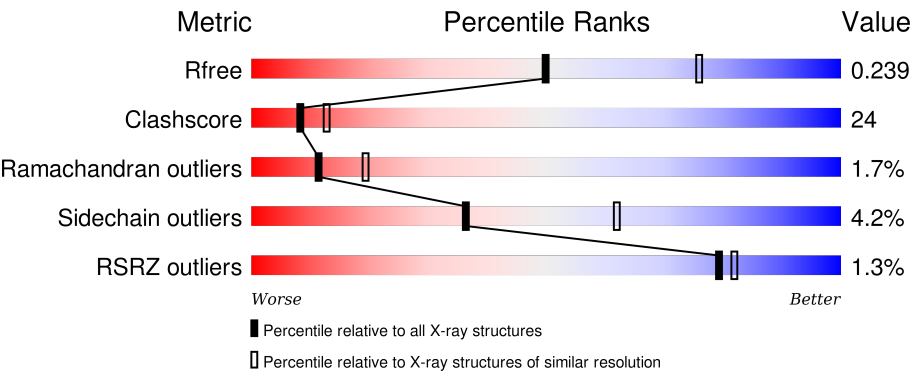
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	387	<div><div>%</div><div>63%33% . ..</div></div>
1	B	387	<div><div>2%</div><div>65%30% . ..</div></div>
1	C	387	<div><div>%</div><div>63%33% . ..</div></div>
1	D	387	<div><div>%</div><div>60%35%5% ..</div></div>
1	E	387	<div><div>2%</div><div>64%32% . ..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	387	
1	G	387	
1	H	387	

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	G39	F	805	-	-	-	X

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23856 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.

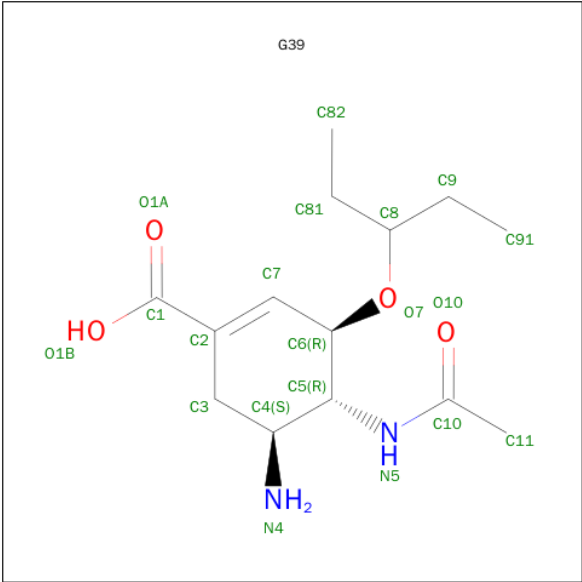
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	B	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	C	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	D	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	E	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	F	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	G	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			
1	H	385	Total	C	N	O	S	0	0	0
			2962	1858	510	573	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	TYR	HIS	ENGINEERED MUTATION	UNP Q6DPL2
B	252	TYR	HIS	ENGINEERED MUTATION	UNP Q6DPL2
C	252	TYR	HIS	ENGINEERED MUTATION	UNP Q6DPL2
D	252	TYR	HIS	ENGINEERED MUTATION	UNP Q6DPL2
E	252	TYR	HIS	ENGINEERED MUTATION	UNP Q6DPL2
F	252	TYR	HIS	ENGINEERED MUTATION	UNP Q6DPL2
G	252	TYR	HIS	ENGINEERED MUTATION	UNP Q6DPL2
H	252	TYR	HIS	ENGINEERED MUTATION	UNP Q6DPL2

- Molecule 2 is (3R,4R,5S)-4-(ACETYLAMINO)-5-AMINO-3-(PENTAN-3-YLOXY)CYCLO HEX-1-ENE-1-CARBOXYLIC ACID (three-letter code: G39) (formula: C₁₄H₂₄N₂O₄).

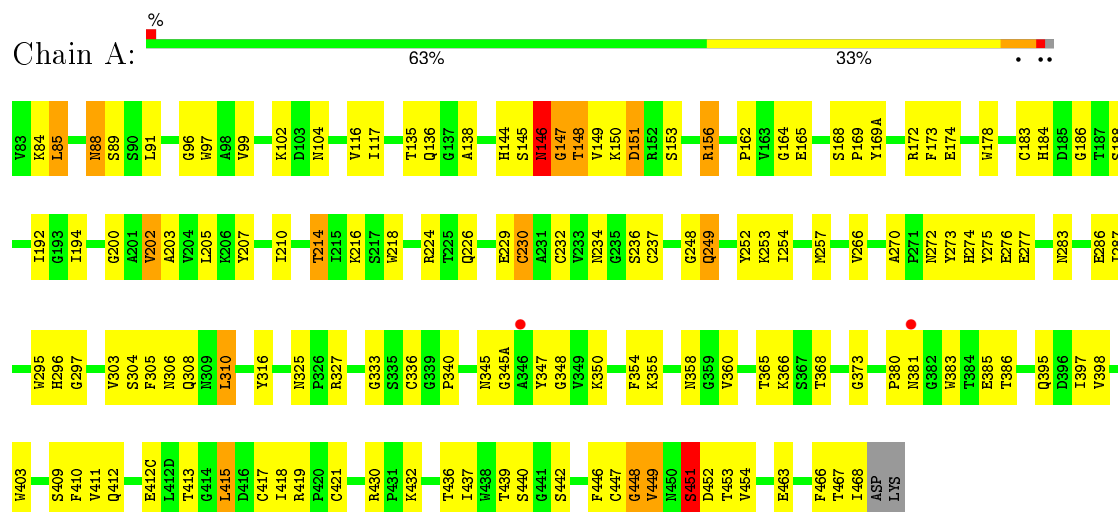


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	14	2	4		
2	B	1	Total	C	N	O	0	0
			20	14	2	4		
2	C	1	Total	C	N	O	0	0
			20	14	2	4		
2	D	1	Total	C	N	O	0	0
			20	14	2	4		
2	E	1	Total	C	N	O	0	0
			20	14	2	4		
2	F	1	Total	C	N	O	0	0
			20	14	2	4		
2	G	1	Total	C	N	O	0	0
			20	14	2	4		
2	H	1	Total	C	N	O	0	0
			20	14	2	4		

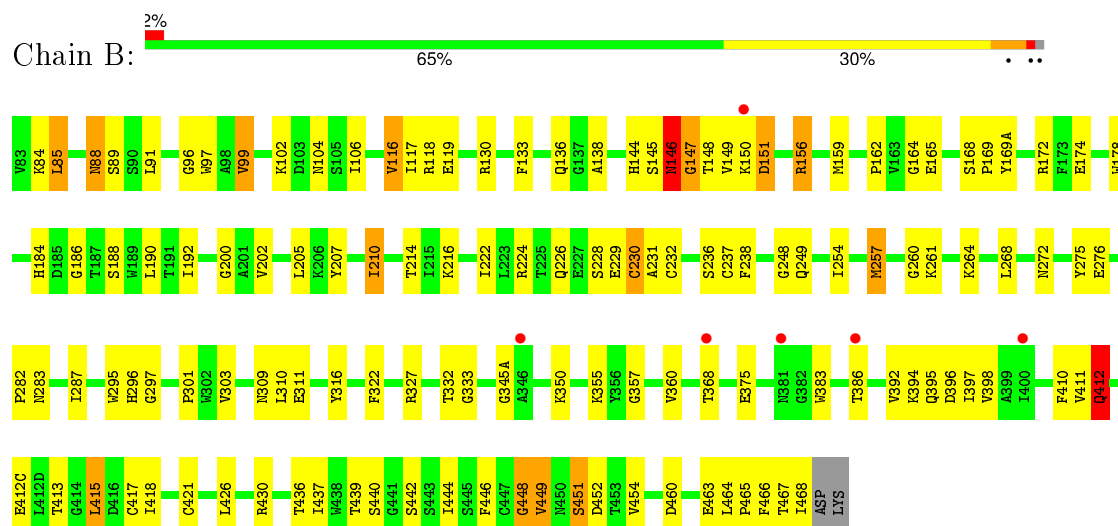
3 Residue-property plots

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

• Molecule 1: Neuraminidase

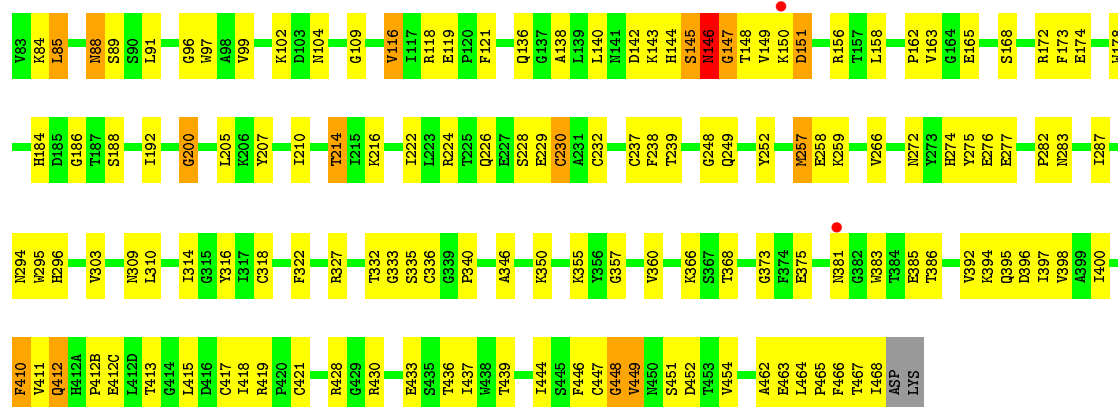


• Molecule 1: Neuraminidase

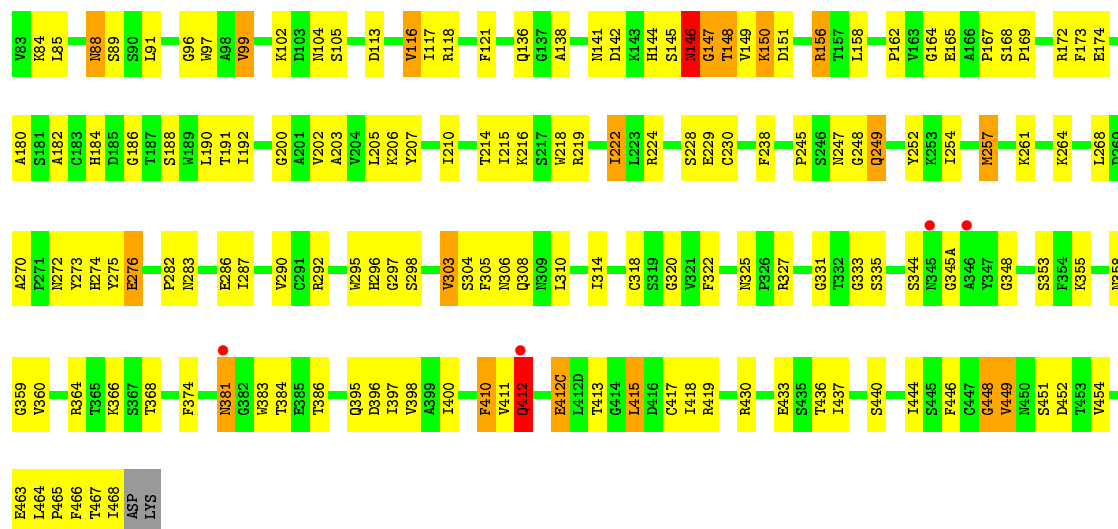


• Molecule 1: Neuraminidase

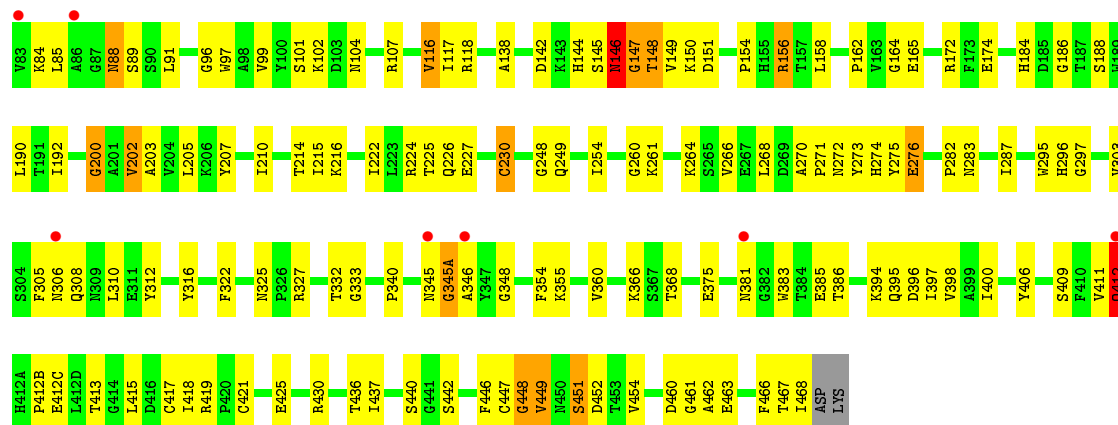




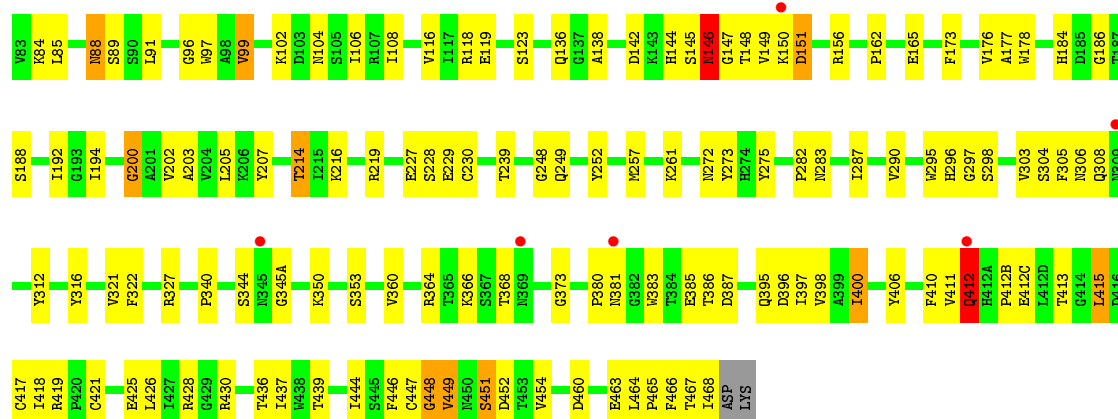
• Molecule 1: Neuraminidase



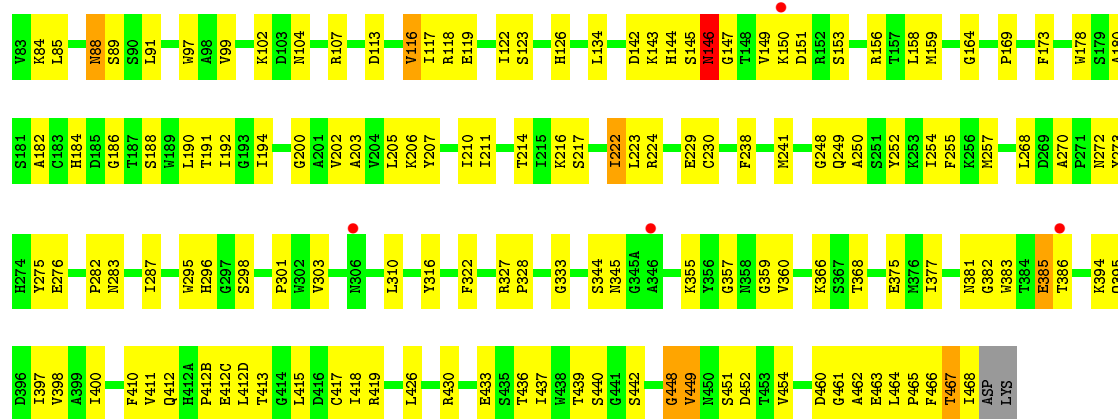
• Molecule 1: Neuraminidase



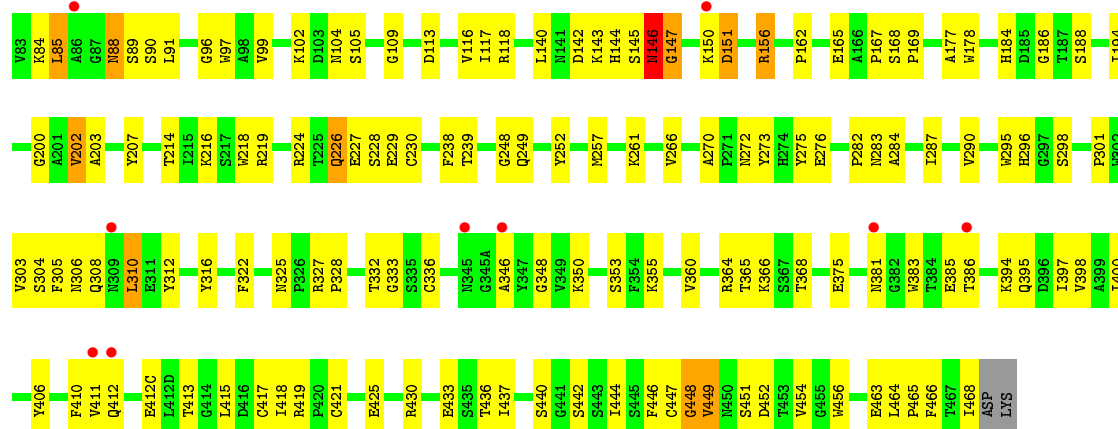
• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	201.06Å 201.24Å 211.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 19.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.50) 93.2 (19.96-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.273 0.240 , 0.239	Depositor DCC
R_{free} test set	6823 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , -3.8	EDS
Estimated twinning fraction	0.079 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 136759 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23856	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G39

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/3045	0.72	0/4141
1	B	0.45	1/3045 (0.0%)	0.74	2/4141 (0.0%)
1	C	0.43	0/3045	0.74	1/4141 (0.0%)
1	D	0.47	2/3045 (0.1%)	0.77	3/4141 (0.1%)
1	E	0.47	1/3045 (0.0%)	0.72	1/4141 (0.0%)
1	F	0.48	1/3045 (0.0%)	0.73	1/4141 (0.0%)
1	G	0.42	0/3045	0.72	0/4141
1	H	0.42	0/3045	0.73	1/4141 (0.0%)
All	All	0.45	5/24360 (0.0%)	0.73	9/33128 (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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	412	GLN	C-N	-11.84	1.06	1.34
1	D	412	GLN	C-N	-10.38	1.10	1.34
1	E	412	GLN	C-N	-9.68	1.11	1.34
1	B	412	GLN	C-N	-9.25	1.12	1.34
1	D	410	PHE	C-N	-5.43	1.21	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	412	GLN	O-C-N	-9.63	107.29	122.70
1	D	412	GLN	CA-C-N	5.84	130.06	117.20
1	B	412	GLN	CB-CA-C	5.44	121.28	110.40
1	F	412	GLN	CB-CA-C	5.42	121.25	110.40
1	E	412	GLN	CB-CA-C	5.41	121.22	110.40
1	C	412	GLN	CB-CA-C	5.41	121.22	110.40
1	D	412	GLN	CB-CA-C	5.38	121.16	110.40
1	H	226	GLN	N-CA-C	5.23	125.12	111.00
1	B	311	GLU	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	412	GLN	Mainchain
1	C	410	PHE	Mainchain
1	D	412	GLN	Mainchain
1	E	412	GLN	Mainchain
1	F	412	GLN	Mainchain

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	2962	0	2783	157	0
1	B	2962	0	2782	155	0
1	C	2962	0	2783	150	0
1	D	2962	0	2781	171	0
1	E	2962	0	2782	166	0
1	F	2962	0	2782	139	0
1	G	2962	0	2783	159	0
1	H	2962	0	2783	143	0
2	A	20	0	23	0	0
2	B	20	0	23	0	0
2	C	20	0	23	0	0
2	D	20	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	20	0	23	0	0
2	F	20	0	23	0	0
2	G	20	0	23	0	0
2	H	20	0	23	0	0
All	All	23856	0	22443	1126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1126) 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:G:327:ARG:O	1:G:368:THR:CG2	1.67	1.42
1:F:327:ARG:O	1:F:368:THR:CG2	1.73	1.37
1:H:327:ARG:O	1:H:368:THR:CG2	1.74	1.36
1:A:327:ARG:O	1:A:368:THR:CG2	1.71	1.35
1:B:327:ARG:O	1:B:368:THR:CG2	1.82	1.28
1:E:327:ARG:O	1:E:368:THR:CG2	1.88	1.21
1:C:327:ARG:O	1:C:368:THR:CG2	1.90	1.20
1:D:412:GLN:OE1	1:D:419:ARG:HD2	1.45	1.14
1:F:327:ARG:O	1:F:368:THR:HG22	1.46	1.14
1:H:327:ARG:O	1:H:368:THR:HG22	1.41	1.11
1:D:327:ARG:O	1:D:368:THR:CG2	2.02	1.07
1:G:327:ARG:O	1:G:368:THR:HG23	1.52	1.06
1:D:411:VAL:HG12	1:D:412:GLN:O	1.55	1.06
1:H:412:GLN:OE1	1:H:419:ARG:HD2	1.54	1.06
1:C:413:THR:HG21	1:C:415:LEU:HD22	1.36	1.06
1:D:358:ASN:O	1:D:381:ASN:HA	1.57	1.05
1:B:413:THR:HG21	1:B:415:LEU:HD22	1.37	1.04
1:F:412:GLN:OE1	1:F:419:ARG:HD2	1.56	1.03
1:A:413:THR:HG21	1:A:415:LEU:HD22	1.38	1.03
1:E:413:THR:HG21	1:E:415:LEU:HD22	1.39	1.03
1:D:359:GLY:HA2	1:D:381:ASN:H	1.23	1.03
1:H:327:ARG:HG3	1:H:368:THR:HG23	1.40	1.03
1:G:327:ARG:O	1:G:368:THR:HG22	1.55	1.01
1:A:411:VAL:HG11	1:A:418:ILE:HG23	1.40	1.01
1:C:327:ARG:O	1:C:368:THR:HG22	1.57	1.00
1:A:327:ARG:O	1:A:368:THR:HG23	1.59	1.00
1:E:452:ASP:HB2	1:G:216:LYS:NZ	1.77	1.00
1:B:327:ARG:O	1:B:368:THR:HG22	1.63	0.98
1:F:91:LEU:HG	1:F:283:ASN:HD22	1.29	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:ARG:O	1:E:368:THR:HG22	1.61	0.97
1:G:413:THR:HG21	1:G:415:LEU:HD22	1.46	0.96
1:G:85:LEU:HD12	1:G:412(C):GLU:HG3	1.47	0.95
1:A:216:LYS:HZ1	1:D:452:ASP:HB2	1.32	0.94
1:A:216:LYS:NZ	1:D:452:ASP:HB2	1.82	0.94
1:E:452:ASP:HB2	1:G:216:LYS:HZ1	1.33	0.94
1:D:413:THR:HG21	1:D:415:LEU:HD22	1.49	0.93
1:A:327:ARG:O	1:A:368:THR:HG22	1.65	0.93
1:B:451:SER:HB2	1:D:214:THR:HB	1.49	0.92
1:A:452:ASP:HB2	1:C:216:LYS:NZ	1.85	0.92
1:B:452:ASP:HB2	1:D:216:LYS:NZ	1.84	0.91
1:H:397:ILE:HG22	1:H:398:VAL:HG23	1.53	0.91
1:B:188:SER:OG	1:B:207:TYR:CZ	2.24	0.91
1:D:359:GLY:CA	1:D:381:ASN:H	1.84	0.90
1:H:89:SER:OG	1:H:417:CYS:HA	1.70	0.90
1:B:249:GLN:HE21	1:B:272:ASN:H	1.14	0.90
1:E:249:GLN:NE2	1:E:272:ASN:H	1.70	0.89
1:F:327:ARG:O	1:F:368:THR:HG23	1.69	0.89
1:B:452:ASP:HB2	1:D:216:LYS:HZ1	1.36	0.88
1:B:91:LEU:HG	1:B:283:ASN:HD22	1.35	0.88
1:D:381:ASN:N	1:D:381:ASN:HD22	1.69	0.88
1:G:397:ILE:HG22	1:G:398:VAL:HG23	1.56	0.87
1:A:452:ASP:HB2	1:C:216:LYS:HZ1	1.38	0.87
1:A:91:LEU:HG	1:A:283:ASN:HD22	1.38	0.87
1:H:413:THR:HG21	1:H:415:LEU:HD22	1.55	0.87
1:C:91:LEU:HG	1:C:283:ASN:HD22	1.40	0.87
1:B:200:GLY:O	1:C:454:VAL:HG11	1.74	0.87
1:E:192:ILE:HG12	1:E:205:LEU:HD22	1.55	0.86
1:A:327:ARG:O	1:A:368:THR:HG21	1.75	0.86
1:E:214:THR:HG21	1:H:452:ASP:O	1.76	0.86
1:A:150:LYS:O	1:A:151:ASP:HB2	1.76	0.86
1:A:85:LEU:HD12	1:A:412(C):GLU:HG3	1.55	0.86
1:B:327:ARG:HG3	1:B:368:THR:HG23	1.58	0.86
1:F:214:THR:HB	1:G:451:SER:OG	1.76	0.86
1:D:327:ARG:O	1:D:368:THR:HG22	1.75	0.85
1:E:452:ASP:O	1:G:214:THR:HG21	1.75	0.85
1:A:192:ILE:HG12	1:A:205:LEU:HD22	1.58	0.85
1:C:188:SER:OG	1:C:207:TYR:CZ	2.29	0.85
1:A:413:THR:HG22	1:A:415:LEU:HD13	1.58	0.85
1:B:249:GLN:NE2	1:B:272:ASN:H	1.75	0.84
1:A:411:VAL:HG11	1:A:418:ILE:CG2	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:LEU:HG	1:G:283:ASN:HD22	1.42	0.84
1:G:413:THR:HG22	1:G:415:LEU:HD13	1.59	0.84
1:H:327:ARG:O	1:H:368:THR:HG21	1.76	0.83
1:B:452:ASP:O	1:D:214:THR:HG21	1.77	0.83
1:F:452:ASP:O	1:H:214:THR:HG21	1.78	0.83
1:B:327:ARG:O	1:B:368:THR:HG23	1.78	0.82
1:D:359:GLY:HA2	1:D:381:ASN:N	1.94	0.82
1:E:200:GLY:O	1:H:454:VAL:HG11	1.79	0.82
1:A:144:HIS:HE1	1:D:463:GLU:H	1.25	0.82
1:A:188:SER:OG	1:A:207:TYR:CZ	2.32	0.82
1:A:452:ASP:O	1:C:214:THR:HG21	1.78	0.81
1:F:413:THR:HG21	1:F:415:LEU:HD22	1.62	0.81
1:B:85:LEU:HD12	1:B:412(C):GLU:HG3	1.63	0.81
1:B:144:HIS:HE1	1:C:463:GLU:H	1.29	0.81
1:B:454:VAL:HG11	1:D:200:GLY:O	1.81	0.81
1:D:327:ARG:O	1:D:368:THR:HG23	1.80	0.81
1:A:327:ARG:HG3	1:A:368:THR:HG23	1.64	0.80
1:E:327:ARG:O	1:E:368:THR:HG23	1.80	0.80
1:C:327:ARG:HG3	1:C:368:THR:HG23	1.63	0.80
1:D:85:LEU:HD12	1:D:412(C):GLU:HG3	1.62	0.80
1:E:144:HIS:HE1	1:H:463:GLU:H	1.27	0.80
1:F:282:PRO:HD2	1:F:411:VAL:HG21	1.62	0.79
1:E:97:TRP:H	1:E:395:GLN:HE22	1.29	0.79
1:G:327:ARG:O	1:G:368:THR:HG21	1.81	0.79
1:A:89:SER:OG	1:A:417:CYS:HA	1.82	0.79
1:D:89:SER:OG	1:D:417:CYS:HA	1.83	0.79
1:C:413:THR:HG22	1:C:415:LEU:HD13	1.64	0.79
1:G:381:ASN:HB3	1:G:385:GLU:HG3	1.65	0.79
1:A:452:ASP:HB3	1:C:216:LYS:HD3	1.64	0.78
1:H:333:GLY:N	1:H:386:THR:HG23	1.99	0.78
1:D:411:VAL:CG1	1:D:412:GLN:O	2.31	0.78
1:A:147:GLY:HA2	1:A:430:ARG:HH12	1.48	0.78
1:E:89:SER:OG	1:E:417:CYS:HA	1.83	0.78
1:A:411:VAL:HG12	1:A:412:GLN:N	1.98	0.78
1:G:381:ASN:O	1:G:385:GLU:HG3	1.83	0.78
1:C:448:GLY:O	1:C:449:VAL:HB	1.84	0.78
1:C:150:LYS:O	1:C:151:ASP:HB2	1.84	0.78
1:E:454:VAL:HG11	1:G:200:GLY:O	1.84	0.77
1:A:214:THR:HG21	1:D:452:ASP:O	1.84	0.77
1:F:327:ARG:HG3	1:F:368:THR:HG23	1.66	0.77
1:F:412:GLN:NE2	1:F:447:CYS:SG	2.58	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLU:H	1:D:144:HIS:HE1	1.32	0.77
1:B:397:ILE:HG22	1:B:398:VAL:HG23	1.67	0.77
1:E:216:LYS:HZ1	1:H:452:ASP:HB2	1.50	0.77
1:H:188:SER:OG	1:H:207:TYR:CZ	2.37	0.76
1:F:412:GLN:OE1	1:F:419:ARG:CD	2.33	0.76
1:F:452:ASP:HB3	1:H:216:LYS:HD3	1.66	0.76
1:F:463:GLU:H	1:H:144:HIS:HE1	1.33	0.76
1:F:150:LYS:O	1:F:151:ASP:HB2	1.86	0.76
1:E:184:HIS:HD2	1:E:186:GLY:H	1.33	0.76
1:E:397:ILE:HG22	1:E:398:VAL:HG23	1.66	0.76
1:E:249:GLN:HE21	1:E:272:ASN:H	1.31	0.76
1:C:89:SER:OG	1:C:417:CYS:HA	1.86	0.76
1:F:214:THR:HG21	1:G:452:ASP:O	1.86	0.75
1:E:85:LEU:HD12	1:E:412(C):GLU:HG3	1.67	0.75
1:G:147:GLY:HA2	1:G:430:ARG:HH12	1.50	0.75
1:C:97:TRP:H	1:C:395:GLN:HE22	1.33	0.75
1:F:97:TRP:H	1:F:395:GLN:HE22	1.34	0.75
1:H:327:ARG:CG	1:H:368:THR:HG23	2.17	0.75
1:B:327:ARG:O	1:B:368:THR:HG21	1.86	0.75
1:E:412:GLN:NE2	1:E:447:CYS:SG	2.59	0.75
1:C:188:SER:OG	1:C:207:TYR:CE1	2.38	0.75
1:E:327:ARG:HG3	1:E:368:THR:HG23	1.69	0.74
1:G:188:SER:OG	1:G:207:TYR:CZ	2.40	0.74
1:D:360:VAL:HG13	1:D:383:TRP:HB2	1.68	0.74
1:B:150:LYS:O	1:B:151:ASP:HB2	1.86	0.74
1:E:463:GLU:H	1:G:144:HIS:HE1	1.34	0.74
1:F:466:PHE:C	1:F:468:ILE:H	1.91	0.74
1:A:397:ILE:HG22	1:A:398:VAL:HG23	1.69	0.74
1:H:412:GLN:NE2	1:H:447:CYS:SG	2.60	0.74
1:A:411:VAL:HG13	1:A:419:ARG:O	1.88	0.74
1:C:327:ARG:O	1:C:368:THR:HG23	1.86	0.73
1:A:216:LYS:HD3	1:D:452:ASP:HB3	1.68	0.73
1:H:147:GLY:HA2	1:H:430:ARG:HH12	1.54	0.73
1:D:188:SER:OG	1:D:207:TYR:CZ	2.42	0.73
1:H:412:GLN:OE1	1:H:419:ARG:CD	2.35	0.73
1:E:282:PRO:HD2	1:E:411:VAL:HG21	1.68	0.73
1:F:216:LYS:NZ	1:G:452:ASP:HB2	2.02	0.73
1:B:413:THR:CG2	1:B:415:LEU:HD22	2.16	0.73
1:G:85:LEU:CD1	1:G:412(C):GLU:HG3	2.19	0.73
1:F:411:VAL:CG1	1:F:418:ILE:HG23	2.19	0.72
1:E:91:LEU:H	1:E:283:ASN:ND2	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:GLN:NE2	1:E:272:ASN:N	2.37	0.72
1:B:360:VAL:HG13	1:B:383:TRP:HB2	1.71	0.72
1:F:411:VAL:HG12	1:F:412:GLN:N	2.05	0.72
1:B:287:ILE:N	1:B:287:ILE:HD12	2.04	0.72
1:B:214:THR:HG21	1:C:452:ASP:O	1.88	0.72
1:G:448:GLY:O	1:G:449:VAL:HB	1.88	0.72
1:B:188:SER:OG	1:B:207:TYR:CE1	2.43	0.72
1:F:452:ASP:HB2	1:H:216:LYS:NZ	2.05	0.71
1:D:192:ILE:HG12	1:D:205:LEU:HD22	1.72	0.71
1:E:91:LEU:H	1:E:283:ASN:HD21	1.39	0.71
1:H:333:GLY:H	1:H:386:THR:HG23	1.55	0.71
1:F:216:LYS:HZ1	1:G:452:ASP:HB2	1.54	0.71
1:B:411:VAL:HG12	1:B:412:GLN:N	2.05	0.71
1:E:150:LYS:O	1:E:151:ASP:HB2	1.90	0.70
1:F:200:GLY:O	1:G:454:VAL:HG11	1.91	0.70
1:E:411:VAL:HG12	1:E:412:GLN:N	2.05	0.70
1:F:142:ASP:O	1:F:145:SER:HB3	1.91	0.70
1:E:188:SER:OG	1:E:207:TYR:CZ	2.43	0.70
1:A:411:VAL:CG1	1:A:418:ILE:HG23	2.18	0.70
1:G:366:LYS:HD3	1:G:400:ILE:HG12	1.73	0.70
1:F:452:ASP:HB2	1:H:216:LYS:HZ1	1.56	0.70
1:B:333:GLY:N	1:B:386:THR:HG23	2.07	0.70
1:A:116:VAL:HG13	1:A:136:GLN:HB2	1.72	0.70
1:D:145:SER:O	1:D:146:ASN:O	2.10	0.70
1:B:192:ILE:HG12	1:B:205:LEU:HD22	1.72	0.70
1:C:149:VAL:HG23	1:C:430:ARG:NH1	2.07	0.69
1:E:116:VAL:HG12	1:E:138:ALA:O	1.92	0.69
1:B:91:LEU:HG	1:B:283:ASN:ND2	2.05	0.69
1:E:214:THR:HB	1:H:451:SER:OG	1.90	0.69
1:C:192:ILE:HG12	1:C:205:LEU:HD22	1.74	0.69
1:D:381:ASN:N	1:D:381:ASN:ND2	2.40	0.69
1:D:261:LYS:NZ	1:D:261:LYS:HB2	2.07	0.69
1:B:190:LEU:HD21	1:B:257:MET:HE3	1.73	0.69
1:A:162:PRO:HG2	1:A:165:GLU:CD	2.13	0.69
1:E:261:LYS:NZ	1:E:261:LYS:HB2	2.08	0.69
1:A:216:LYS:NZ	1:D:452:ASP:CB	2.55	0.69
1:F:413:THR:HG22	1:F:415:LEU:HD13	1.74	0.69
1:B:216:LYS:NZ	1:C:452:ASP:HB2	2.07	0.69
1:A:214:THR:HB	1:D:451:SER:OG	1.93	0.69
1:A:188:SER:OG	1:A:207:TYR:CE1	2.45	0.69
1:F:396:ASP:O	1:F:397:ILE:HD12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:LYS:O	1:H:151:ASP:HB2	1.93	0.68
1:E:275:TYR:CE2	1:E:303:VAL:HG23	2.29	0.68
1:E:184:HIS:CD2	1:E:186:GLY:H	2.11	0.68
1:B:214:THR:HB	1:C:451:SER:OG	1.94	0.68
1:C:91:LEU:HG	1:C:283:ASN:ND2	2.07	0.68
1:G:91:LEU:HG	1:G:283:ASN:ND2	2.07	0.68
1:B:411:VAL:CG1	1:B:418:ILE:HG23	2.24	0.68
1:A:360:VAL:HG13	1:A:383:TRP:HB2	1.73	0.68
1:B:89:SER:OG	1:B:417:CYS:HA	1.94	0.68
1:D:97:TRP:HD1	1:D:395:GLN:NE2	1.91	0.68
1:H:360:VAL:HG11	1:H:383:TRP:HE3	1.59	0.68
1:F:91:LEU:HG	1:F:283:ASN:ND2	2.06	0.68
1:D:413:THR:HG22	1:D:415:LEU:HD13	1.75	0.68
1:A:184:HIS:HD2	1:A:186:GLY:H	1.40	0.68
1:F:192:ILE:HG12	1:F:205:LEU:HD22	1.74	0.67
1:C:184:HIS:HD2	1:C:186:GLY:H	1.42	0.67
1:E:386:THR:HG22	1:E:386:THR:O	1.94	0.67
1:G:333:GLY:H	1:G:386:THR:HG23	1.60	0.67
1:D:412:GLN:CD	1:D:419:ARG:HD2	2.15	0.67
1:C:413:THR:CG2	1:C:415:LEU:HD13	2.23	0.67
1:E:216:LYS:NZ	1:H:452:ASP:HB2	2.08	0.67
1:A:452:ASP:CB	1:C:216:LYS:NZ	2.58	0.67
1:F:406:TYR:HB2	1:F:425:GLU:OE1	1.94	0.67
1:C:147:GLY:HA2	1:C:430:ARG:HH12	1.59	0.67
1:F:448:GLY:O	1:F:449:VAL:HB	1.95	0.67
1:D:85:LEU:CD1	1:D:412(C):GLU:HG3	2.24	0.67
1:A:463:GLU:H	1:C:144:HIS:HE1	1.43	0.67
1:F:249:GLN:NE2	1:F:272:ASN:H	1.93	0.67
1:F:249:GLN:HE21	1:F:272:ASN:H	1.43	0.67
1:F:454:VAL:HG11	1:H:200:GLY:O	1.95	0.67
1:B:162:PRO:HG2	1:B:165:GLU:CD	2.15	0.67
1:D:147:GLY:HA2	1:D:430:ARG:HH12	1.59	0.67
1:A:413:THR:CG2	1:A:415:LEU:HD22	2.20	0.66
1:E:452:ASP:CB	1:G:216:LYS:NZ	2.58	0.66
1:C:145:SER:O	1:C:146:ASN:O	2.13	0.66
1:A:88:ASN:HD22	1:A:88:ASN:H	1.44	0.66
1:H:88:ASN:N	1:H:88:ASN:HD22	1.93	0.66
1:H:249:GLN:HE21	1:H:272:ASN:H	1.42	0.66
1:D:190:LEU:HD21	1:D:257:MET:HE3	1.77	0.66
1:A:91:LEU:HG	1:A:283:ASN:ND2	2.08	0.66
1:B:145:SER:O	1:B:146:ASN:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:SER:CB	1:D:214:THR:HB	2.25	0.66
1:H:386:THR:O	1:H:386:THR:HG22	1.95	0.66
1:H:88:ASN:H	1:H:88:ASN:ND2	1.92	0.66
1:E:360:VAL:HG11	1:E:383:TRP:HE3	1.59	0.66
1:C:360:VAL:HG11	1:C:383:TRP:HE3	1.60	0.66
1:D:275:TYR:CE2	1:D:303:VAL:HG22	2.31	0.66
1:C:142:ASP:O	1:C:145:SER:HB3	1.96	0.66
1:F:464:LEU:HB3	1:F:465:PRO:HA	1.78	0.66
1:G:287:ILE:N	1:G:287:ILE:HD12	2.12	0.65
1:H:184:HIS:HD2	1:H:186:GLY:H	1.44	0.65
1:E:451:SER:OG	1:G:214:THR:HB	1.96	0.65
1:B:216:LYS:NZ	1:C:452:ASP:CB	2.60	0.65
1:C:360:VAL:CG1	1:C:383:TRP:HE3	2.10	0.65
1:D:397:ILE:HG22	1:D:398:VAL:HG23	1.78	0.65
1:C:116:VAL:HG12	1:C:138:ALA:O	1.96	0.65
1:G:184:HIS:HD2	1:G:186:GLY:H	1.45	0.65
1:B:216:LYS:HZ1	1:C:452:ASP:HB2	1.61	0.64
1:H:413:THR:HG22	1:H:415:LEU:HD13	1.79	0.64
1:F:85:LEU:HD13	1:F:186:GLY:HA2	1.79	0.64
1:B:261:LYS:HB2	1:B:261:LYS:NZ	2.12	0.64
1:G:89:SER:OG	1:G:417:CYS:HA	1.98	0.64
1:G:411:VAL:HG12	1:G:412:GLN:N	2.12	0.64
1:E:270:ALA:HB1	1:E:273:TYR:HB2	1.80	0.64
1:F:84:LYS:HD2	1:F:84:LYS:H	1.62	0.64
1:E:451:SER:CB	1:G:214:THR:HB	2.27	0.64
1:B:85:LEU:CD1	1:B:412(C):GLU:HG3	2.28	0.64
1:C:412:GLN:NE2	1:C:447:CYS:SG	2.71	0.64
1:F:451:SER:CB	1:H:214:THR:HB	2.27	0.64
1:F:466:PHE:C	1:F:468:ILE:N	2.49	0.64
1:D:146:ASN:O	1:D:148:THR:N	2.28	0.64
1:A:448:GLY:O	1:A:449:VAL:HB	1.96	0.64
1:H:411:VAL:HG12	1:H:412:GLN:N	2.12	0.64
1:B:360:VAL:CG1	1:B:383:TRP:HE3	2.11	0.64
1:D:360:VAL:CG1	1:D:383:TRP:HE3	2.09	0.64
1:B:144:HIS:CE1	1:C:463:GLU:H	2.15	0.63
1:A:145:SER:O	1:A:146:ASN:O	2.16	0.63
1:D:202:VAL:HG23	1:D:214:THR:HG23	1.80	0.63
1:E:413:THR:HG22	1:E:415:LEU:HD13	1.80	0.63
1:C:360:VAL:HG13	1:C:383:TRP:HB2	1.79	0.63
1:F:116:VAL:HG13	1:F:136:GLN:HB2	1.79	0.63
1:A:88:ASN:HD22	1:A:88:ASN:N	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:GLU:HG3	1:G:143:LYS:NZ	2.14	0.63
1:C:85:LEU:HD12	1:C:412(C):GLU:HG3	1.80	0.63
1:G:184:HIS:CD2	1:G:186:GLY:H	2.16	0.63
1:G:375:GLU:OE1	1:G:394:LYS:HE3	1.98	0.63
1:F:147:GLY:HA2	1:F:430:ARG:HH12	1.63	0.62
1:D:366:LYS:HD3	1:D:400:ILE:HG12	1.81	0.62
1:E:142:ASP:O	1:E:145:SER:HB3	1.99	0.62
1:B:452:ASP:CB	1:D:216:LYS:NZ	2.62	0.62
1:F:451:SER:OG	1:H:214:THR:HB	1.99	0.62
1:E:452:ASP:HB3	1:G:216:LYS:HD3	1.80	0.62
1:G:150:LYS:O	1:G:151:ASP:HB2	1.98	0.62
1:B:249:GLN:NE2	1:B:272:ASN:N	2.47	0.62
1:E:172:ARG:HD2	1:E:174:GLU:OE1	2.00	0.62
1:G:463:GLU:O	1:G:463:GLU:HG3	1.97	0.62
1:E:360:VAL:HG13	1:E:383:TRP:HB2	1.82	0.62
1:D:358:ASN:C	1:D:381:ASN:HA	2.20	0.62
1:G:360:VAL:HG11	1:G:383:TRP:HE3	1.63	0.62
1:F:327:ARG:O	1:F:368:THR:HG21	1.90	0.62
1:C:184:HIS:CD2	1:C:186:GLY:H	2.17	0.62
1:H:327:ARG:O	1:H:368:THR:HG23	1.89	0.62
1:C:412:GLN:NE2	1:C:421:CYS:SG	2.73	0.62
1:B:214:THR:HB	1:C:451:SER:CB	2.30	0.62
1:H:322:PHE:CD1	1:H:328:PRO:HG2	2.35	0.62
1:D:411:VAL:CG1	1:D:418:ILE:HG23	2.30	0.62
1:H:184:HIS:CD2	1:H:186:GLY:H	2.18	0.62
1:A:454:VAL:HG11	1:C:200:GLY:O	2.00	0.61
1:G:229:GLU:OE1	1:G:410:PHE:HA	2.00	0.61
1:F:412:GLN:NE2	1:F:421:CYS:SG	2.72	0.61
1:A:411:VAL:CG1	1:A:412:GLN:N	2.63	0.61
1:E:411:VAL:HG13	1:E:418:ILE:HG23	1.81	0.61
1:C:396:ASP:O	1:C:397:ILE:HD12	2.00	0.61
1:B:91:LEU:H	1:B:283:ASN:ND2	1.99	0.61
1:C:411:VAL:HG12	1:C:412:GLN:N	2.15	0.61
1:E:202:VAL:HG23	1:E:214:THR:HG23	1.82	0.61
1:H:360:VAL:HG13	1:H:383:TRP:HB2	1.81	0.61
1:C:397:ILE:HG22	1:C:398:VAL:HG23	1.82	0.61
1:F:360:VAL:CG1	1:F:383:TRP:HE3	2.12	0.61
1:B:97:TRP:H	1:B:395:GLN:HE22	1.48	0.61
1:B:249:GLN:HE21	1:B:272:ASN:N	1.94	0.61
1:G:411:VAL:CG1	1:G:412:GLN:N	2.64	0.61
1:D:287:ILE:HD12	1:D:287:ILE:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:ILE:HG22	1:F:398:VAL:HG23	1.82	0.61
1:A:97:TRP:H	1:A:395:GLN:HE22	1.48	0.61
1:B:452:ASP:HB3	1:D:216:LYS:HD3	1.83	0.61
1:A:287:ILE:N	1:A:287:ILE:HD12	2.15	0.61
1:E:413:THR:CG2	1:E:415:LEU:HD22	2.25	0.61
1:B:216:LYS:HZ2	1:C:452:ASP:CB	2.14	0.61
1:G:360:VAL:CG1	1:G:383:TRP:HE3	2.13	0.60
1:E:266:VAL:HG23	1:E:310:LEU:HD23	1.81	0.60
1:H:316:TYR:HB2	1:H:336:CYS:O	2.01	0.60
1:H:411:VAL:CG1	1:H:412:GLN:N	2.64	0.60
1:H:89:SER:HG	1:H:417:CYS:HA	1.66	0.60
1:B:156:ARG:HG2	1:B:178:TRP:HA	1.82	0.60
1:B:136:GLN:HG3	1:B:148:THR:HB	1.83	0.60
1:E:97:TRP:N	1:E:395:GLN:HE22	1.97	0.60
1:B:216:LYS:HZ2	1:C:452:ASP:HB3	1.64	0.60
1:F:373:GLY:HA2	1:F:398:VAL:HG12	1.84	0.60
1:F:287:ILE:HD12	1:F:287:ILE:N	2.16	0.60
1:H:360:VAL:CG1	1:H:383:TRP:HE3	2.15	0.60
1:E:360:VAL:CG1	1:E:383:TRP:HE3	2.14	0.60
1:E:261:LYS:HB2	1:E:261:LYS:HZ3	1.67	0.60
1:F:396:ASP:C	1:F:397:ILE:HD12	2.22	0.60
1:D:102:LYS:HG3	1:D:444:ILE:HG22	1.84	0.60
1:H:88:ASN:HD22	1:H:88:ASN:H	1.45	0.60
1:A:360:VAL:HG11	1:A:383:TRP:HE3	1.65	0.60
1:F:102:LYS:HG3	1:F:444:ILE:HG22	1.82	0.60
1:C:162:PRO:HG2	1:C:165:GLU:CD	2.22	0.60
1:C:277:GLU:HB3	1:C:350:LYS:HD2	1.84	0.60
1:E:88:ASN:HD22	1:E:88:ASN:H	1.50	0.60
1:H:229:GLU:OE1	1:H:410:PHE:HA	2.01	0.60
1:H:366:LYS:HD3	1:H:400:ILE:HG12	1.83	0.60
1:H:327:ARG:C	1:H:368:THR:CG2	2.66	0.59
1:E:249:GLN:HG2	1:E:295:TRP:CH2	2.37	0.59
1:F:451:SER:HB2	1:H:214:THR:HB	1.83	0.59
1:E:463:GLU:H	1:G:144:HIS:CE1	2.18	0.59
1:B:411:VAL:HG11	1:B:418:ILE:HG23	1.84	0.59
1:D:158:LEU:HD22	1:D:180:ALA:HB1	1.83	0.59
1:A:102:LYS:HZ2	1:A:104:ASN:HD21	1.48	0.59
1:H:322:PHE:HB2	1:H:327:ARG:HD2	1.84	0.59
1:H:88:ASN:O	1:H:284:ALA:HA	2.02	0.59
1:E:188:SER:OG	1:E:207:TYR:CE1	2.54	0.59
1:A:164:GLY:HA3	1:C:173:PHE:CG	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:PRO:HG2	1:F:165:GLU:CD	2.22	0.59
1:A:149:VAL:HG22	1:A:439:THR:OG1	2.02	0.59
1:H:109:GLY:HA3	1:H:140:LEU:HD12	1.84	0.59
1:B:411:VAL:CG1	1:B:412:GLN:N	2.65	0.59
1:H:97:TRP:HD1	1:H:395:GLN:NE2	2.00	0.59
1:E:88:ASN:ND2	1:E:88:ASN:H	2.01	0.59
1:A:229:GLU:OE1	1:A:410:PHE:HA	2.03	0.59
1:A:207:TYR:O	1:A:210:ILE:HG12	2.03	0.59
1:G:411:VAL:CG1	1:G:418:ILE:HG23	2.31	0.59
1:F:466:PHE:O	1:F:468:ILE:N	2.36	0.59
1:F:188:SER:OG	1:F:207:TYR:CZ	2.56	0.59
1:D:162:PRO:HG2	1:D:165:GLU:CD	2.22	0.59
1:F:411:VAL:CG1	1:F:412:GLN:N	2.65	0.59
1:G:145:SER:O	1:G:146:ASN:O	2.21	0.59
1:A:366:LYS:HD2	1:A:398:VAL:O	2.03	0.59
1:E:412:GLN:OE1	1:E:419:ARG:HD2	2.03	0.58
1:A:249:GLN:HE21	1:A:272:ASN:H	1.51	0.58
1:B:430:ARG:HD2	1:B:436:THR:O	2.02	0.58
1:G:327:ARG:HG3	1:G:368:THR:HG23	1.84	0.58
1:A:411:VAL:HG12	1:A:412:GLN:H	1.67	0.58
1:G:149:VAL:HG22	1:G:439:THR:OG1	2.03	0.58
1:E:411:VAL:CG1	1:E:418:ILE:HG23	2.33	0.58
1:E:466:PHE:C	1:E:468:ILE:N	2.56	0.58
1:H:145:SER:O	1:H:146:ASN:O	2.22	0.58
1:G:107:ARG:HD2	1:G:461:GLY:HA3	1.85	0.58
1:H:102:LYS:HG3	1:H:444:ILE:HG22	1.86	0.58
1:G:413:THR:CG2	1:G:415:LEU:HD22	2.29	0.58
1:E:146:ASN:ND2	1:E:437:ILE:HB	2.19	0.58
1:D:91:LEU:HG	1:D:283:ASN:HD22	1.69	0.58
1:E:207:TYR:O	1:E:210:ILE:HG12	2.04	0.58
1:B:130:ARG:HG2	1:B:130:ARG:HH21	1.69	0.58
1:A:200:GLY:O	1:D:454:VAL:HG11	2.03	0.58
1:E:451:SER:HB2	1:G:214:THR:HB	1.86	0.58
1:E:411:VAL:CG1	1:E:412:GLN:N	2.65	0.58
1:A:368:THR:HG22	1:A:368:THR:O	2.02	0.58
1:E:249:GLN:HE21	1:E:272:ASN:N	1.95	0.58
1:C:467:THR:O	1:C:468:ILE:HB	2.03	0.58
1:G:249:GLN:HE21	1:G:272:ASN:H	1.48	0.58
1:F:327:ARG:C	1:F:368:THR:HG23	2.23	0.58
1:C:316:TYR:CZ	1:C:340:PRO:HG3	2.39	0.58
1:A:116:VAL:HG23	1:A:440:SER:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:TYR:HB2	1:C:336:CYS:O	2.04	0.57
1:A:270:ALA:HB1	1:A:273:TYR:HB2	1.84	0.57
1:B:228:SER:HB3	1:B:350:LYS:CE	2.33	0.57
1:E:226:GLN:HE22	1:E:230:CYS:HA	1.68	0.57
1:E:332:THR:HG23	1:E:386:THR:HG22	1.87	0.57
1:E:466:PHE:C	1:E:468:ILE:H	2.07	0.57
1:G:322:PHE:HB2	1:G:327:ARG:HD2	1.86	0.57
1:H:188:SER:OG	1:H:207:TYR:CE2	2.57	0.57
1:F:228:SER:HB3	1:F:350:LYS:CE	2.34	0.57
1:G:466:PHE:C	1:G:468:ILE:H	2.06	0.57
1:A:116:VAL:HG12	1:A:138:ALA:O	2.05	0.57
1:H:146:ASN:ND2	1:H:437:ILE:HB	2.19	0.57
1:E:381:ASN:O	1:E:385:GLU:HB2	2.04	0.57
1:H:290:VAL:HG21	1:H:353:SER:HB2	1.87	0.57
1:G:91:LEU:H	1:G:283:ASN:ND2	2.02	0.57
1:H:84:LYS:HD2	1:H:84:LYS:N	2.20	0.57
1:F:463:GLU:O	1:F:463:GLU:HG3	2.03	0.57
1:D:249:GLN:HE21	1:D:272:ASN:H	1.50	0.57
1:F:151:ASP:O	1:F:156:ARG:NH2	2.38	0.57
1:G:118:ARG:HB3	1:G:119:GLU:CD	2.25	0.57
1:B:282:PRO:HD2	1:B:411:VAL:HG21	1.87	0.57
1:E:84:LYS:HD2	1:E:84:LYS:H	1.70	0.57
1:B:192:ILE:HD11	1:B:257:MET:HE3	1.87	0.56
1:A:146:ASN:O	1:A:148:THR:N	2.32	0.56
1:H:84:LYS:HD2	1:H:84:LYS:H	1.69	0.56
1:C:411:VAL:CG1	1:C:418:ILE:HG23	2.36	0.56
1:D:184:HIS:CD2	1:D:186:GLY:H	2.24	0.56
1:H:224:ARG:NE	1:H:276:GLU:OE1	2.34	0.56
1:C:266:VAL:HG23	1:C:310:LEU:HD23	1.87	0.56
1:E:248:GLY:HA2	1:E:295:TRP:CD1	2.40	0.56
1:C:282:PRO:HD2	1:C:411:VAL:HG21	1.87	0.56
1:C:146:ASN:O	1:C:148:THR:N	2.37	0.56
1:E:88:ASN:HD22	1:E:88:ASN:N	2.01	0.56
1:G:466:PHE:C	1:G:468:ILE:N	2.57	0.56
1:F:306:ASN:CG	1:F:308:GLN:N	2.58	0.56
1:B:467:THR:O	1:B:468:ILE:HB	2.05	0.56
1:F:123:SER:HB2	1:F:229:GLU:HB3	1.87	0.56
1:H:142:ASP:O	1:H:145:SER:HB3	2.04	0.56
1:G:467:THR:O	1:G:468:ILE:HB	2.04	0.56
1:B:466:PHE:C	1:B:468:ILE:N	2.59	0.56
1:H:249:GLN:HE21	1:H:272:ASN:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLU:C	1:A:287:ILE:HD12	2.26	0.56
1:H:162:PRO:HG2	1:H:165:GLU:CD	2.26	0.56
1:F:275:TYR:CE2	1:F:303:VAL:HG23	2.41	0.56
1:F:216:LYS:NZ	1:G:452:ASP:CB	2.69	0.56
1:F:89:SER:OG	1:F:417:CYS:HA	2.05	0.56
1:A:333:GLY:N	1:A:386:THR:HG23	2.20	0.56
1:H:301:PRO:HB3	1:H:316:TYR:CZ	2.41	0.56
1:G:188:SER:OG	1:G:207:TYR:CE1	2.59	0.56
1:F:85:LEU:HD13	1:F:186:GLY:CA	2.35	0.56
1:D:118:ARG:HB2	1:D:156:ARG:HH12	1.71	0.56
1:C:333:GLY:N	1:C:386:THR:HG23	2.21	0.56
1:A:360:VAL:CG1	1:A:383:TRP:HB2	2.36	0.56
1:G:275:TYR:CE2	1:G:303:VAL:HG22	2.41	0.56
1:H:322:PHE:CE1	1:H:328:PRO:HG2	2.41	0.55
1:E:146:ASN:O	1:E:148:THR:N	2.33	0.55
1:G:116:VAL:HG23	1:G:440:SER:HB2	1.88	0.55
1:G:191:THR:OG1	1:G:206:LYS:HB2	2.06	0.55
1:G:327:ARG:C	1:G:368:THR:HG23	2.26	0.55
1:H:282:PRO:HD2	1:H:411:VAL:HG21	1.88	0.55
1:H:85:LEU:HD12	1:H:412(C):GLU:HG3	1.88	0.55
1:F:306:ASN:CG	1:F:308:GLN:H	2.08	0.55
1:B:333:GLY:H	1:B:386:THR:HG23	1.70	0.55
1:D:116:VAL:HG13	1:D:136:GLN:HB2	1.87	0.55
1:B:254:ILE:HD11	1:B:268:LEU:HD21	1.86	0.55
1:H:218:TRP:CD1	1:H:219:ARG:HG2	2.41	0.55
1:E:216:LYS:NZ	1:H:452:ASP:CB	2.69	0.55
1:C:412:GLN:OE1	1:C:419:ARG:HD2	2.06	0.55
1:F:452:ASP:CB	1:H:216:LYS:NZ	2.69	0.55
1:B:360:VAL:CG1	1:B:383:TRP:HB2	2.36	0.55
1:C:149:VAL:CG2	1:C:430:ARG:NH1	2.69	0.55
1:B:146:ASN:ND2	1:B:437:ILE:HB	2.22	0.55
1:B:466:PHE:C	1:B:468:ILE:H	2.10	0.55
1:E:144:HIS:CE1	1:H:463:GLU:H	2.16	0.55
1:E:396:ASP:O	1:E:397:ILE:HD12	2.06	0.55
1:F:146:ASN:O	1:F:437:ILE:O	2.25	0.55
1:B:360:VAL:HG11	1:B:383:TRP:HE3	1.70	0.55
1:B:147:GLY:HA2	1:B:430:ARG:HH12	1.71	0.55
1:D:306:ASN:CG	1:D:308:GLN:H	2.10	0.55
1:E:145:SER:O	1:E:146:ASN:O	2.23	0.55
1:F:188:SER:OG	1:F:207:TYR:CE1	2.60	0.55
1:B:229:GLU:OE1	1:B:410:PHE:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:430:ARG:HD2	1:H:436:THR:O	2.06	0.55
1:D:464:LEU:HB3	1:D:465:PRO:HA	1.88	0.55
1:H:406:TYR:HB2	1:H:425:GLU:OE1	2.06	0.54
1:G:381:ASN:HB3	1:G:385:GLU:CG	2.36	0.54
1:A:102:LYS:HZ2	1:A:104:ASN:ND2	2.04	0.54
1:H:91:LEU:HG	1:H:283:ASN:HD22	1.71	0.54
1:F:194:ILE:HG12	1:F:203:ALA:HB2	1.89	0.54
1:G:84:LYS:N	1:G:84:LYS:HD2	2.23	0.54
1:C:381:ASN:O	1:C:385:GLU:HB2	2.07	0.54
1:A:411:VAL:CG1	1:A:412:GLN:H	2.21	0.54
1:E:412:GLN:NE2	1:E:421:CYS:SG	2.80	0.54
1:D:116:VAL:HG12	1:D:138:ALA:O	2.08	0.54
1:H:275:TYR:CE2	1:H:303:VAL:CG2	2.89	0.54
1:B:464:LEU:HB3	1:B:465:PRO:HA	1.88	0.54
1:H:202:VAL:HG23	1:H:214:THR:HG23	1.90	0.54
1:G:333:GLY:N	1:G:386:THR:HG23	2.22	0.54
1:D:172:ARG:HD2	1:D:174:GLU:OE1	2.08	0.54
1:D:191:THR:OG1	1:D:206:LYS:HB2	2.08	0.54
1:C:355:LYS:NZ	1:C:357:GLY:O	2.38	0.54
1:G:355:LYS:HD2	1:G:383:TRP:CE2	2.42	0.54
1:G:84:LYS:HD2	1:G:84:LYS:H	1.73	0.54
1:C:375:GLU:OE1	1:C:394:LYS:HE3	2.06	0.54
1:E:254:ILE:HD11	1:E:268:LEU:HD21	1.88	0.54
1:F:261:LYS:HB2	1:F:261:LYS:NZ	2.23	0.54
1:D:84:LYS:HD2	1:D:84:LYS:N	2.22	0.54
1:H:261:LYS:NZ	1:H:261:LYS:HB2	2.23	0.54
1:D:254:ILE:HD13	1:D:305:PHE:CD2	2.43	0.54
1:H:411:VAL:CG1	1:H:418:ILE:HG23	2.38	0.54
1:F:144:HIS:HE1	1:G:463:GLU:H	1.55	0.54
1:C:332:THR:HG23	1:C:386:THR:CG2	2.36	0.54
1:A:358:ASN:O	1:A:381:ASN:HA	2.07	0.54
1:B:164:GLY:HA3	1:D:173:PHE:CG	2.43	0.54
1:C:274:HIS:HB2	1:C:295:TRP:HE3	1.73	0.54
1:B:248:GLY:HA2	1:B:295:TRP:CD2	2.42	0.54
1:H:421:CYS:HB3	1:H:446:PHE:O	2.08	0.54
1:E:452:ASP:HB2	1:G:216:LYS:HZ2	1.69	0.54
1:B:91:LEU:H	1:B:283:ASN:HD21	1.53	0.54
1:A:430:ARG:HD2	1:A:436:THR:O	2.08	0.54
1:A:360:VAL:CG1	1:A:383:TRP:HE3	2.22	0.53
1:A:96:GLY:O	1:A:448:GLY:O	2.26	0.53
1:F:360:VAL:HG13	1:F:383:TRP:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:ARG:HB2	1:E:156:ARG:NH1	2.23	0.53
1:D:466:PHE:C	1:D:468:ILE:N	2.61	0.53
1:F:411:VAL:HG11	1:F:418:ILE:HG23	1.90	0.53
1:G:156:ARG:HG2	1:G:178:TRP:HA	1.88	0.53
1:E:162:PRO:HG2	1:E:165:GLU:CD	2.28	0.53
1:B:275:TYR:CE2	1:B:303:VAL:HG23	2.44	0.53
1:B:413:THR:HG22	1:B:415:LEU:HD13	1.90	0.53
1:F:360:VAL:HG11	1:F:383:TRP:HE3	1.73	0.53
1:C:156:ARG:HG2	1:C:178:TRP:HA	1.91	0.53
1:C:84:LYS:N	1:C:84:LYS:HD2	2.24	0.53
1:A:88:ASN:H	1:A:88:ASN:ND2	2.05	0.53
1:H:464:LEU:HB3	1:H:465:PRO:HA	1.89	0.53
1:G:411:VAL:HG13	1:G:418:ILE:HG23	1.88	0.53
1:D:202:VAL:CG2	1:D:214:THR:HG23	2.39	0.53
1:D:142:ASP:O	1:D:145:SER:HB3	2.08	0.53
1:A:202:VAL:HG12	1:D:454:VAL:HG22	1.90	0.53
1:G:282:PRO:HD2	1:G:411:VAL:HG21	1.91	0.53
1:D:355:LYS:HD2	1:D:383:TRP:CE2	2.44	0.53
1:F:96:GLY:O	1:F:448:GLY:O	2.27	0.53
1:F:275:TYR:CE2	1:F:303:VAL:CG2	2.92	0.53
1:C:248:GLY:HA2	1:C:295:TRP:CG	2.44	0.53
1:D:322:PHE:HB2	1:D:327:ARG:HD2	1.90	0.53
1:D:147:GLY:C	1:D:149:VAL:H	2.11	0.53
1:G:151:ASP:O	1:G:156:ARG:NH2	2.41	0.53
1:C:248:GLY:HA2	1:C:295:TRP:CD1	2.44	0.53
1:C:226:GLN:HE22	1:C:230:CYS:HA	1.74	0.53
1:A:452:ASP:CB	1:C:216:LYS:HZ2	2.22	0.53
1:H:224:ARG:NH1	1:H:276:GLU:OE1	2.39	0.53
1:E:214:THR:HB	1:H:451:SER:CB	2.39	0.52
1:C:88:ASN:HD22	1:C:88:ASN:N	2.05	0.52
1:G:466:PHE:O	1:G:468:ILE:N	2.42	0.52
1:A:413:THR:HG21	1:A:415:LEU:CD2	2.23	0.52
1:A:85:LEU:HD13	1:A:186:GLY:HA2	1.91	0.52
1:D:396:ASP:C	1:D:397:ILE:HD12	2.29	0.52
1:A:266:VAL:HG23	1:A:310:LEU:HD23	1.90	0.52
1:D:282:PRO:HD2	1:D:411:VAL:HG21	1.91	0.52
1:F:411:VAL:HG13	1:F:418:ILE:HG23	1.92	0.52
1:E:462:ALA:HA	1:G:144:HIS:CE1	2.44	0.52
1:H:366:LYS:HD2	1:H:398:VAL:O	2.10	0.52
1:A:216:LYS:HD3	1:D:452:ASP:CB	2.38	0.52
1:B:149:VAL:HG22	1:B:439:THR:OG1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:VAL:HG13	1:C:136:GLN:HB2	1.92	0.52
1:C:303:VAL:HG13	1:C:314:ILE:HG22	1.91	0.52
1:D:218:TRP:CD1	1:D:219:ARG:HG2	2.45	0.52
1:B:216:LYS:HD3	1:C:452:ASP:HB3	1.91	0.52
1:E:118:ARG:HB2	1:E:156:ARG:HH12	1.73	0.52
1:D:411:VAL:HG12	1:D:412:GLN:N	2.24	0.52
1:H:88:ASN:HD22	1:H:89:SER:H	1.58	0.52
1:D:463:GLU:HG3	1:D:463:GLU:O	2.09	0.52
1:C:96:GLY:O	1:C:448:GLY:O	2.28	0.52
1:C:97:TRP:N	1:C:395:GLN:HE22	2.06	0.52
1:F:430:ARG:HD2	1:F:436:THR:O	2.09	0.52
1:A:146:ASN:ND2	1:A:437:ILE:HB	2.24	0.52
1:D:158:LEU:HD22	1:D:180:ALA:CB	2.40	0.52
1:F:162:PRO:HG2	1:F:165:GLU:OE2	2.10	0.52
1:D:162:PRO:HG2	1:D:165:GLU:OE2	2.10	0.52
1:H:156:ARG:HG2	1:H:178:TRP:HA	1.92	0.52
1:B:96:GLY:O	1:B:448:GLY:O	2.28	0.52
1:A:216:LYS:HZ2	1:D:452:ASP:CB	2.23	0.52
1:F:227:GLU:O	1:F:350:LYS:HE2	2.09	0.52
1:B:99:VAL:HG13	1:B:446:PHE:CE2	2.45	0.52
1:C:368:THR:O	1:C:368:THR:HG22	2.10	0.52
1:C:318:CYS:HA	1:C:335:SER:O	2.09	0.52
1:D:150:LYS:O	1:D:151:ASP:HB2	2.10	0.52
1:E:368:THR:O	1:E:368:THR:HG22	2.09	0.51
1:C:355:LYS:HD2	1:C:383:TRP:CE2	2.45	0.51
1:B:116:VAL:HG13	1:B:136:GLN:HB2	1.92	0.51
1:G:102:LYS:HZ2	1:G:104:ASN:HD21	1.57	0.51
1:G:97:TRP:H	1:G:395:GLN:HE22	1.58	0.51
1:G:333:GLY:H	1:G:386:THR:CG2	2.22	0.51
1:A:467:THR:O	1:A:468:ILE:HB	2.09	0.51
1:C:411:VAL:CG1	1:C:412:GLN:N	2.73	0.51
1:D:396:ASP:O	1:D:397:ILE:HD12	2.10	0.51
1:C:84:LYS:H	1:C:84:LYS:HD2	1.75	0.51
1:D:333:GLY:N	1:D:386:THR:HG23	2.25	0.51
1:A:252:TYR:OH	1:A:274:HIS:HA	2.10	0.51
1:H:96:GLY:O	1:H:448:GLY:O	2.28	0.51
1:H:227:GLU:OE1	1:H:227:GLU:HA	2.09	0.51
1:F:91:LEU:HA	1:F:418:ILE:O	2.10	0.51
1:B:355:LYS:NZ	1:B:357:GLY:O	2.41	0.51
1:H:466:PHE:C	1:H:468:ILE:N	2.62	0.51
1:E:214:THR:CG2	1:E:215:ILE:N	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:466:PHE:O	1:H:468:ILE:HG13	2.11	0.51
1:H:226:GLN:NE2	1:H:239:THR:OG1	2.44	0.51
1:C:322:PHE:HB2	1:C:327:ARG:HD2	1.93	0.51
1:F:216:LYS:HZ2	1:G:452:ASP:CB	2.24	0.51
1:G:97:TRP:HD1	1:G:395:GLN:NE2	2.09	0.51
1:G:126:HIS:HA	1:G:412(D):LEU:HB2	1.92	0.51
1:H:305:PHE:HB3	1:H:312:TYR:HB3	1.93	0.51
1:B:463:GLU:H	1:D:144:HIS:CE1	2.21	0.51
1:H:466:PHE:C	1:H:468:ILE:H	2.13	0.51
1:D:318:CYS:HA	1:D:335:SER:O	2.10	0.51
1:H:194:ILE:HG12	1:H:203:ALA:HB2	1.91	0.51
1:F:228:SER:HB3	1:F:350:LYS:HE2	1.92	0.51
1:H:113:ASP:O	1:H:169:PRO:HD2	2.11	0.51
1:F:411:VAL:CG1	1:F:412:GLN:H	2.24	0.51
1:B:224:ARG:NE	1:B:276:GLU:OE1	2.41	0.50
1:B:144:HIS:HE1	1:C:463:GLU:N	2.03	0.50
1:B:287:ILE:CD1	1:B:287:ILE:N	2.73	0.50
1:B:411:VAL:CG1	1:B:412:GLN:H	2.24	0.50
1:D:261:LYS:HB2	1:D:261:LYS:HZ2	1.74	0.50
1:D:467:THR:O	1:D:468:ILE:HB	2.12	0.50
1:E:452:ASP:CB	1:G:216:LYS:HD3	2.41	0.50
1:E:411:VAL:CG1	1:E:412:GLN:H	2.24	0.50
1:B:214:THR:HB	1:C:451:SER:HB2	1.94	0.50
1:E:306:ASN:CG	1:E:308:GLN:N	2.65	0.50
1:F:298:SER:OG	1:F:344:SER:O	2.29	0.50
1:B:248:GLY:O	1:B:249:GLN:C	2.48	0.50
1:G:381:ASN:O	1:G:385:GLU:CG	2.57	0.50
1:B:192:ILE:HD11	1:B:257:MET:CE	2.40	0.50
1:H:355:LYS:HD2	1:H:383:TRP:CD2	2.46	0.50
1:B:228:SER:HB3	1:B:350:LYS:NZ	2.26	0.50
1:C:121:PHE:CG	1:C:228:SER:HA	2.47	0.50
1:A:327:ARG:CG	1:A:368:THR:HG23	2.40	0.50
1:A:355:LYS:HD2	1:A:383:TRP:CE2	2.47	0.50
1:A:97:TRP:N	1:A:395:GLN:HE22	2.09	0.50
1:D:411:VAL:HG11	1:D:418:ILE:HG23	1.93	0.50
1:D:117:ILE:O	1:D:440:SER:HA	2.11	0.50
1:G:355:LYS:NZ	1:G:357:GLY:O	2.42	0.50
1:B:355:LYS:HB2	1:B:383:TRP:CE3	2.47	0.50
1:H:228:SER:HB3	1:H:350:LYS:CE	2.42	0.50
1:D:466:PHE:C	1:D:468:ILE:H	2.13	0.49
1:A:365:THR:HA	1:A:373:GLY:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:238:PHE:N	1:G:238:PHE:CD1	2.80	0.49
1:F:411:VAL:CG1	1:F:418:ILE:CG2	2.89	0.49
1:H:146:ASN:O	1:H:437:ILE:O	2.30	0.49
1:F:176:VAL:O	1:F:177:ALA:HB2	2.11	0.49
1:G:224:ARG:NE	1:G:276:GLU:OE1	2.42	0.49
1:G:464:LEU:HB3	1:G:465:PRO:HA	1.94	0.49
1:H:188:SER:OG	1:H:207:TYR:CE1	2.63	0.49
1:F:144:HIS:CE1	1:G:462:ALA:HA	2.47	0.49
1:F:273:TYR:CD2	1:F:316:TYR:HE1	2.29	0.49
1:G:322:PHE:CE1	1:G:328:PRO:HG2	2.47	0.49
1:D:184:HIS:HD2	1:D:186:GLY:H	1.60	0.49
1:D:290:VAL:HG11	1:D:353:SER:HB2	1.94	0.49
1:F:380:PRO:O	1:F:381:ASN:C	2.49	0.49
1:B:228:SER:HB3	1:B:350:LYS:HE2	1.93	0.49
1:E:184:HIS:HD2	1:E:186:GLY:N	2.06	0.49
1:H:248:GLY:HA2	1:H:295:TRP:CG	2.47	0.49
1:B:84:LYS:H	1:B:84:LYS:HD2	1.76	0.49
1:D:360:VAL:HG11	1:D:383:TRP:HE3	1.76	0.49
1:B:355:LYS:HD2	1:B:383:TRP:CE2	2.48	0.49
1:C:147:GLY:HA2	1:C:430:ARG:NH1	2.27	0.49
1:E:316:TYR:CZ	1:E:340:PRO:HG3	2.47	0.49
1:C:102:LYS:HZ2	1:C:104:ASN:HD21	1.60	0.49
1:C:102:LYS:NZ	1:C:104:ASN:ND2	2.60	0.49
1:C:366:LYS:HD2	1:C:398:VAL:O	2.13	0.49
1:D:286:GLU:C	1:D:287:ILE:HD12	2.33	0.49
1:B:88:ASN:N	1:B:88:ASN:HD22	2.10	0.49
1:D:327:ARG:HG3	1:D:368:THR:HG23	1.94	0.49
1:E:452:ASP:CB	1:G:216:LYS:HZ2	2.24	0.49
1:F:413:THR:CG2	1:F:415:LEU:HD22	2.39	0.49
1:D:188:SER:OG	1:D:207:TYR:CE2	2.65	0.49
1:B:146:ASN:HD22	1:B:437:ILE:HB	1.78	0.49
1:A:333:GLY:CA	1:A:386:THR:HG23	2.43	0.49
1:G:102:LYS:HZ2	1:G:104:ASN:ND2	2.11	0.49
1:E:287:ILE:N	1:E:287:ILE:HD12	2.28	0.49
1:F:366:LYS:HD3	1:F:400:ILE:HG12	1.95	0.48
1:D:121:PHE:CG	1:D:228:SER:HA	2.48	0.48
1:B:130:ARG:NH2	1:B:130:ARG:HG2	2.27	0.48
1:D:386:THR:O	1:D:386:THR:HG22	2.14	0.48
1:B:309:ASN:O	1:B:310:LEU:HB2	2.12	0.48
1:D:88:ASN:HD22	1:D:88:ASN:H	1.61	0.48
1:D:203:ALA:HB3	1:D:215:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:PHE:C	1:C:468:ILE:N	2.67	0.48
1:C:386:THR:HG22	1:C:386:THR:O	2.12	0.48
1:D:192:ILE:HD11	1:D:257:MET:HE1	1.94	0.48
1:C:430:ARG:HD2	1:C:436:THR:O	2.13	0.48
1:B:106:ILE:HD12	1:B:460:ASP:OD2	2.14	0.48
1:D:229:GLU:OE1	1:D:410:PHE:HA	2.12	0.48
1:B:375:GLU:OE1	1:B:394:LYS:HE3	2.14	0.48
1:A:84:LYS:H	1:A:84:LYS:HD2	1.79	0.48
1:G:430:ARG:HD2	1:G:436:THR:O	2.13	0.48
1:G:97:TRP:N	1:G:395:GLN:HE22	2.11	0.48
1:H:325:ASN:O	1:H:348:GLY:HA2	2.13	0.48
1:C:207:TYR:O	1:C:210:ILE:HG12	2.14	0.48
1:G:413:THR:CG2	1:G:415:LEU:HD13	2.37	0.48
1:E:366:LYS:HD2	1:E:398:VAL:O	2.13	0.48
1:F:97:TRP:N	1:F:395:GLN:HE22	2.07	0.48
1:C:224:ARG:NE	1:C:276:GLU:OE1	2.42	0.48
1:G:88:ASN:HD22	1:G:88:ASN:N	2.11	0.48
1:F:322:PHE:HB2	1:F:327:ARG:HD2	1.94	0.48
1:E:248:GLY:HA2	1:E:295:TRP:CG	2.49	0.48
1:G:222:ILE:O	1:G:224:ARG:NH2	2.44	0.48
1:G:254:ILE:HD11	1:G:268:LEU:HD21	1.94	0.48
1:A:183:CYS:HB3	1:A:230:CYS:O	2.14	0.48
1:D:97:TRP:HD1	1:D:395:GLN:HE22	1.58	0.48
1:D:147:GLY:O	1:D:149:VAL:N	2.42	0.48
1:E:305:PHE:HB3	1:E:312:TYR:HB3	1.96	0.48
1:H:375:GLU:OE1	1:H:394:LYS:HE3	2.13	0.48
1:D:91:LEU:HA	1:D:418:ILE:O	2.14	0.48
1:F:249:GLN:HE21	1:F:272:ASN:N	2.09	0.48
1:D:84:LYS:HD2	1:D:84:LYS:H	1.79	0.48
1:B:421:CYS:HB3	1:B:446:PHE:O	2.13	0.48
1:B:392:VAL:HG12	1:B:394:LYS:N	2.28	0.48
1:B:297:GLY:C	1:B:345(A):GLY:HA3	2.34	0.48
1:E:327:ARG:O	1:E:368:THR:HG21	2.01	0.47
1:B:452:ASP:CB	1:D:216:LYS:HZ2	2.26	0.47
1:B:426:LEU:HD13	1:B:460:ASP:N	2.29	0.47
1:B:301:PRO:HB3	1:B:316:TYR:CZ	2.49	0.47
1:G:158:LEU:HD22	1:G:180:ALA:HB1	1.95	0.47
1:D:411:VAL:CG1	1:D:412:GLN:N	2.76	0.47
1:D:287:ILE:O	1:D:304:SER:HA	2.14	0.47
1:D:306:ASN:CG	1:D:308:GLN:N	2.67	0.47
1:A:224:ARG:NH1	1:A:276:GLU:OE1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:ALA:HB3	1:E:215:ILE:HB	1.96	0.47
1:A:466:PHE:C	1:A:468:ILE:N	2.66	0.47
1:A:224:ARG:NE	1:A:276:GLU:OE1	2.44	0.47
1:A:149:VAL:HG23	1:A:430:ARG:NH1	2.28	0.47
1:E:91:LEU:N	1:E:283:ASN:ND2	2.60	0.47
1:B:448:GLY:O	1:B:449:VAL:HB	2.13	0.47
1:D:99:VAL:HG13	1:D:446:PHE:CE2	2.50	0.47
1:G:118:ARG:HB2	1:G:156:ARG:NH1	2.29	0.47
1:E:158:LEU:O	1:E:174:GLU:HB2	2.15	0.47
1:B:116:VAL:HG12	1:B:138:ALA:O	2.15	0.47
1:A:380:PRO:O	1:A:381:ASN:C	2.53	0.47
1:F:136:GLN:O	1:G:107:ARG:NH1	2.43	0.47
1:D:254:ILE:CD1	1:D:268:LEU:HD21	2.45	0.47
1:F:316:TYR:CZ	1:F:340:PRO:HG3	2.50	0.47
1:F:327:ARG:C	1:F:368:THR:CG2	2.70	0.47
1:D:412:GLN:HB2	1:D:419:ARG:HB3	1.97	0.47
1:H:411:VAL:HG13	1:H:418:ILE:HG23	1.96	0.47
1:G:381:ASN:CB	1:G:385:GLU:HG3	2.38	0.47
1:C:332:THR:HG23	1:C:386:THR:HG22	1.97	0.47
1:A:316:TYR:CZ	1:A:340:PRO:HG3	2.50	0.47
1:D:96:GLY:O	1:D:448:GLY:O	2.33	0.47
1:D:320:GLY:HA3	1:D:331:GLY:O	2.15	0.47
1:G:301:PRO:HB3	1:G:316:TYR:CZ	2.50	0.47
1:E:448:GLY:O	1:E:449:VAL:HB	2.15	0.47
1:G:412(B):PRO:HB3	1:G:415:LEU:O	2.15	0.47
1:A:147:GLY:HA2	1:A:430:ARG:NH1	2.24	0.47
1:C:88:ASN:HD22	1:C:88:ASN:H	1.63	0.47
1:E:264:LYS:HG2	1:E:310:LEU:HD22	1.96	0.47
1:C:277:GLU:OE1	1:C:350:LYS:HB2	2.14	0.47
1:G:249:GLN:HE21	1:G:272:ASN:N	2.13	0.47
1:B:275:TYR:CE2	1:B:303:VAL:CG2	2.98	0.47
1:C:239:THR:CG2	1:C:257:MET:HE1	2.45	0.47
1:E:345:ASN:O	1:E:346:ALA:N	2.44	0.47
1:F:411:VAL:HG13	1:F:418:ILE:CG2	2.45	0.47
1:D:355:LYS:HB2	1:D:383:TRP:CZ3	2.50	0.47
1:F:249:GLN:NE2	1:F:272:ASN:N	2.60	0.47
1:A:234:ASN:CG	1:A:234:ASN:O	2.53	0.47
1:E:226:GLN:O	1:E:227:GLU:HB2	2.14	0.47
1:G:275:TYR:CE2	1:G:303:VAL:CG2	2.97	0.47
1:H:448:GLY:O	1:H:449:VAL:HB	2.14	0.47
1:H:295:TRP:O	1:H:346:ALA:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:THR:HG22	1:C:257:MET:CE	2.45	0.47
1:A:421:CYS:HB3	1:A:446:PHE:O	2.15	0.47
1:B:248:GLY:HA2	1:B:295:TRP:CG	2.49	0.46
1:E:91:LEU:HG	1:E:283:ASN:ND2	2.31	0.46
1:E:102:LYS:NZ	1:E:104:ASN:ND2	2.63	0.46
1:C:238:PHE:CD1	1:C:238:PHE:N	2.83	0.46
1:H:117:ILE:O	1:H:440:SER:HA	2.14	0.46
1:G:202:VAL:HG23	1:G:214:THR:HG23	1.97	0.46
1:F:156:ARG:HG2	1:F:178:TRP:HA	1.97	0.46
1:B:332:THR:HG23	1:B:386:THR:CG2	2.46	0.46
1:B:190:LEU:HD13	1:B:260:GLY:HA2	1.97	0.46
1:E:333:GLY:N	1:E:386:THR:HG23	2.30	0.46
1:E:146:ASN:HA	1:E:437:ILE:CD1	2.45	0.46
1:B:149:VAL:HG23	1:B:430:ARG:NH1	2.30	0.46
1:C:109:GLY:HA3	1:C:140:LEU:HD12	1.97	0.46
1:E:147:GLY:HA2	1:E:430:ARG:HH12	1.80	0.46
1:B:238:PHE:N	1:B:238:PHE:CD1	2.83	0.46
1:A:403:TRP:CZ3	1:A:432:LYS:HG3	2.50	0.46
1:E:413:THR:HA	1:G:210:ILE:HD12	1.97	0.46
1:F:85:LEU:HD12	1:F:412(C):GLU:HG3	1.97	0.46
1:G:359:GLY:HA2	1:G:382:GLY:H	1.81	0.46
1:E:406:TYR:HB2	1:E:425:GLU:OE1	2.15	0.46
1:D:248:GLY:HA2	1:D:295:TRP:CG	2.50	0.46
1:E:117:ILE:O	1:E:440:SER:HA	2.15	0.46
1:A:306:ASN:CG	1:A:308:GLN:N	2.69	0.46
1:H:412:GLN:HB2	1:H:419:ARG:HB3	1.98	0.46
1:E:274:HIS:HB2	1:E:295:TRP:HE3	1.81	0.46
1:D:85:LEU:HD13	1:D:186:GLY:HA2	1.98	0.46
1:E:421:CYS:HB3	1:E:446:PHE:O	2.16	0.46
1:H:275:TYR:CE2	1:H:303:VAL:HG23	2.51	0.46
1:G:270:ALA:HB1	1:G:273:TYR:HB2	1.98	0.46
1:C:249:GLN:NE2	1:C:272:ASN:H	2.14	0.46
1:A:194:ILE:HG12	1:A:203:ALA:HB2	1.97	0.46
1:H:306:ASN:CG	1:H:308:GLN:H	2.17	0.46
1:A:452:ASP:CB	1:C:216:LYS:HD3	2.41	0.46
1:F:149:VAL:HG22	1:F:439:THR:OG1	2.16	0.46
1:D:97:TRP:H	1:D:395:GLN:HE22	1.64	0.46
1:D:430:ARG:HD2	1:D:436:THR:O	2.15	0.46
1:G:224:ARG:NH1	1:G:276:GLU:OE1	2.45	0.46
1:E:96:GLY:O	1:E:448:GLY:O	2.33	0.46
1:A:173:PHE:CG	1:D:164:GLY:HA3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:VAL:CG2	1:H:214:THR:HG23	2.46	0.46
1:D:146:ASN:ND2	1:D:437:ILE:HB	2.31	0.46
1:E:146:ASN:HA	1:E:437:ILE:HD12	1.97	0.46
1:E:88:ASN:ND2	1:E:88:ASN:N	2.61	0.46
1:G:102:LYS:NZ	1:G:104:ASN:ND2	2.64	0.46
1:E:306:ASN:CG	1:E:308:GLN:H	2.19	0.46
1:A:306:ASN:CG	1:A:308:GLN:H	2.19	0.46
1:E:375:GLU:OE1	1:E:394:LYS:HE3	2.15	0.46
1:H:381:ASN:O	1:H:385:GLU:HB2	2.16	0.46
1:A:117:ILE:HG22	1:A:135:THR:HA	1.97	0.46
1:C:327:ARG:O	1:C:368:THR:HG21	2.05	0.46
1:H:332:THR:HG23	1:H:386:THR:HG21	1.98	0.46
1:H:85:LEU:HD13	1:H:186:GLY:CA	2.46	0.46
1:H:143:LYS:C	1:H:145:SER:H	2.17	0.46
1:H:118:ARG:NE	1:H:425:GLU:OE2	2.35	0.46
1:H:248:GLY:HA2	1:H:295:TRP:CD1	2.51	0.46
1:D:88:ASN:N	1:D:88:ASN:HD22	2.12	0.46
1:A:84:LYS:N	1:A:84:LYS:HD2	2.31	0.46
1:D:261:LYS:HZ3	1:D:261:LYS:HB2	1.78	0.46
1:B:146:ASN:O	1:B:437:ILE:O	2.34	0.46
1:E:466:PHE:O	1:E:468:ILE:N	2.49	0.46
1:A:202:VAL:CG1	1:D:454:VAL:HG22	2.45	0.46
1:B:88:ASN:H	1:B:88:ASN:ND2	2.14	0.46
1:G:182:ALA:HA	1:G:190:LEU:O	2.16	0.46
1:A:453:THR:O	1:A:454:VAL:HG13	2.16	0.46
1:E:467:THR:O	1:E:468:ILE:HB	2.16	0.46
1:G:248:GLY:HA2	1:G:295:TRP:CD1	2.51	0.46
1:H:156:ARG:HB3	1:H:177:ALA:O	2.15	0.46
1:H:306:ASN:CG	1:H:308:GLN:N	2.69	0.46
1:H:270:ALA:HB1	1:H:273:TYR:HB2	1.98	0.46
1:B:184:HIS:CD2	1:B:186:GLY:H	2.34	0.46
1:D:381:ASN:HD22	1:D:381:ASN:H	1.58	0.45
1:C:88:ASN:ND2	1:C:88:ASN:H	2.14	0.45
1:E:102:LYS:HZ2	1:E:104:ASN:HD21	1.64	0.45
1:E:102:LYS:HZ2	1:E:104:ASN:ND2	2.14	0.45
1:A:172:ARG:HD2	1:A:174:GLU:OE1	2.15	0.45
1:D:333:GLY:H	1:D:386:THR:HG23	1.82	0.45
1:A:226:GLN:HE22	1:A:230:CYS:HA	1.82	0.45
1:H:85:LEU:HD13	1:H:186:GLY:HA2	1.98	0.45
1:D:249:GLN:NE2	1:D:272:ASN:H	2.14	0.45
1:D:297:GLY:C	1:D:345(A):GLY:HA3	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:CYS:HB3	1:C:446:PHE:O	2.17	0.45
1:G:91:LEU:HA	1:G:418:ILE:O	2.17	0.45
1:F:184:HIS:CD2	1:F:186:GLY:H	2.34	0.45
1:B:226:GLN:HE22	1:B:230:CYS:HA	1.81	0.45
1:E:225:THR:OG1	1:E:226:GLN:N	2.49	0.45
1:D:433:GLU:CD	1:D:464:LEU:HD12	2.36	0.45
1:G:322:PHE:CD1	1:G:328:PRO:HG2	2.52	0.45
1:H:433:GLU:CD	1:H:464:LEU:HD12	2.36	0.45
1:C:275:TYR:CE2	1:C:303:VAL:HG22	2.51	0.45
1:D:290:VAL:HG21	1:D:353:SER:HB2	1.97	0.45
1:B:232:CYS:HA	1:B:237:CYS:HA	1.99	0.45
1:A:413:THR:HA	1:C:210:ILE:HD12	1.99	0.45
1:A:147:GLY:C	1:A:149:VAL:H	2.20	0.45
1:G:150:LYS:HE3	1:G:153:SER:HB3	1.98	0.45
1:C:102:LYS:HZ2	1:C:104:ASN:ND2	2.14	0.45
1:E:430:ARG:HD2	1:E:436:THR:O	2.17	0.45
1:B:102:LYS:HG3	1:B:444:ILE:HG22	1.99	0.45
1:D:276:GLU:O	1:D:292:ARG:HB3	2.17	0.45
1:A:452:ASP:CG	1:A:453:THR:H	2.20	0.45
1:F:145:SER:O	1:F:146:ASN:O	2.34	0.45
1:H:261:LYS:HZ3	1:H:261:LYS:HB2	1.82	0.45
1:A:248:GLY:HA2	1:A:295:TRP:CD1	2.51	0.45
1:E:297:GLY:C	1:E:345(A):GLY:HA3	2.37	0.45
1:F:239:THR:CG2	1:F:257:MET:HE1	2.47	0.45
1:A:97:TRP:N	1:A:453:THR:HG21	2.32	0.45
1:B:411:VAL:HG13	1:B:418:ILE:HG23	1.96	0.45
1:A:218:TRP:CE2	1:A:253:LYS:HE3	2.52	0.45
1:C:85:LEU:HD13	1:C:186:GLY:HA2	2.00	0.44
1:B:261:LYS:HB2	1:B:261:LYS:HZ2	1.80	0.44
1:A:102:LYS:NZ	1:A:104:ASN:ND2	2.65	0.44
1:H:248:GLY:HA2	1:H:295:TRP:CD2	2.52	0.44
1:A:254:ILE:HD13	1:A:305:PHE:CD2	2.52	0.44
1:C:428:ARG:HB3	1:C:464:LEU:HD11	1.97	0.44
1:A:89:SER:HG	1:A:417:CYS:HA	1.80	0.44
1:G:147:GLY:HA2	1:G:430:ARG:NH1	2.26	0.44
1:B:202:VAL:HG23	1:B:214:THR:HG23	1.98	0.44
1:H:91:LEU:HG	1:H:283:ASN:ND2	2.32	0.44
1:A:232:CYS:HA	1:A:237:CYS:HA	1.99	0.44
1:D:102:LYS:NZ	1:D:104:ASN:ND2	2.65	0.44
1:E:466:PHE:O	1:E:468:ILE:HG13	2.17	0.44
1:H:102:LYS:HZ2	1:H:104:ASN:HD21	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HA	1:B:446:PHE:CD2	2.52	0.44
1:H:412:GLN:NE2	1:H:421:CYS:SG	2.90	0.44
1:D:355:LYS:HB2	1:D:383:TRP:CE3	2.52	0.44
1:G:333:GLY:N	1:G:386:THR:CG2	2.81	0.44
1:A:287:ILE:O	1:A:304:SER:HA	2.17	0.44
1:E:216:LYS:HZ2	1:H:452:ASP:CB	2.30	0.44
1:G:248:GLY:HA2	1:G:295:TRP:CG	2.52	0.44
1:D:298:SER:OG	1:D:344:SER:O	2.33	0.44
1:F:88:ASN:HD22	1:F:88:ASN:N	2.14	0.44
1:D:146:ASN:HD22	1:D:437:ILE:HB	1.82	0.44
1:C:162:PRO:HG2	1:C:165:GLU:OE2	2.16	0.44
1:E:254:ILE:HD13	1:E:305:PHE:CD2	2.53	0.44
1:B:168:SER:OG	1:B:169:PRO:HD2	2.18	0.44
1:G:368:THR:HG22	1:G:368:THR:O	2.17	0.44
1:E:447:CYS:HB2	1:G:211:ILE:HD12	1.99	0.44
1:D:192:ILE:HG23	1:D:205:LEU:CD2	2.48	0.44
1:B:264:LYS:HG2	1:B:310:LEU:HD22	1.99	0.44
1:G:122:ILE:HG22	1:G:123:SER:N	2.31	0.44
1:G:192:ILE:HG23	1:G:205:LEU:CD2	2.48	0.44
1:G:375:GLU:OE2	1:G:377:ILE:HD11	2.17	0.44
1:E:147:GLY:C	1:E:149:VAL:H	2.21	0.44
1:F:321:VAL:HG13	1:F:364:ARG:NH2	2.33	0.44
1:G:119:GLU:HB2	1:G:134:LEU:HD12	2.00	0.44
1:B:144:HIS:CE1	1:C:462:ALA:HA	2.53	0.43
1:G:118:ARG:HB3	1:G:119:GLU:OE2	2.18	0.43
1:C:316:TYR:CE1	1:C:340:PRO:HG3	2.53	0.43
1:E:97:TRP:HD1	1:E:395:GLN:NE2	2.16	0.43
1:B:355:LYS:HB2	1:B:383:TRP:CZ3	2.53	0.43
1:E:333:GLY:C	1:E:386:THR:HG23	2.39	0.43
1:A:88:ASN:N	1:A:88:ASN:ND2	2.64	0.43
1:C:373:GLY:HA2	1:C:398:VAL:HG12	2.00	0.43
1:B:88:ASN:HD22	1:B:88:ASN:H	1.64	0.43
1:A:325:ASN:O	1:A:348:GLY:HA2	2.18	0.43
1:F:116:VAL:CG1	1:F:136:GLN:HB2	2.46	0.43
1:A:287:ILE:N	1:A:287:ILE:CD1	2.82	0.43
1:F:99:VAL:HG13	1:F:446:PHE:CE2	2.53	0.43
1:A:156:ARG:HG2	1:A:178:TRP:HA	1.99	0.43
1:G:113:ASP:O	1:G:169:PRO:HD2	2.18	0.43
1:D:264:LYS:HG2	1:D:310:LEU:HD22	1.99	0.43
1:C:248:GLY:HA2	1:C:295:TRP:CD2	2.54	0.43
1:F:381:ASN:O	1:F:385:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:PHE:CG	1:G:164:GLY:HA3	2.53	0.43
1:E:84:LYS:HD2	1:E:84:LYS:N	2.33	0.43
1:C:102:LYS:HG3	1:C:444:ILE:HG22	2.01	0.43
1:A:232:CYS:HA	1:A:236:SER:O	2.19	0.43
1:H:364:ARG:HG3	1:H:365:THR:O	2.17	0.43
1:E:412(B):PRO:HB3	1:E:415:LEU:O	2.18	0.43
1:F:192:ILE:HG23	1:F:205:LEU:CD2	2.49	0.43
1:C:222:ILE:O	1:C:224:ARG:NH2	2.50	0.43
1:A:421:CYS:HA	1:A:447:CYS:HA	2.00	0.43
1:B:133:PHE:CE1	1:B:159:MET:HB2	2.54	0.43
1:E:325:ASN:O	1:E:348:GLY:HA2	2.18	0.43
1:G:355:LYS:HD2	1:G:383:TRP:CD2	2.54	0.43
1:F:386:THR:O	1:F:387:ASP:HB3	2.18	0.43
1:A:451:SER:OG	1:C:214:THR:HB	2.19	0.43
1:B:396:ASP:O	1:B:397:ILE:HD12	2.18	0.43
1:E:446:PHE:N	1:E:446:PHE:CD1	2.86	0.43
1:E:463:GLU:N	1:G:144:HIS:HE1	2.07	0.43
1:F:437:ILE:HD13	1:F:468:ILE:HG23	2.00	0.43
1:C:146:ASN:O	1:C:437:ILE:O	2.36	0.43
1:G:250:ALA:HB3	1:G:252:TYR:CE2	2.52	0.43
1:A:169:PRO:HG2	1:A:169(A):TYR:CE2	2.53	0.43
1:F:426:LEU:HD13	1:F:460:ASP:N	2.34	0.43
1:D:411:VAL:HG13	1:D:418:ILE:HG23	2.00	0.43
1:A:91:LEU:HA	1:A:418:ILE:O	2.19	0.43
1:G:411:VAL:HG11	1:G:418:ILE:HG23	1.99	0.43
1:F:366:LYS:NZ	1:F:396:ASP:OD1	2.46	0.43
1:F:287:ILE:O	1:F:304:SER:HA	2.18	0.43
1:H:332:THR:HG23	1:H:386:THR:CG2	2.48	0.43
1:E:463:GLU:HG3	1:G:143:LYS:HZ1	1.84	0.43
1:B:332:THR:HG23	1:B:386:THR:HG22	2.00	0.43
1:G:249:GLN:HG2	1:G:295:TRP:CH2	2.54	0.43
1:A:162:PRO:HG2	1:A:165:GLU:OE2	2.17	0.42
1:F:116:VAL:HG12	1:F:138:ALA:O	2.19	0.42
1:A:466:PHE:C	1:A:468:ILE:H	2.22	0.42
1:H:266:VAL:HG23	1:H:310:LEU:HD23	2.00	0.42
1:F:106:ILE:HD13	1:F:428:ARG:HB2	2.01	0.42
1:C:287:ILE:HD12	1:C:287:ILE:N	2.34	0.42
1:D:364:ARG:O	1:D:374:PHE:HA	2.19	0.42
1:H:168:SER:OG	1:H:169:PRO:HD2	2.19	0.42
1:D:222:ILE:O	1:D:224:ARG:NH2	2.51	0.42
1:G:217:SER:HB2	1:G:223:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:THR:CG2	1:A:368:THR:O	2.66	0.42
1:E:396:ASP:C	1:E:397:ILE:HD12	2.39	0.42
1:E:85:LEU:CD1	1:E:412(C):GLU:HG3	2.44	0.42
1:G:287:ILE:N	1:G:287:ILE:CD1	2.81	0.42
1:F:248:GLY:HA2	1:F:295:TRP:CG	2.54	0.42
1:H:90:SER:O	1:H:417:CYS:HB2	2.19	0.42
1:F:146:ASN:HB3	1:F:147:GLY:H	1.69	0.42
1:G:249:GLN:NE2	1:G:272:ASN:H	2.16	0.42
1:C:332:THR:HG23	1:C:386:THR:HG21	2.01	0.42
1:D:88:ASN:ND2	1:D:88:ASN:H	2.17	0.42
1:D:245:PRO:C	1:D:247:ASN:H	2.17	0.42
1:C:294:ASN:O	1:C:346:ALA:O	2.37	0.42
1:C:88:ASN:ND2	1:C:88:ASN:N	2.67	0.42
1:B:216:LYS:NZ	1:C:452:ASP:HB3	2.28	0.42
1:E:355:LYS:HD2	1:E:383:TRP:CE2	2.54	0.42
1:H:368:THR:HG22	1:H:368:THR:O	2.18	0.42
1:B:368:THR:HG22	1:B:368:THR:O	2.19	0.42
1:G:412:GLN:OE1	1:G:419:ARG:HD2	2.19	0.42
1:C:433:GLU:CD	1:C:464:LEU:HD12	2.40	0.42
1:G:426:LEU:HD13	1:G:460:ASP:N	2.35	0.42
1:A:210:ILE:HD12	1:D:413:THR:HA	2.01	0.42
1:D:303:VAL:HG13	1:D:314:ILE:HG22	2.01	0.42
1:G:360:VAL:HG13	1:G:383:TRP:HB2	2.00	0.42
1:E:149:VAL:HG21	1:E:430:ARG:CZ	2.50	0.42
1:B:232:CYS:HA	1:B:236:SER:O	2.20	0.42
1:E:107:ARG:HD2	1:E:461:GLY:HA3	2.02	0.42
1:D:325:ASN:O	1:D:348:GLY:HA2	2.20	0.42
1:G:194:ILE:HG12	1:G:203:ALA:HB2	2.00	0.42
1:E:154:PRO:HG3	1:H:456:TRP:CH2	2.55	0.42
1:E:190:LEU:HD13	1:E:260:GLY:HA2	2.02	0.42
1:D:238:PHE:N	1:D:238:PHE:CD1	2.88	0.42
1:A:327:ARG:C	1:A:368:THR:HG23	2.34	0.42
1:C:91:LEU:HA	1:C:418:ILE:O	2.20	0.42
1:D:383:TRP:HD1	1:D:384:THR:HG23	1.84	0.42
1:B:162:PRO:HG2	1:B:165:GLU:OE2	2.19	0.42
1:E:164:GLY:HA3	1:G:173:PHE:CG	2.55	0.42
1:A:85:LEU:HD13	1:A:186:GLY:CA	2.50	0.42
1:F:412(B):PRO:HB3	1:F:415:LEU:O	2.20	0.42
1:C:88:ASN:HD22	1:C:89:SER:N	2.17	0.42
1:D:188:SER:OG	1:D:207:TYR:CE1	2.67	0.42
1:F:84:LYS:HD2	1:F:84:LYS:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:PHE:C	1:C:468:ILE:H	2.23	0.42
1:C:309:ASN:O	1:C:310:LEU:HB2	2.19	0.42
1:A:347:TYR:CG	1:A:348:GLY:N	2.87	0.42
1:E:101:SER:HA	1:G:173:PHE:CZ	2.55	0.42
1:B:322:PHE:HB2	1:B:327:ARG:HD2	2.02	0.41
1:C:143:LYS:C	1:C:145:SER:H	2.22	0.41
1:C:392:VAL:HG12	1:C:394:LYS:N	2.34	0.41
1:C:118:ARG:HB3	1:C:119:GLU:CD	2.41	0.41
1:D:448:GLY:O	1:D:449:VAL:HB	2.20	0.41
1:B:102:LYS:HZ2	1:B:104:ASN:HD21	1.68	0.41
1:A:354:PHE:CZ	1:A:409:SER:HB2	2.55	0.41
1:C:229:GLU:OE1	1:C:410:PHE:HA	2.20	0.41
1:F:305:PHE:HB3	1:F:312:TYR:HB3	2.02	0.41
1:H:327:ARG:C	1:H:368:THR:HG23	2.38	0.41
1:D:287:ILE:CD1	1:D:287:ILE:N	2.83	0.41
1:F:229:GLU:OE1	1:F:410:PHE:HA	2.20	0.41
1:D:466:PHE:O	1:D:468:ILE:N	2.53	0.41
1:E:345:ASN:C	1:E:346:ALA:H	2.21	0.41
1:A:275:TYR:CE2	1:A:303:VAL:HG23	2.55	0.41
1:F:412:GLN:HB2	1:F:419:ARG:HB3	2.02	0.41
1:E:150:LYS:O	1:E:151:ASP:CB	2.65	0.41
1:D:433:GLU:OE1	1:D:464:LEU:HD12	2.21	0.41
1:F:290:VAL:HG21	1:F:353:SER:HB2	2.02	0.41
1:C:232:CYS:HA	1:C:237:CYS:HA	2.02	0.41
1:C:158:LEU:O	1:C:174:GLU:HB2	2.20	0.41
1:C:172:ARG:HD2	1:C:174:GLU:OE1	2.20	0.41
1:H:238:PHE:CD1	1:H:238:PHE:N	2.88	0.41
1:E:322:PHE:HB2	1:E:327:ARG:HD2	2.03	0.41
1:B:463:GLU:HG3	1:B:463:GLU:O	2.19	0.41
1:A:116:VAL:CG1	1:A:136:GLN:HB2	2.44	0.41
1:C:396:ASP:C	1:C:397:ILE:HD12	2.41	0.41
1:F:287:ILE:CD1	1:F:287:ILE:N	2.83	0.41
1:A:333:GLY:C	1:A:386:THR:HG23	2.41	0.41
1:D:252:TYR:OH	1:D:274:HIS:HA	2.19	0.41
1:D:105:SER:HB3	1:D:167:PRO:HD2	2.02	0.41
1:D:360:VAL:CG1	1:D:383:TRP:HB2	2.45	0.41
1:A:249:GLN:HE21	1:A:272:ASN:N	2.17	0.41
1:B:149:VAL:CG2	1:B:430:ARG:NH1	2.83	0.41
1:E:226:GLN:O	1:E:227:GLU:CB	2.68	0.41
1:C:258:GLU:O	1:C:259:LYS:C	2.59	0.41
1:D:366:LYS:HD2	1:D:398:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LYS:HZ2	1:D:104:ASN:ND2	2.18	0.41
1:A:316:TYR:HB2	1:A:336:CYS:O	2.21	0.41
1:B:169:PRO:HG2	1:B:169(A):TYR:CE2	2.56	0.41
1:F:104:ASN:O	1:F:108:ILE:HG13	2.19	0.41
1:B:118:ARG:HB3	1:B:119:GLU:CD	2.41	0.41
1:E:354:PHE:CZ	1:E:409:SER:HB2	2.56	0.41
1:B:327:ARG:C	1:B:368:THR:HG23	2.40	0.41
1:B:360:VAL:HG12	1:B:383:TRP:HE3	1.84	0.41
1:F:261:LYS:HZ3	1:F:261:LYS:HB2	1.86	0.41
1:B:102:LYS:HZ2	1:B:104:ASN:ND2	2.18	0.41
1:C:464:LEU:HB3	1:C:465:PRO:HA	2.02	0.41
1:F:219:ARG:HA	1:F:219:ARG:HD3	1.92	0.41
1:B:117:ILE:O	1:B:440:SER:HA	2.21	0.41
1:A:216:LYS:CD	1:D:452:ASP:HB3	2.44	0.41
1:C:411:VAL:HG13	1:C:418:ILE:CG2	2.51	0.41
1:G:146:ASN:O	1:G:437:ILE:O	2.39	0.41
1:E:146:ASN:HA	1:E:437:ILE:HG13	2.03	0.41
1:A:333:GLY:N	1:A:386:THR:CG2	2.84	0.41
1:G:84:LYS:H	1:G:84:LYS:CD	2.33	0.41
1:A:466:PHE:O	1:A:468:ILE:HG13	2.21	0.41
1:E:224:ARG:NH1	1:E:276:GLU:OE1	2.52	0.41
1:D:270:ALA:HB1	1:D:273:TYR:HB2	2.03	0.41
1:E:411:VAL:HG12	1:E:412:GLN:H	1.80	0.41
1:F:147:GLY:C	1:F:149:VAL:H	2.24	0.41
1:D:146:ASN:HD22	1:D:146:ASN:HA	1.64	0.41
1:C:149:VAL:HG22	1:C:439:THR:OG1	2.21	0.41
1:E:275:TYR:CZ	1:E:303:VAL:CG2	3.04	0.41
1:E:333:GLY:O	1:E:386:THR:HG23	2.20	0.41
1:G:248:GLY:HA2	1:G:295:TRP:CD2	2.56	0.41
1:H:91:LEU:H	1:H:283:ASN:ND2	2.19	0.41
1:E:162:PRO:HG2	1:E:165:GLU:OE2	2.21	0.41
1:C:118:ARG:HB2	1:C:156:ARG:NH1	2.35	0.41
1:C:275:TYR:CE2	1:C:303:VAL:CG2	3.03	0.41
1:D:248:GLY:HA2	1:D:295:TRP:CD2	2.55	0.41
1:F:118:ARG:HB3	1:F:119:GLU:CD	2.41	0.41
1:E:271:PRO:O	1:E:272:ASN:HB3	2.21	0.41
1:A:144:HIS:CE1	1:D:463:GLU:H	2.18	0.41
1:H:105:SER:HB3	1:H:167:PRO:HD2	2.02	0.41
1:A:413:THR:CG2	1:A:415:LEU:HD13	2.41	0.40
1:D:162:PRO:CG	1:D:165:GLU:OE2	2.68	0.40
1:A:333:GLY:H	1:A:386:THR:HG23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:ILE:O	1:G:440:SER:HA	2.21	0.40
1:A:274:HIS:CE1	1:A:276:GLU:OE2	2.73	0.40
1:D:182:ALA:O	1:D:229:GLU:HA	2.21	0.40
1:G:159:MET:HG2	1:G:173:PHE:HA	2.02	0.40
1:G:241:MET:HB2	1:G:255:PHE:HE1	1.86	0.40
1:G:298:SER:OG	1:G:344:SER:O	2.36	0.40
1:A:277:GLU:OE1	1:A:350:LYS:HB2	2.21	0.40
1:B:172:ARG:HD2	1:B:174:GLU:OE1	2.22	0.40
1:B:248:GLY:HA2	1:B:295:TRP:CE2	2.55	0.40
1:G:146:ASN:HB3	1:G:147:GLY:H	1.67	0.40
1:G:142:ASP:OD2	1:G:144:HIS:HD2	2.04	0.40
1:G:433:GLU:OE2	1:G:464:LEU:HD12	2.20	0.40
1:B:231:ALA:O	1:B:237:CYS:HA	2.20	0.40
1:A:297:GLY:C	1:A:345(A):GLY:HA3	2.41	0.40
1:B:207:TYR:O	1:B:210:ILE:HG12	2.19	0.40
1:A:184:HIS:CD2	1:A:186:GLY:H	2.28	0.40
1:F:214:THR:HG22	1:G:451:SER:HB2	2.02	0.40
1:A:381:ASN:O	1:A:385:GLU:HB2	2.20	0.40
1:C:252:TYR:OH	1:C:274:HIS:HA	2.21	0.40
1:A:169:PRO:HG2	1:A:169(A):TYR:CD2	2.57	0.40
1:D:113:ASP:O	1:D:169:PRO:HD2	2.21	0.40
1:A:452:ASP:HB3	1:C:216:LYS:CD	2.42	0.40
1:E:271:PRO:O	1:E:272:ASN:CB	2.70	0.40
1:B:84:LYS:N	1:B:84:LYS:HD2	2.36	0.40
1:F:297:GLY:C	1:F:345(A):GLY:HA3	2.42	0.40
1:E:216:LYS:HZ2	1:H:452:ASP:HB3	1.85	0.40
1:F:452:ASP:HB3	1:H:216:LYS:CD	2.45	0.40
1:G:147:GLY:C	1:G:149:VAL:H	2.24	0.40
1:B:386:THR:O	1:B:386:THR:HG22	2.21	0.40
1:D:116:VAL:HG23	1:D:440:SER:HB2	2.03	0.40
1:H:287:ILE:O	1:H:304:SER:HA	2.22	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	383/387 (99%)	350 (91%)	26 (7%)	7 (2%)	11	18
1	B	383/387 (99%)	347 (91%)	30 (8%)	6 (2%)	12	21
1	C	383/387 (99%)	348 (91%)	29 (8%)	6 (2%)	12	21
1	D	383/387 (99%)	347 (91%)	29 (8%)	7 (2%)	11	18
1	E	383/387 (99%)	338 (88%)	37 (10%)	8 (2%)	9	14
1	F	383/387 (99%)	344 (90%)	32 (8%)	7 (2%)	11	18
1	G	383/387 (99%)	348 (91%)	30 (8%)	5 (1%)	15	26
1	H	383/387 (99%)	345 (90%)	33 (9%)	5 (1%)	15	26
All	All	3064/3096 (99%)	2767 (90%)	246 (8%)	51 (2%)	11	19

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	B	146	ASN
1	C	146	ASN
1	C	448	GLY
1	D	146	ASN
1	E	146	ASN
1	F	146	ASN
1	F	448	GLY
1	G	146	ASN
1	H	146	ASN
1	A	147	GLY
1	A	151	ASP
1	A	448	GLY
1	A	449	VAL
1	B	448	GLY
1	B	449	VAL
1	C	147	GLY
1	C	449	VAL
1	D	147	GLY
1	D	148	THR
1	D	448	GLY
1	D	449	VAL
1	E	147	GLY
1	E	448	GLY

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Mol	Chain	Res	Type
1	E	449	VAL
1	F	449	VAL
1	G	448	GLY
1	G	449	VAL
1	H	448	GLY
1	H	449	VAL
1	B	151	ASP
1	D	150	LYS
1	E	148	THR
1	F	467	THR
1	G	467	THR
1	H	151	ASP
1	A	148	THR
1	C	151	ASP
1	C	200	GLY
1	F	148	THR
1	F	151	ASP
1	F	200	GLY
1	A	451	SER
1	E	345(A)	GLY
1	E	200	GLY
1	H	147	GLY
1	B	147	GLY
1	G	222	ILE
1	D	222	ILE
1	B	222	ILE
1	E	222	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/331 (99%)	311 (94%)	18 (6%)	27	48
1	B	329/331 (99%)	316 (96%)	13 (4%)	38	64
1	C	329/331 (99%)	315 (96%)	14 (4%)	35	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	329/331 (99%)	312 (95%)	17 (5%)	29	51
1	E	329/331 (99%)	316 (96%)	13 (4%)	38	64
1	F	329/331 (99%)	318 (97%)	11 (3%)	45	73
1	G	329/331 (99%)	318 (97%)	11 (3%)	45	73
1	H	329/331 (99%)	315 (96%)	14 (4%)	35	61
All	All	2632/2648 (99%)	2521 (96%)	111 (4%)	36	62

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	88	ASN
1	A	99	VAL
1	A	146	ASN
1	A	153	SER
1	A	156	ARG
1	A	168	SER
1	A	202	VAL
1	A	214	THR
1	A	230	CYS
1	A	249	GLN
1	A	257	MET
1	A	296	HIS
1	A	310	LEU
1	A	345	ASN
1	A	415	LEU
1	A	442	SER
1	A	451	SER
1	B	85	LEU
1	B	88	ASN
1	B	99	VAL
1	B	116	VAL
1	B	146	ASN
1	B	156	ARG
1	B	210	ILE
1	B	230	CYS
1	B	257	MET
1	B	296	HIS
1	B	415	LEU
1	B	442	SER

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Mol	Chain	Res	Type
1	B	451	SER
1	C	85	LEU
1	C	88	ASN
1	C	99	VAL
1	C	116	VAL
1	C	145	SER
1	C	146	ASN
1	C	163	VAL
1	C	168	SER
1	C	214	THR
1	C	230	CYS
1	C	257	MET
1	C	296	HIS
1	C	400	ILE
1	C	412(B)	PRO
1	D	88	ASN
1	D	99	VAL
1	D	116	VAL
1	D	141	ASN
1	D	146	ASN
1	D	156	ARG
1	D	168	SER
1	D	210	ILE
1	D	230	CYS
1	D	249	GLN
1	D	257	MET
1	D	276	GLU
1	D	296	HIS
1	D	303	VAL
1	D	381	ASN
1	D	412(C)	GLU
1	D	415	LEU
1	E	88	ASN
1	E	99	VAL
1	E	116	VAL
1	E	146	ASN
1	E	156	ARG
1	E	202	VAL
1	E	230	CYS
1	E	276	GLU
1	E	296	HIS
1	E	400	ILE

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Mol	Chain	Res	Type
1	E	442	SER
1	E	451	SER
1	E	460	ASP
1	F	88	ASN
1	F	99	VAL
1	F	146	ASN
1	F	202	VAL
1	F	214	THR
1	F	230	CYS
1	F	252	TYR
1	F	296	HIS
1	F	400	ILE
1	F	415	LEU
1	F	451	SER
1	G	88	ASN
1	G	99	VAL
1	G	116	VAL
1	G	146	ASN
1	G	230	CYS
1	G	257	MET
1	G	296	HIS
1	G	310	LEU
1	G	345	ASN
1	G	385	GLU
1	G	442	SER
1	H	85	LEU
1	H	88	ASN
1	H	99	VAL
1	H	116	VAL
1	H	146	ASN
1	H	156	ARG
1	H	202	VAL
1	H	230	CYS
1	H	252	TYR
1	H	257	MET
1	H	296	HIS
1	H	298	SER
1	H	310	LEU
1	H	442	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	104	ASN
1	A	144	HIS
1	A	146	ASN
1	A	155	HIS
1	A	184	HIS
1	A	226	GLN
1	A	249	GLN
1	A	283	ASN
1	A	313	GLN
1	A	395	GLN
1	B	88	ASN
1	B	104	ASN
1	B	144	HIS
1	B	146	ASN
1	B	155	HIS
1	B	184	HIS
1	B	226	GLN
1	B	249	GLN
1	B	283	ASN
1	B	313	GLN
1	B	395	GLN
1	C	88	ASN
1	C	104	ASN
1	C	144	HIS
1	C	146	ASN
1	C	155	HIS
1	C	184	HIS
1	C	226	GLN
1	C	249	GLN
1	C	283	ASN
1	C	313	GLN
1	C	395	GLN
1	D	88	ASN
1	D	104	ASN
1	D	144	HIS
1	D	146	ASN
1	D	155	HIS
1	D	184	HIS
1	D	208	ASN
1	D	226	GLN
1	D	249	GLN
1	D	283	ASN

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Mol	Chain	Res	Type
1	D	313	GLN
1	D	381	ASN
1	D	395	GLN
1	D	450	ASN
1	E	88	ASN
1	E	104	ASN
1	E	144	HIS
1	E	146	ASN
1	E	155	HIS
1	E	184	HIS
1	E	226	GLN
1	E	249	GLN
1	E	283	ASN
1	E	313	GLN
1	E	395	GLN
1	F	88	ASN
1	F	104	ASN
1	F	144	HIS
1	F	146	ASN
1	F	155	HIS
1	F	184	HIS
1	F	226	GLN
1	F	249	GLN
1	F	283	ASN
1	F	296	HIS
1	F	313	GLN
1	F	395	GLN
1	G	88	ASN
1	G	104	ASN
1	G	144	HIS
1	G	146	ASN
1	G	184	HIS
1	G	226	GLN
1	G	249	GLN
1	G	283	ASN
1	G	313	GLN
1	G	395	GLN
1	G	412(A)	HIS
1	H	88	ASN
1	H	104	ASN
1	H	144	HIS
1	H	146	ASN

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Mol	Chain	Res	Type
1	H	184	HIS
1	H	226	GLN
1	H	249	GLN
1	H	272	ASN
1	H	283	ASN
1	H	313	GLN
1	H	395	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	G39	A	800	-	16,20,20	3.12	7 (43%)	12,27,27	1.98	2 (16%)
2	G39	B	801	-	16,20,20	3.07	7 (43%)	12,27,27	2.05	2 (16%)
2	G39	C	802	-	16,20,20	3.09	7 (43%)	12,27,27	1.96	2 (16%)
2	G39	D	803	-	16,20,20	3.20	7 (43%)	12,27,27	1.93	1 (8%)
2	G39	E	804	-	16,20,20	3.11	7 (43%)	12,27,27	1.85	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G39	F	805	-	16,20,20	3.09	7 (43%)	12,27,27	1.95	2 (16%)
2	G39	G	806	-	16,20,20	3.13	7 (43%)	12,27,27	1.98	2 (16%)
2	G39	H	807	-	16,20,20	3.22	7 (43%)	12,27,27	1.93	2 (16%)

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	G39	A	800	-	-	0/12/32/32	0/1/1/1
2	G39	B	801	-	-	0/12/32/32	0/1/1/1
2	G39	C	802	-	-	0/12/32/32	0/1/1/1
2	G39	D	803	-	-	0/12/32/32	0/1/1/1
2	G39	E	804	-	-	0/12/32/32	0/1/1/1
2	G39	F	805	-	-	0/12/32/32	0/1/1/1
2	G39	G	806	-	-	0/12/32/32	0/1/1/1
2	G39	H	807	-	-	0/12/32/32	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	804	G39	C1-C2	-4.08	1.44	1.51
2	C	802	G39	C1-C2	-3.97	1.44	1.51
2	F	805	G39	C1-C2	-3.87	1.44	1.51
2	D	803	G39	C1-C2	-3.83	1.44	1.51
2	A	800	G39	C1-C2	-3.70	1.44	1.51
2	B	801	G39	C1-C2	-3.63	1.45	1.51
2	G	806	G39	C1-C2	-3.54	1.45	1.51
2	H	807	G39	C1-C2	-3.15	1.45	1.51
2	B	801	G39	O7-C6	2.00	1.49	1.44
2	C	802	G39	O7-C6	2.14	1.50	1.44
2	H	807	G39	O7-C6	2.17	1.50	1.44
2	F	805	G39	O7-C6	2.19	1.50	1.44
2	A	800	G39	O7-C6	2.21	1.50	1.44
2	E	804	G39	O7-C6	2.22	1.50	1.44
2	D	803	G39	O7-C6	2.31	1.50	1.44
2	G	806	G39	C3-C4	2.39	1.58	1.54
2	C	802	G39	C3-C4	2.52	1.58	1.54
2	G	806	G39	O7-C6	2.52	1.51	1.44
2	B	801	G39	C3-C4	2.78	1.59	1.54
2	E	804	G39	C3-C4	2.87	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	805	G39	C3-C4	2.89	1.59	1.54
2	D	803	G39	C3-C4	2.95	1.59	1.54
2	F	805	G39	O7-C8	2.97	1.49	1.44
2	A	800	G39	O7-C8	3.00	1.49	1.44
2	D	803	G39	C5-N5	3.03	1.50	1.45
2	E	804	G39	C5-N5	3.05	1.50	1.45
2	A	800	G39	C3-C4	3.09	1.59	1.54
2	B	801	G39	O7-C8	3.15	1.49	1.44
2	H	807	G39	C5-N5	3.25	1.51	1.45
2	H	807	G39	C3-C4	3.30	1.60	1.54
2	G	806	G39	C5-N5	3.31	1.51	1.45
2	C	802	G39	C5-N5	3.35	1.51	1.45
2	C	802	G39	O7-C8	3.37	1.49	1.44
2	B	801	G39	C5-N5	3.55	1.51	1.45
2	H	807	G39	O7-C8	3.58	1.50	1.44
2	A	800	G39	C5-N5	3.60	1.51	1.45
2	E	804	G39	O7-C8	3.61	1.50	1.44
2	G	806	G39	O7-C8	3.62	1.50	1.44
2	D	803	G39	O7-C8	3.75	1.50	1.44
2	F	805	G39	C5-N5	3.76	1.52	1.45
2	A	800	G39	C7-C2	5.63	1.43	1.34
2	F	805	G39	C7-C2	5.71	1.43	1.34
2	B	801	G39	C7-C2	5.79	1.43	1.34
2	C	802	G39	C7-C2	5.94	1.43	1.34
2	E	804	G39	C7-C2	5.98	1.43	1.34
2	G	806	G39	C7-C2	6.01	1.43	1.34
2	D	803	G39	C7-C2	6.26	1.44	1.34
2	H	807	G39	C7-C2	6.37	1.44	1.34
2	E	804	G39	C3-C2	7.88	1.63	1.50
2	C	802	G39	C3-C2	7.94	1.63	1.50
2	F	805	G39	C3-C2	7.95	1.63	1.50
2	B	801	G39	C3-C2	8.04	1.63	1.50
2	G	806	G39	C3-C2	8.10	1.63	1.50
2	D	803	G39	C3-C2	8.19	1.63	1.50
2	A	800	G39	C3-C2	8.29	1.64	1.50
2	H	807	G39	C3-C2	8.43	1.64	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	806	G39	C4-C5-N5	-2.48	105.63	110.39
2	A	800	G39	C4-C5-N5	-2.42	105.76	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	805	G39	C4-C5-N5	-2.23	106.11	110.39
2	C	802	G39	O10-C10-C11	-2.15	118.11	122.06
2	H	807	G39	O10-C10-C11	-2.03	118.34	122.06
2	B	801	G39	O10-C10-C11	-2.01	118.38	122.06
2	E	804	G39	C4-C3-C2	5.08	116.11	109.65
2	F	805	G39	C4-C3-C2	5.19	116.25	109.65
2	G	806	G39	C4-C3-C2	5.28	116.37	109.65
2	C	802	G39	C4-C3-C2	5.29	116.37	109.65
2	D	803	G39	C4-C3-C2	5.38	116.49	109.65
2	A	800	G39	C4-C3-C2	5.43	116.56	109.65
2	H	807	G39	C4-C3-C2	5.56	116.72	109.65
2	B	801	G39	C4-C3-C2	5.69	116.89	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	385/387 (99%)	-0.37	2 (0%) 91 92	9, 18, 28, 40	0
1	B	385/387 (99%)	-0.33	6 (1%) 74 78	8, 18, 28, 40	0
1	C	385/387 (99%)	-0.34	2 (0%) 91 92	10, 18, 28, 41	0
1	D	385/387 (99%)	-0.34	4 (1%) 84 86	10, 18, 29, 43	0
1	E	385/387 (99%)	-0.22	7 (1%) 71 75	15, 24, 33, 43	0
1	F	385/387 (99%)	-0.20	6 (1%) 74 78	12, 25, 35, 44	0
1	G	385/387 (99%)	-0.25	4 (1%) 84 86	9, 21, 32, 43	0
1	H	385/387 (99%)	-0.19	9 (2%) 64 67	14, 23, 34, 44	0
All	All	3080/3096 (99%)	-0.28	40 (1%) 79 82	8, 21, 32, 44	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	381	ASN	5.5
1	H	381	ASN	4.6
1	E	345	ASN	4.5
1	C	381	ASN	4.4
1	H	345	ASN	4.0
1	B	381	ASN	3.8
1	E	346	ALA	3.7
1	B	346	ALA	3.4
1	F	345	ASN	3.3
1	H	150	LYS	3.0
1	F	381	ASN	2.9
1	E	381	ASN	2.8
1	A	346	ALA	2.8
1	B	150	LYS	2.7
1	G	306	ASN	2.7
1	D	412	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	346	ALA	2.7
1	H	411	VAL	2.6
1	G	150	LYS	2.5
1	E	412	GLN	2.5
1	D	346	ALA	2.5
1	F	150	LYS	2.4
1	F	369	ASN	2.4
1	B	368	THR	2.4
1	H	346	ALA	2.4
1	D	345	ASN	2.3
1	F	412	GLN	2.3
1	G	386	THR	2.3
1	E	86	ALA	2.2
1	F	309	ASN	2.2
1	B	386	THR	2.2
1	A	381	ASN	2.1
1	C	150	LYS	2.1
1	B	400	ILE	2.1
1	H	86	ALA	2.1
1	E	83	VAL	2.1
1	H	309	ASN	2.1
1	H	412	GLN	2.0
1	H	386	THR	2.0
1	E	306	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	G39	F	805	20/20	0.94	0.19	2.07	25,29,32,33	0
2	G39	C	802	20/20	0.94	0.18	1.98	24,26,28,31	0
2	G39	E	804	20/20	0.89	0.18	1.36	21,24,26,26	0
2	G39	H	807	20/20	0.92	0.17	1.29	20,27,29,29	0
2	G39	B	801	20/20	0.95	0.17	1.12	17,25,29,30	0
2	G39	D	803	20/20	0.93	0.15	0.76	17,22,23,24	0
2	G39	G	806	20/20	0.94	0.15	0.49	18,21,23,23	0
2	G39	A	800	20/20	0.92	0.14	0.01	20,24,26,26	0

6.5 Other polymers

There are no such residues in this entry.