



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:30 am GMT

PDB ID : 1MWA
Title : 2C/H-2KBM3/DEV8 ALLOGENEIC COMPLEX
Authors : Luz, J.G.; Huang, M.D.; Garcia, K.C.; Rudolph, M.G.; Teyton, L.; Wilson, I.A.
Deposited on : 2002-09-27
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

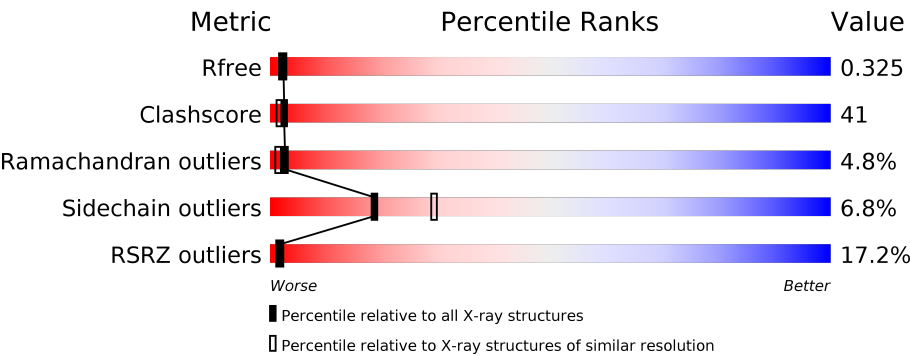
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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





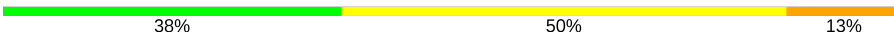

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	202	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>55%40%5%</div></div>
1	C	202	<div><div>44%</div><div><div></div><div></div><div></div><div></div></div><div>33%56%9%</div></div>
2	B	237	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>60%36%</div></div>
2	D	237	<div><div>60%</div><div><div></div><div></div><div></div><div></div></div><div>28%60%11%</div></div>
3	H	275	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>55%39%5%</div></div>
3	I	275	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>37%54%8%</div></div>

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Mol	Chain	Length	Quality of chain
4	L	99	
4	M	99	
5	P	8	
5	Q	8	

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
10	NAG	B	809	-	-	X	X
11	ACY	P	1001	-	-	-	X
6	NAG	A	803	-	-	-	X
7	NAG	A	805	-	-	X	X
7	NAG	B	808	X	-	-	-
7	NAG	H	812	X	-	-	-
9	GOL	A	902	-	-	-	X
9	GOL	L	901	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 13973 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 2C T CELL RECEPTOR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			
1	C	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	GLN	SEE REMARK 999	GB 224220
A	165	ALA	LYS	SEE REMARK 999	GB 224220
C	127	ALA	GLN	SEE REMARK 999	GB 224220
C	165	ALA	LYS	SEE REMARK 999	GB 224220

- Molecule 2 is a protein called 2C T CELL RECEPTOR BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			
2	D	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLY	GLN	SEE REMARK 999	GB 1791255
B	?	-	ARG	SEE REMARK 999	GB 1791255
B	?	-	ALA	SEE REMARK 999	GB 1791255
B	105	THR	GLU	SEE REMARK 999	GB 1791255
B	106	LEU	GLN	SEE REMARK 999	GB 1791255
B	107	TYR	PHE	SEE REMARK 999	GB 1791255
B	110	ALA	PRO	SEE REMARK 999	GB 1791255
B	115	SER	THR	SEE REMARK 999	GB 1791255

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Chain	Residue	Modelled	Actual	Comment	Reference
D	97	GLY	GLN	SEE REMARK 999	GB 1791255
D	?	-	ARG	SEE REMARK 999	GB 1791255
D	?	-	ALA	SEE REMARK 999	GB 1791255
D	105	THR	GLU	SEE REMARK 999	GB 1791255
D	106	LEU	GLN	SEE REMARK 999	GB 1791255
D	107	TYR	PHE	SEE REMARK 999	GB 1791255
D	110	ALA	PRO	SEE REMARK 999	GB 1791255
D	115	SER	THR	SEE REMARK 999	GB 1791255

- Molecule 3 is a protein called H-2KBM3 MHC CLASS I MOLECULE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	274	Total	C	N	O	S	0	0	0
			2225	1404	392	420	9			
3	I	274	Total	C	N	O	S	0	0	0
			2224	1404	392	419	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	77	SER	ASP	CONFLICT	UNP P01901
H	89	ALA	LYS	CONFLICT	UNP P01901
H	275	ARG	GLU	CONFLICT	UNP P01901
I	77	SER	ASP	CONFLICT	UNP P01901
I	89	ALA	LYS	CONFLICT	UNP P01901
I	275	ARG	GLU	CONFLICT	UNP P01901

- Molecule 4 is a protein called MICROGLOBULIN MHC LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
4	M	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

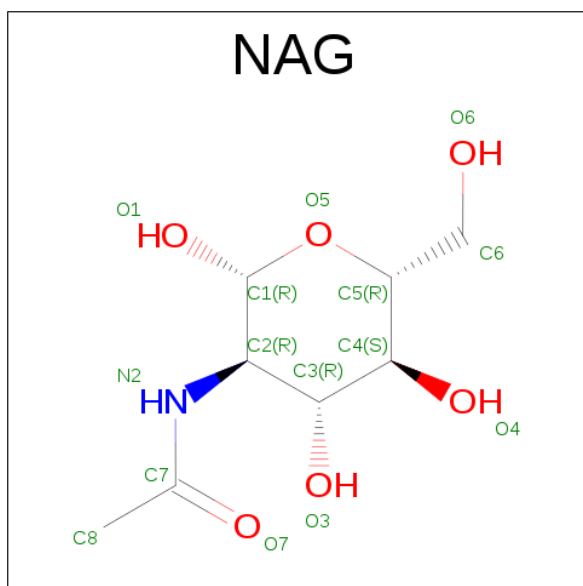
- Molecule 5 is a protein called DEV8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	8	Total	C	N	O	0	0	0
			76	51	10	15			
5	Q	8	Total	C	N	O	0	0	0
			76	51	10	15			

- Molecule 6 is a polymer of unknown type called SUGAR (NAG-NAG).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

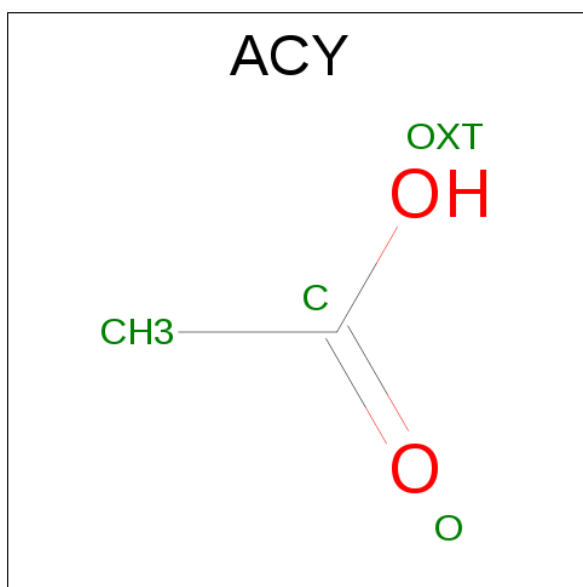


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	I	1	Total	C	O	0	0
			6	3	3		
9	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	3	Total	C	N	O	0	0
			39	22	2	15		
10	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	P	1	Total	C	O	0	0
			4	2	2		

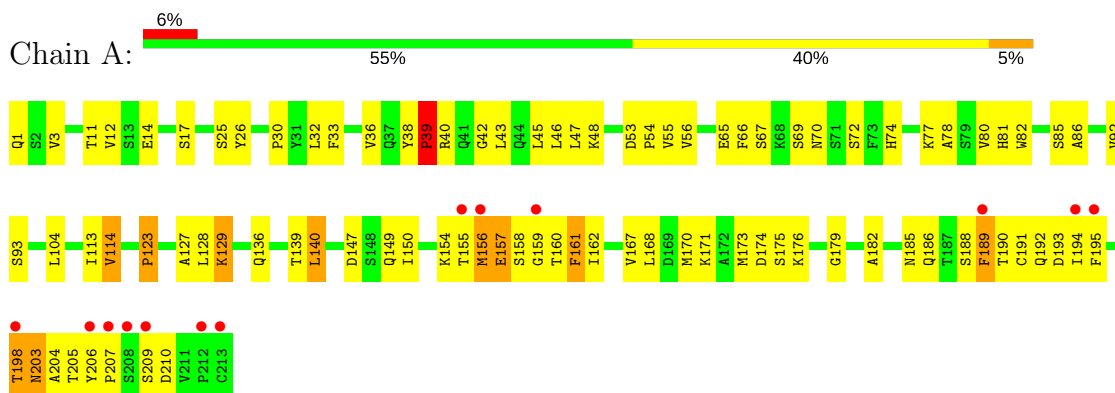
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	106	Total	O	0	0
			106	106		
12	C	41	Total	O	0	0
			41	41		
12	B	118	Total	O	0	0
			118	118		
12	D	10	Total	O	0	0
			10	10		
12	H	183	Total	O	0	0
			183	183		
12	I	107	Total	O	0	0
			107	107		
12	L	62	Total	O	0	0
			62	62		
12	M	44	Total	O	0	0
			44	44		
12	P	2	Total	O	0	0
			2	2		
12	Q	2	Total	O	0	0
			2	2		

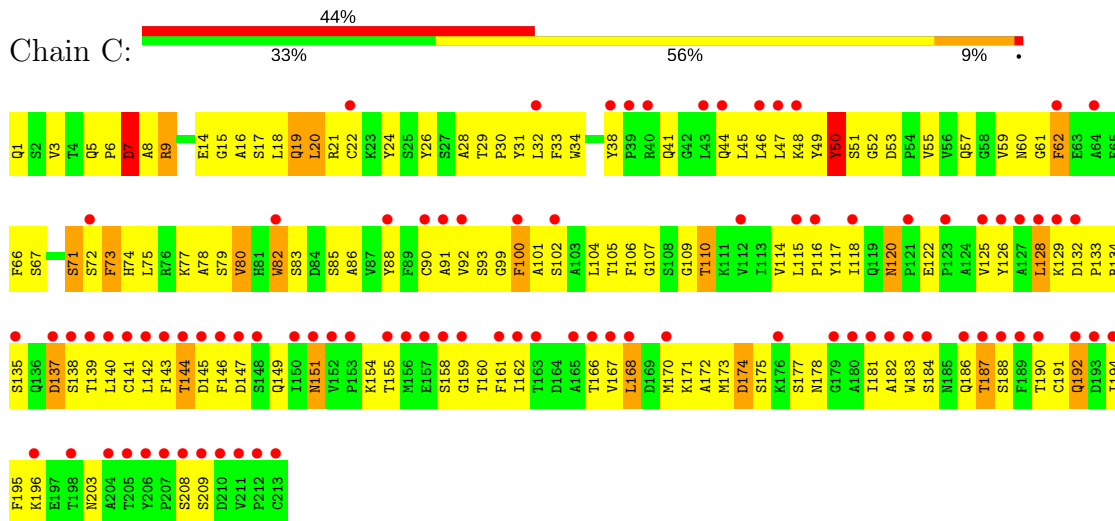
3 Residue-property plots [i](#)

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

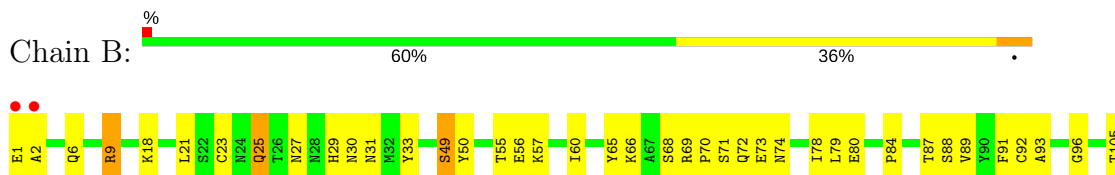
• Molecule 1: 2C T CELL RECEPTOR ALPHA CHAIN

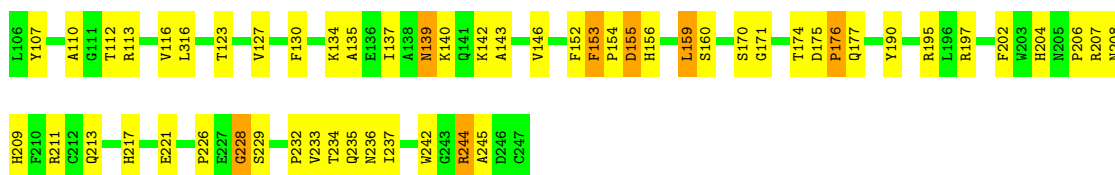


• Molecule 1: 2C T CELL RECEPTOR ALPHA CHAIN

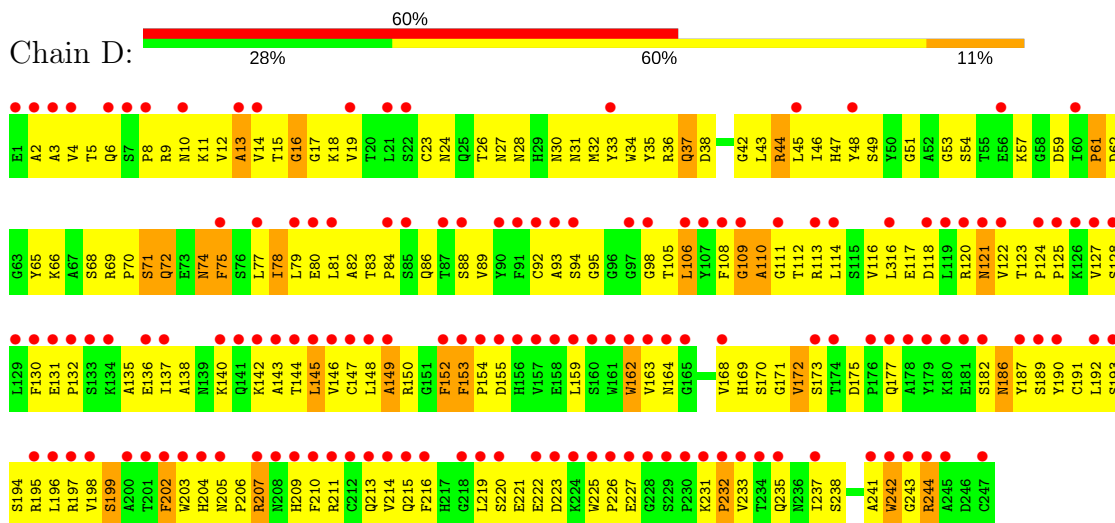


• Molecule 2: 2C T CELL RECEPTOR BETA CHAIN

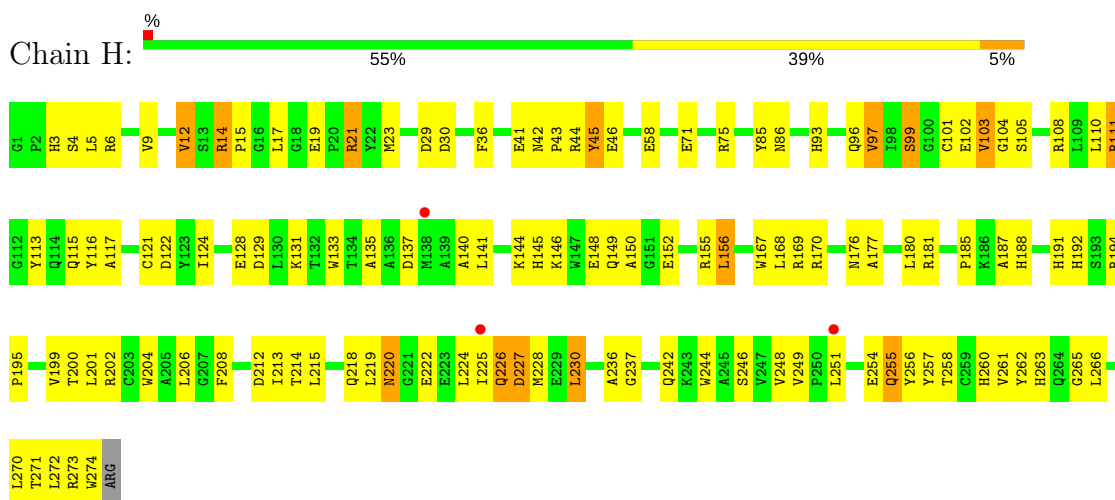




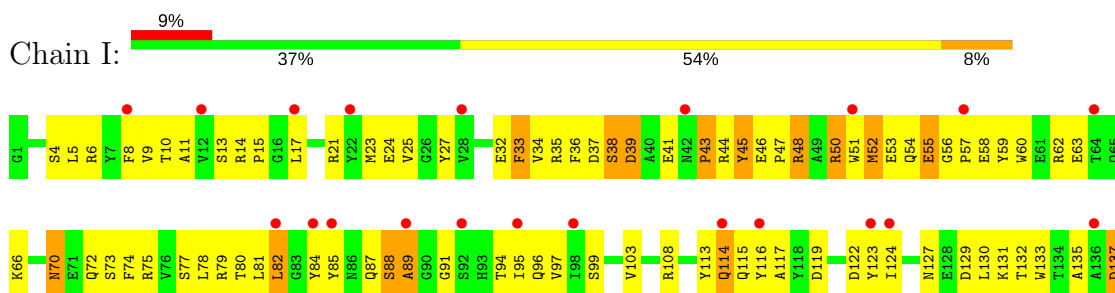
• Molecule 2: 2C T CELL RECEPTOR BETA CHAIN

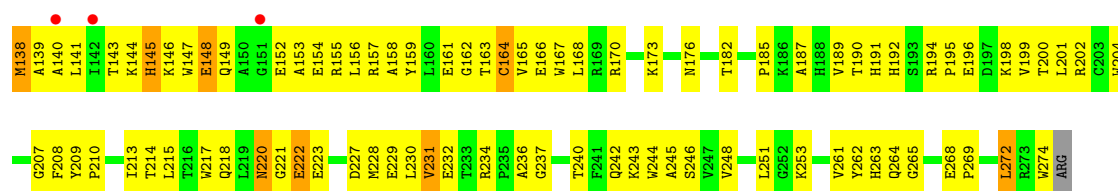


• Molecule 3: H-2KBM3 MHC CLASS I MOLECULE HEAVY CHAIN



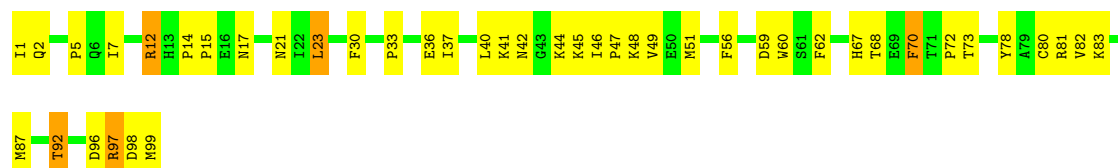
• Molecule 3: H-2KBM3 MHC CLASS I MOLECULE HEAVY CHAIN





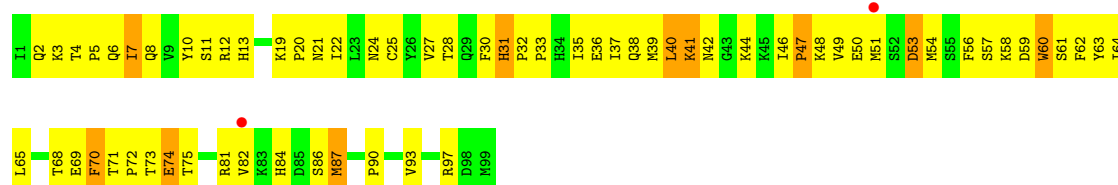
● Molecule 4: MICROGLOBULIN MHC LIGHT CHAIN

Chain L: 56% 39% 5%



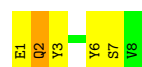
● Molecule 4: MICROGLOBULIN MHC LIGHT CHAIN

Chain M: 33% 57% 10%



● Molecule 5: DEV8

Chain P: 38% 50% 13%



● Molecule 5: DEV8

Chain Q: 63% 38% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	297.90Å 95.94Å 84.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.40 49.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.39-2.40) 99.6 (49.65-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.284 , 0.313 0.294 , 0.325	Depositor DCC
R_{free} test set	4781 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 89.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13973	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACY, BMA, 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	0.44	0/1611	0.76	0/2193
1	C	0.34	0/1611	0.66	0/2193
2	B	0.43	0/1904	0.75	2/2586 (0.1%)
2	D	0.27	0/1904	0.56	0/2586
3	H	0.41	0/2286	0.71	0/3106
3	I	0.38	1/2285 (0.0%)	0.71	1/3105 (0.0%)
4	L	0.44	0/847	0.77	0/1148
4	M	0.33	0/847	0.72	0/1148
5	P	0.50	0/78	0.77	0/102
5	Q	0.61	0/78	0.88	0/102
All	All	0.39	1/13451 (0.0%)	0.70	3/18269 (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
3	I	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	220	ASN	C-N	-5.16	1.23	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	228	GLY	N-CA-C	-7.15	95.22	113.10
3	I	220	ASN	CA-C-N	-6.59	103.03	116.20
2	B	9	ARG	NE-CZ-NH1	-5.36	117.62	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	50	TYR	Peptide
3	I	220	ASN	Mainchain

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	1570	0	1503	91	0
1	C	1570	0	1503	153	1
2	B	1853	0	1761	102	0
2	D	1853	0	1763	229	0
3	H	2225	0	2115	120	0
3	I	2224	0	2113	236	0
4	L	821	0	796	39	0
4	M	821	0	796	98	0
5	P	76	0	70	8	0
5	Q	76	0	70	28	0
6	A	28	0	25	1	0
7	A	14	0	13	11	0
7	B	14	0	13	0	0
7	H	28	0	26	5	0
8	A	25	0	21	5	0
9	A	6	0	8	0	0
9	I	6	0	8	0	0
9	L	6	0	8	0	0
10	B	39	0	33	13	0
10	C	39	0	34	4	0
11	P	4	0	3	0	0
12	A	106	0	0	8	0
12	B	118	0	0	10	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	41	0	0	14	0
12	D	10	0	0	1	0
12	H	183	0	0	9	0
12	I	107	0	0	16	0
12	L	62	0	0	3	0
12	M	44	0	0	19	0
12	P	2	0	0	0	0
12	Q	2	0	0	0	0
All	All	13973	0	12682	1051	1

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 41.

All (1051) 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)
2:B:236:ASN:HD21	10:B:809:NAG:C1	1.18	1.50
10:B:810:NAG:H61	10:B:811:BMA:C2	1.52	1.34
10:B:810:NAG:C6	10:B:811:BMA:H2	1.32	1.32
1:A:185:ASN:HD21	7:A:805:NAG:C2	1.53	1.20
1:A:185:ASN:ND2	7:A:805:NAG:C2	2.07	1.18
2:B:236:ASN:HD21	10:B:809:NAG:C2	1.57	1.15
2:B:9:ARG:HH12	2:B:110:ALA:HB3	1.12	1.13
3:H:180:LEU:CD1	7:H:813:NAG:H81	1.79	1.12
1:A:185:ASN:HD21	7:A:805:NAG:H2	1.07	1.09
3:H:177:ALA:HB3	12:H:924:HOH:O	1.52	1.09
3:I:78:LEU:HG	3:I:95:ILE:HD11	1.23	1.09
3:H:180:LEU:HD13	7:H:813:NAG:H81	1.12	1.08
2:D:4:VAL:H	2:D:109:GLY:HA3	1.21	1.06
3:H:9:VAL:HB	3:H:97:VAL:HG13	1.36	1.05
3:I:66:LYS:HB2	12:I:967:HOH:O	1.56	1.03
2:B:130:PHE:HB2	2:B:146:VAL:HG13	1.37	1.02
3:I:189:VAL:HG23	3:I:274:TRP:HD1	1.20	1.01
3:H:14:ARG:HB2	3:H:17:LEU:HB2	1.41	1.00
4:L:45:LYS:HE2	4:L:81:ARG:HH22	1.24	0.99
3:I:50:ARG:O	3:I:53:GLU:HG2	1.63	0.98
3:I:218:GLN:HB2	3:I:222:GLU:O	1.66	0.95
2:D:16:GLY:HA2	2:D:81:LEU:HA	1.48	0.94
1:A:185:ASN:ND2	7:A:805:NAG:H2	1.75	0.94
3:H:111:ARG:HG3	3:H:111:ARG:HH11	1.30	0.93
2:D:121:ASN:ND2	2:D:153:PHE:CE2	2.38	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:57:PRO:HA	3:I:60:TRP:HB2	1.51	0.92
4:M:2:GLN:HA	4:M:31:HIS:O	1.69	0.91
1:C:31:TYR:HB2	1:C:93:SER:HB3	1.51	0.91
3:I:145:HIS:HB3	3:I:149:GLN:NE2	1.86	0.90
4:M:31:HIS:HD1	4:M:32:PRO:HA	1.37	0.90
2:D:6:GLN:HE21	2:D:111:GLY:HA2	1.37	0.89
8:A:806:NAG:O3	8:A:807:BMA:O5	1.89	0.89
2:B:9:ARG:HH12	2:B:110:ALA:CB	1.84	0.89
3:I:234:ARG:HH11	4:M:8:GLN:NE2	1.71	0.88
2:B:204:HIS:HA	2:B:244:ARG:O	1.74	0.87
4:M:73:THR:HG22	4:M:75:THR:H	1.37	0.87
1:A:185:ASN:CG	7:A:805:NAG:C1	2.44	0.86
1:C:170:MET:H	1:C:175:SER:HB3	1.39	0.86
4:L:45:LYS:HE2	4:L:81:ARG:NH2	1.89	0.86
1:C:6:PRO:HB2	1:C:21:ARG:HE	1.38	0.86
1:C:155:THR:HG21	1:C:161:PHE:HA	1.55	0.86
5:Q:2:GLN:NE2	5:Q:3:TYR:H	1.73	0.86
3:H:180:LEU:HD13	7:H:813:NAG:C8	2.01	0.85
1:C:1:GLN:HE21	1:C:105:THR:HG23	1.42	0.85
7:H:812:NAG:H62	7:H:813:NAG:H82	1.59	0.84
2:D:46:ILE:HG22	2:D:47:HIS:ND1	1.91	0.84
3:H:104:GLY:HA3	12:H:836:HOH:O	1.76	0.84
1:C:45:LEU:HD12	1:C:46:LEU:N	1.93	0.83
4:M:37:ILE:HG22	4:M:82:VAL:HG12	1.59	0.83
3:I:77:SER:O	3:I:81:LEU:HG	1.78	0.83
3:I:131:LYS:HA	12:I:949:HOH:O	1.79	0.83
2:B:236:ASN:ND2	10:B:809:NAG:C2	2.32	0.82
3:I:11:ALA:HB3	3:I:95:ILE:HD12	1.60	0.82
2:D:14:VAL:HB	2:D:17:GLY:H	1.44	0.82
2:B:9:ARG:NH1	2:B:110:ALA:HB3	1.93	0.82
1:C:18:LEU:HB3	1:C:77:LYS:HB3	1.61	0.82
3:I:253:LYS:HE3	12:I:971:HOH:O	1.78	0.82
1:C:9:ARG:HD3	1:C:9:ARG:O	1.80	0.81
2:D:164:ASN:ND2	2:D:209:HIS:HB3	1.95	0.81
5:Q:2:GLN:HE21	5:Q:3:TYR:H	1.26	0.81
3:I:194:ARG:HG3	3:I:195:PRO:HD2	1.60	0.81
1:A:194:ILE:HG23	1:A:195:PHE:HD1	1.44	0.80
2:D:68:SER:O	2:D:70:PRO:HD3	1.79	0.80
3:I:218:GLN:CB	3:I:222:GLU:O	2.29	0.80
3:I:48:ARG:HA	12:I:939:HOH:O	1.80	0.80
2:D:146:VAL:HG23	2:D:194:SER:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:185:PRO:HB3	3:I:208:PHE:HB3	1.64	0.80
4:M:63:TYR:HB3	12:M:281:HOH:O	1.83	0.78
4:M:7:ILE:HB	4:M:93:VAL:HG21	1.66	0.78
3:I:130:LEU:HB3	12:I:948:HOH:O	1.83	0.78
2:D:37:GLN:HB2	2:D:43:LEU:CD1	2.13	0.78
2:D:30:ASN:OD1	3:I:146:LYS:HE3	1.82	0.78
3:I:263:HIS:CD2	3:I:265:GLY:H	2.02	0.78
3:I:96:GLN:HG2	12:I:962:HOH:O	1.83	0.78
3:I:159:TYR:CE2	5:Q:3:TYR:HB2	2.18	0.78
2:D:9:ARG:HA	2:D:112:THR:HG22	1.65	0.78
3:I:182:THR:HG22	3:I:210:PRO:HD3	1.66	0.78
1:C:67:SER:OG	10:C:814:NAG:H82	1.84	0.77
1:A:53:ASP:OD2	1:A:55:VAL:HG22	1.84	0.77
2:D:4:VAL:H	2:D:109:GLY:CA	1.96	0.77
2:D:18:LYS:HA	2:D:80:GLU:HA	1.65	0.77
3:I:14:ARG:HH21	3:I:21:ARG:HD2	1.47	0.77
4:L:40:LEU:HD21	4:L:81:ARG:HH21	1.49	0.77
3:I:189:VAL:HG23	3:I:274:TRP:CD1	2.13	0.77
5:P:2:GLN:NE2	5:P:3:TYR:H	1.83	0.76
2:D:145:LEU:HD23	2:D:145:LEU:H	1.49	0.76
3:I:124:ILE:HB	3:I:140:ALA:HB1	1.67	0.76
1:C:8:ALA:HA	1:C:110:THR:HA	1.68	0.76
4:M:21:ASN:HB3	4:M:70:PHE:CE1	2.21	0.76
4:M:21:ASN:HD22	4:M:22:ILE:H	1.33	0.76
1:C:186:GLN:HG3	1:C:187:THR:H	1.51	0.76
1:A:185:ASN:ND2	7:A:805:NAG:O5	2.18	0.76
1:C:170:MET:HG2	1:C:171:LYS:H	1.50	0.75
1:A:72:SER:HB2	1:A:74:HIS:CE1	2.21	0.75
8:A:806:NAG:C3	8:A:807:BMA:O5	2.35	0.75
1:C:20:LEU:HD23	1:C:20:LEU:H	1.50	0.75
1:A:81:HIS:HB2	12:A:937:HOH:O	1.86	0.75
1:C:132:ASP:HB3	1:C:135:SER:HB3	1.69	0.75
2:D:198:VAL:HB	2:D:202:PHE:HB3	1.67	0.75
7:A:805:NAG:HO4	8:A:806:NAG:C1	1.98	0.74
2:B:236:ASN:CG	10:B:809:NAG:C1	2.55	0.74
2:D:122:VAL:O	2:D:232:PRO:HG2	1.88	0.74
2:B:27:ASN:HB3	2:B:29:HIS:CE1	2.22	0.74
2:D:6:GLN:NE2	2:D:111:GLY:HA2	2.02	0.74
4:L:67:HIS:HD2	12:L:938:HOH:O	1.69	0.74
2:D:37:GLN:HA	2:D:43:LEU:HA	1.70	0.73
2:D:45:LEU:HD21	2:D:48:TYR:HD2	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:42:ASN:OD1	3:H:44:ARG:HD3	1.88	0.73
2:D:4:VAL:N	2:D:109:GLY:HA3	2.01	0.73
4:M:31:HIS:ND1	4:M:32:PRO:HA	2.02	0.73
2:D:18:LYS:HG3	2:D:80:GLU:HG3	1.71	0.73
3:H:219:LEU:O	3:H:220:ASN:ND2	2.22	0.73
3:I:145:HIS:HA	3:I:148:GLU:HB3	1.69	0.73
3:I:231:VAL:HG13	3:I:232:GLU:O	1.89	0.73
2:D:6:GLN:HE21	2:D:111:GLY:CA	2.02	0.72
1:C:53:ASP:OD1	1:C:55:VAL:HG22	1.89	0.72
3:H:249:VAL:CG2	3:H:254:GLU:HG3	2.20	0.72
2:D:32:MET:HG3	12:D:317:HOH:O	1.90	0.72
2:D:242:TRP:HB3	2:D:244:ARG:NH1	2.03	0.72
2:B:84:PRO:HA	2:B:116:VAL:HB	1.71	0.72
2:D:78:ILE:H	2:D:78:ILE:HD12	1.55	0.71
4:M:87:MET:HB2	12:M:375:HOH:O	1.91	0.71
1:C:20:LEU:HD11	1:C:75:LEU:HD23	1.73	0.71
1:C:26:TYR:HD2	1:C:28:ALA:H	1.36	0.71
3:H:237:GLY:HA3	12:L:931:HOH:O	1.91	0.71
1:C:80:VAL:HG23	1:C:80:VAL:O	1.91	0.71
2:D:83:THR:HG22	2:D:86:GLN:HG3	1.72	0.71
4:M:19:LYS:O	4:M:72:PRO:HD2	1.91	0.71
2:D:125:PRO:HG3	2:D:216:PHE:HB2	1.73	0.70
3:I:54:GLN:NE2	12:I:1000:HOH:O	2.24	0.70
3:I:147:TRP:HE1	5:Q:8:VAL:C	1.94	0.70
3:H:249:VAL:HG21	3:H:254:GLU:HG3	1.73	0.70
3:I:194:ARG:NH1	3:I:248:VAL:HG11	2.06	0.70
2:D:46:ILE:HG21	2:D:77:LEU:HD11	1.73	0.70
1:C:142:LEU:HD11	2:D:144:THR:HB	1.72	0.70
1:C:45:LEU:HD12	1:C:46:LEU:H	1.57	0.70
1:A:40:ARG:HD2	12:A:993:HOH:O	1.92	0.70
7:H:812:NAG:C6	7:H:813:NAG:H82	2.22	0.70
5:P:2:GLN:HA	5:P:2:GLN:HE21	1.57	0.70
1:C:166:THR:HB	2:D:173:SER:OG	1.91	0.69
1:C:115:LEU:H	1:C:115:LEU:HD22	1.57	0.69
3:H:6:ARG:NE	12:H:898:HOH:O	2.24	0.69
1:A:159:GLY:HA3	7:A:805:NAG:H82	1.74	0.69
2:D:152:PHE:O	2:D:189:SER:HA	1.92	0.69
5:Q:2:GLN:HE21	5:Q:3:TYR:N	1.90	0.69
3:H:14:ARG:HB2	3:H:17:LEU:CB	2.20	0.69
1:C:82:TRP:HA	1:C:114:VAL:HG13	1.73	0.69
1:C:32:LEU:HD23	1:C:92:VAL:HG12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:PRO:HG2	2:D:62:ASP:H	1.57	0.69
3:H:111:ARG:HG3	3:H:111:ARG:NH1	2.07	0.69
3:I:215:LEU:HD23	3:I:261:VAL:HG13	1.74	0.69
1:A:77:LYS:HD3	1:A:80:VAL:HG12	1.76	0.69
1:C:82:TRP:HA	1:C:114:VAL:CG1	2.23	0.69
1:C:3:VAL:HG21	1:C:90:CYS:O	1.92	0.69
3:I:230:LEU:HD12	3:I:245:ALA:HB2	1.73	0.68
3:I:46:GLU:HG3	3:I:47:PRO:HD2	1.75	0.68
4:M:12:ARG:HE	4:M:13:HIS:CE1	2.11	0.68
4:M:73:THR:CG2	4:M:75:THR:HG22	2.22	0.68
1:C:47:LEU:O	1:C:47:LEU:HD12	1.94	0.68
2:B:153:PHE:O	2:B:154:PRO:C	2.30	0.68
2:B:2:ALA:HA	2:B:27:ASN:OD1	1.94	0.67
4:M:69:GLU:HB2	12:M:599:HOH:O	1.93	0.67
4:M:21:ASN:HB3	4:M:70:PHE:HE1	1.59	0.67
4:M:87:MET:CB	12:M:375:HOH:O	2.41	0.67
1:A:67:SER:HB2	6:A:803:NAG:H82	1.76	0.67
2:D:244:ARG:HD2	2:D:244:ARG:N	2.10	0.67
3:I:36:PHE:HE1	3:I:43:PRO:C	1.97	0.67
2:D:13:ALA:HB3	2:D:116:VAL:HG12	1.75	0.67
1:C:6:PRO:HB2	1:C:21:ARG:NE	2.07	0.67
2:D:79:LEU:HD12	2:D:86:GLN:OE1	1.93	0.67
3:H:137:ASP:HB2	12:H:858:HOH:O	1.95	0.67
3:I:129:ASP:OD2	3:I:131:LYS:HB2	1.95	0.67
10:C:814:NAG:O3	10:C:815:NAG:O5	2.13	0.67
3:I:159:TYR:HA	3:I:163:THR:HB	1.75	0.67
2:D:68:SER:OG	2:D:78:ILE:HD11	1.95	0.66
3:H:167:TRP:NE1	5:P:1:GLU:OE2	2.27	0.66
4:M:73:THR:HG21	4:M:75:THR:HG22	1.77	0.66
3:I:129:ASP:O	3:I:131:LYS:HG3	1.96	0.66
2:B:209:HIS:ND1	12:B:875:HOH:O	2.28	0.66
2:D:37:GLN:HA	2:D:42:GLY:O	1.95	0.66
3:H:41:GLU:HB3	12:H:864:HOH:O	1.95	0.66
3:H:41:GLU:O	3:H:43:PRO:HD3	1.95	0.66
3:I:116:TYR:HH	5:Q:5:PHE:HD2	1.44	0.66
3:H:219:LEU:HB3	3:H:224:LEU:HD21	1.76	0.66
10:B:810:NAG:C6	10:B:811:BMA:C2	2.25	0.66
3:I:13:SER:HB3	3:I:78:LEU:HD13	1.77	0.66
3:I:96:GLN:HG3	3:I:117:ALA:HB3	1.76	0.66
1:A:162:ILE:HB	12:A:941:HOH:O	1.95	0.66
1:A:150:ILE:HG13	12:A:940:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4:SER:O	3:I:168:LEU:HD13	1.96	0.66
2:D:37:GLN:HB2	2:D:43:LEU:HD13	1.77	0.65
2:D:47:HIS:HE1	2:D:65:TYR:HB2	1.61	0.65
3:I:189:VAL:CG2	3:I:274:TRP:HD1	2.03	0.65
3:H:58:GLU:H	3:H:58:GLU:CD	2.00	0.65
1:C:92:VAL:HG22	12:C:822:HOH:O	1.97	0.65
2:D:159:LEU:HD12	2:D:159:LEU:H	1.60	0.65
4:M:59:ASP:O	4:M:60:TRP:CD1	2.50	0.65
1:C:24:TYR:HH	1:C:66:PHE:HE2	1.43	0.65
2:D:37:GLN:HB2	2:D:43:LEU:HD12	1.78	0.65
3:I:15:PRO:HG2	3:I:91:GLY:O	1.96	0.65
10:C:814:NAG:O3	10:C:815:NAG:H61	1.97	0.65
1:C:44:GLN:HG3	12:C:854:HOH:O	1.96	0.64
2:D:127:VAL:HG12	2:D:237:ILE:HG22	1.79	0.64
4:M:36:GLU:HB3	12:M:657:HOH:O	1.97	0.64
3:I:62:ARG:NH1	5:Q:1:GLU:OE1	2.30	0.64
2:D:3:ALA:HB1	2:D:109:GLY:HA2	1.79	0.64
3:I:123:TYR:CZ	3:I:140:ALA:HA	2.32	0.64
3:I:143:THR:HG23	5:Q:8:VAL:O	1.98	0.64
4:M:35:ILE:HG23	4:M:37:ILE:HG23	1.78	0.64
3:H:129:ASP:OD2	3:H:131:LYS:HB2	1.97	0.64
1:C:126:TYR:CE2	2:D:136:GLU:HB3	2.33	0.64
2:D:125:PRO:HD3	2:D:216:PHE:CD1	2.33	0.64
3:I:194:ARG:CG	3:I:195:PRO:HD2	2.28	0.64
3:I:8:PHE:CD1	3:I:27:TYR:HD1	2.16	0.64
5:P:2:GLN:HE21	5:P:3:TYR:H	1.43	0.64
4:M:51:MET:HE3	4:M:64:ILE:HD11	1.79	0.64
3:I:94:THR:HG22	3:I:95:ILE:N	2.13	0.63
1:A:171:LYS:HE3	2:B:170:SER:HB2	1.80	0.63
12:I:962:HOH:O	4:M:62:PHE:HZ	1.81	0.63
2:B:236:ASN:ND2	10:B:809:NAG:O5	2.29	0.63
3:I:14:ARG:NH2	3:I:21:ARG:HD2	2.14	0.63
2:D:131:GLU:HB2	2:D:132:PRO:HD2	1.81	0.63
5:Q:2:GLN:HA	5:Q:2:GLN:HE21	1.64	0.63
2:D:121:ASN:OD1	2:D:122:VAL:HG13	1.99	0.63
4:M:44:LYS:HG3	4:M:44:LYS:O	1.98	0.63
3:H:144:LYS:O	3:H:148:GLU:HG3	1.98	0.63
1:C:32:LEU:HD12	1:C:49:TYR:HD2	1.64	0.63
3:H:129:ASP:O	3:H:131:LYS:HG3	1.99	0.63
4:M:44:LYS:HE2	12:M:649:HOH:O	1.97	0.63
1:A:210:ASP:OD1	2:B:134:LYS:HE3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:137:ASP:O	3:I:141:LEU:HD13	1.99	0.62
2:D:5:THR:HB	2:D:24:ASN:HB2	1.80	0.62
1:C:50:TYR:N	12:C:827:HOH:O	2.31	0.62
3:I:103:VAL:HG11	3:I:165:VAL:HG13	1.82	0.62
2:B:33:TYR:O	2:B:92:CYS:HA	1.99	0.62
1:C:67:SER:O	1:C:71:SER:N	2.31	0.62
3:I:52:MET:HE2	3:I:52:MET:HA	1.81	0.62
4:M:48:LYS:O	4:M:68:THR:HG22	2.00	0.62
4:M:5:PRO:HB3	4:M:30:PHE:HB3	1.81	0.62
1:C:208:SER:HA	2:D:135:ALA:HB2	1.81	0.62
2:D:32:MET:HA	2:D:93:ALA:O	1.99	0.62
1:A:55:VAL:O	1:A:55:VAL:HG23	1.97	0.62
10:B:810:NAG:H61	10:B:811:BMA:H2	0.63	0.62
2:D:49:SER:CB	2:D:69:ARG:HE	2.12	0.62
4:M:13:HIS:H	4:M:21:ASN:HD21	1.46	0.62
1:A:33:PHE:CE1	1:A:104:LEU:HD22	2.35	0.62
1:C:22:CYS:H	1:C:74:HIS:CD2	2.18	0.62
3:H:111:ARG:CG	3:H:111:ARG:HH11	2.06	0.62
3:I:162:GLY:O	3:I:166:GLU:HG3	2.00	0.62
1:A:36:VAL:HG22	1:A:46:LEU:HD11	1.82	0.62
1:C:77:LYS:HD2	1:C:78:ALA:H	1.65	0.62
3:H:219:LEU:CB	3:H:224:LEU:HD21	2.30	0.62
2:B:142:LYS:HD3	2:B:197:ARG:HD3	1.80	0.62
1:A:40:ARG:HH11	2:B:113:ARG:HH22	1.48	0.61
1:C:142:LEU:HD23	1:C:181:ILE:HG12	1.82	0.61
2:B:18:LYS:HD2	2:B:80:GLU:HA	1.82	0.61
1:C:3:VAL:HG13	1:C:107:GLY:CA	2.30	0.61
1:C:128:LEU:N	1:C:128:LEU:HD23	2.15	0.61
3:H:135:ALA:HB1	3:H:140:ALA:HB3	1.81	0.61
4:M:2:GLN:O	4:M:2:GLN:HG3	2.00	0.61
4:M:41:LYS:O	4:M:42:ASN:HB2	1.99	0.61
2:D:242:TRP:HB3	2:D:244:ARG:HH12	1.65	0.61
1:A:191:CYS:HA	1:A:194:ILE:HG22	1.83	0.61
8:A:806:NAG:O3	8:A:807:BMA:C1	2.49	0.61
2:B:18:LYS:HE3	2:B:80:GLU:HG2	1.82	0.61
3:I:96:GLN:CG	3:I:117:ALA:HB3	2.30	0.61
3:I:145:HIS:O	3:I:149:GLN:HB2	2.00	0.61
1:A:158:SER:O	7:A:805:NAG:H82	2.01	0.61
1:C:17:SER:HA	12:C:820:HOH:O	2.00	0.61
3:I:62:ARG:NH1	3:I:63:GLU:OE2	2.34	0.61
3:I:96:GLN:NE2	4:M:31:HIS:NE2	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:7:SER:O	5:Q:8:VAL:C	2.37	0.61
2:D:124:PRO:HD3	2:D:232:PRO:HG3	1.82	0.61
3:I:152:GLU:C	3:I:154:GLU:H	2.04	0.61
2:B:27:ASN:HB3	2:B:29:HIS:ND1	2.15	0.61
3:H:191:HIS:HB2	3:H:274:TRP:NE1	2.15	0.61
2:D:13:ALA:HB2	2:D:19:VAL:HG21	1.83	0.61
2:D:74:ASN:O	2:D:75:PHE:HB2	2.01	0.61
3:I:144:LYS:HG2	3:I:148:GLU:OE2	2.01	0.61
1:C:32:LEU:HD12	1:C:49:TYR:CD2	2.36	0.60
1:C:66:PHE:CB	12:C:835:HOH:O	2.48	0.60
3:I:147:TRP:C	3:I:149:GLN:H	2.05	0.60
2:D:149:ALA:HB2	2:D:214:VAL:HG22	1.82	0.60
2:D:226:PRO:HG2	2:D:227:GLU:OE1	2.00	0.60
1:A:127:ALA:C	1:A:128:LEU:HD12	2.22	0.60
1:C:140:LEU:HB3	1:C:183:TRP:CB	2.31	0.60
2:D:6:GLN:HG3	2:D:111:GLY:N	2.17	0.60
2:B:57:LYS:HD2	12:B:896:HOH:O	2.01	0.60
1:C:140:LEU:HB3	1:C:183:TRP:HB3	1.83	0.60
4:M:21:ASN:ND2	4:M:22:ILE:H	2.00	0.60
2:B:236:ASN:ND2	10:B:809:NAG:H2	2.14	0.60
2:D:23:CYS:HB3	2:D:75:PHE:O	2.02	0.60
1:C:45:LEU:HD13	12:C:825:HOH:O	2.01	0.60
2:B:130:PHE:HB2	2:B:146:VAL:CG1	2.23	0.60
2:B:236:ASN:OD1	10:B:809:NAG:C1	2.50	0.60
2:B:232:PRO:HA	12:B:884:HOH:O	2.01	0.60
3:I:209:TYR:HA	3:I:210:PRO:O	2.02	0.59
3:I:215:LEU:CD2	3:I:261:VAL:HG13	2.32	0.59
2:D:27:ASN:O	2:D:28:ASN:HB2	2.01	0.59
2:D:32:MET:HB3	2:D:75:PHE:CD2	2.37	0.59
3:I:130:LEU:HD22	3:I:130:LEU:N	2.18	0.59
2:B:211:ARG:NH2	2:B:213:GLN:OE1	2.35	0.59
1:C:20:LEU:N	1:C:20:LEU:HD23	2.16	0.59
3:I:189:VAL:HG13	3:I:272:LEU:HD12	1.83	0.59
2:D:242:TRP:HD1	2:D:243:GLY:H	1.49	0.59
1:C:16:ALA:O	1:C:80:VAL:HG22	2.03	0.59
1:C:3:VAL:HG12	12:C:822:HOH:O	2.02	0.59
1:A:194:ILE:HG23	1:A:195:PHE:CD1	2.34	0.59
2:D:122:VAL:HA	2:D:153:PHE:HB3	1.85	0.59
2:D:45:LEU:HD21	2:D:48:TYR:CD2	2.36	0.59
3:I:35:ARG:HB3	3:I:48:ARG:CD	2.33	0.59
1:C:196:LYS:NZ	1:C:196:LYS:HB2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:ASN:HD22	2:D:209:HIS:HB3	1.66	0.58
1:C:194:ILE:HG23	1:C:195:PHE:CD2	2.38	0.58
1:C:22:CYS:H	1:C:74:HIS:HD2	1.50	0.58
2:D:121:ASN:CG	2:D:153:PHE:CD2	2.76	0.58
2:D:171:GLY:HA3	2:D:196:LEU:HD12	1.86	0.58
2:B:30:ASN:HD21	3:H:146:LYS:NZ	2.01	0.58
3:I:96:GLN:HB2	3:I:117:ALA:HB3	1.86	0.58
3:I:227:ASP:O	3:I:227:ASP:OD1	2.21	0.58
1:C:191:CYS:O	1:C:192:GLN:HG3	2.03	0.58
2:D:150:ARG:HG2	2:D:190:TYR:O	2.03	0.58
3:H:263:HIS:CD2	3:H:265:GLY:H	2.21	0.58
4:M:25:CYS:O	4:M:65:LEU:HD12	2.04	0.58
2:D:34:TRP:O	2:D:46:ILE:N	2.34	0.58
3:I:194:ARG:NH1	3:I:248:VAL:HG21	2.18	0.58
2:D:4:VAL:HG13	2:D:24:ASN:O	2.04	0.58
3:H:169:ARG:HH21	3:I:269:PRO:HD2	1.67	0.58
2:D:78:ILE:N	2:D:78:ILE:HD12	2.18	0.58
3:H:185:PRO:HB3	3:H:208:PHE:HB3	1.86	0.58
2:B:96:GLY:HA3	3:H:150:ALA:HB1	1.84	0.58
1:C:66:PHE:HB2	12:C:835:HOH:O	2.03	0.58
2:D:81:LEU:O	2:D:81:LEU:HD23	2.03	0.58
1:C:44:GLN:HA	1:C:44:GLN:OE1	2.03	0.58
2:D:3:ALA:HB1	2:D:109:GLY:CA	2.34	0.58
5:Q:6:TYR:O	5:Q:8:VAL:N	2.37	0.58
1:A:40:ARG:HH11	2:B:113:ARG:NH2	2.01	0.57
2:B:232:PRO:CA	12:B:884:HOH:O	2.51	0.57
2:D:153:PHE:HD1	2:D:187:TYR:O	1.85	0.57
3:I:114:GLN:C	3:I:115:GLN:HG3	2.24	0.57
2:D:128:SER:HB2	2:D:148:LEU:HD22	1.85	0.57
3:I:79:ARG:HB2	12:I:960:HOH:O	2.03	0.57
4:M:54:MET:SD	4:M:62:PHE:HD2	2.27	0.57
3:H:108:ARG:NH2	3:I:214:THR:OG1	2.37	0.57
5:P:2:GLN:CA	5:P:2:GLN:HE21	2.18	0.57
1:C:82:TRP:CH2	1:C:167:VAL:HG21	2.39	0.57
3:I:147:TRP:HB3	3:I:152:GLU:HB3	1.85	0.57
3:I:263:HIS:HD2	3:I:265:GLY:H	1.47	0.57
3:I:23:MET:HA	3:I:36:PHE:O	2.04	0.57
1:A:48:LYS:HD3	2:B:105:THR:CG2	2.35	0.57
2:B:25:GLN:OE1	2:B:27:ASN:HB2	2.05	0.57
1:C:142:LEU:HD22	1:C:143:PHE:N	2.18	0.57
3:I:194:ARG:HH12	3:I:248:VAL:HG21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:45:TYR:HB3	3:I:60:TRP:CE3	2.39	0.57
4:M:73:THR:HG22	4:M:75:THR:N	2.14	0.57
1:C:168:LEU:N	1:C:168:LEU:HD23	2.19	0.57
2:D:37:GLN:C	2:D:37:GLN:NE2	2.58	0.57
1:A:185:ASN:HD21	7:A:805:NAG:C7	2.16	0.57
3:I:97:VAL:HG11	5:Q:5:PHE:CE2	2.39	0.57
3:I:234:ARG:HH11	4:M:8:GLN:HE21	1.50	0.57
1:C:170:MET:N	1:C:175:SER:HB3	2.17	0.57
2:D:94:SER:O	2:D:106:LEU:HB3	2.05	0.57
2:D:82:ALA:HB1	2:D:116:VAL:HG11	1.87	0.57
2:D:137:ILE:HG12	2:D:137:ILE:O	2.05	0.57
2:D:35:TYR:HA	2:D:44:ARG:O	2.04	0.57
2:D:150:ARG:HG3	2:D:191:CYS:HA	1.87	0.57
2:D:150:ARG:CG	2:D:191:CYS:HA	2.35	0.57
4:M:2:GLN:HB3	4:M:32:PRO:HD3	1.87	0.56
1:A:206:TYR:HB3	2:B:135:ALA:HB1	1.86	0.56
3:I:135:ALA:HB1	3:I:137:ASP:OD2	2.05	0.56
1:A:156:MET:HB3	12:A:956:HOH:O	2.05	0.56
1:C:128:LEU:HD21	1:C:140:LEU:HG	1.86	0.56
3:I:62:ARG:HH12	5:Q:1:GLU:HB2	1.70	0.56
3:I:194:ARG:HH11	3:I:248:VAL:CG1	2.19	0.56
3:I:66:LYS:HG2	3:I:70:ASN:HD21	1.70	0.56
3:I:8:PHE:HB2	3:I:25:VAL:HG23	1.87	0.56
4:M:37:ILE:HG22	4:M:82:VAL:CG1	2.32	0.56
1:A:190:THR:HG23	1:A:191:CYS:N	2.21	0.56
1:A:190:THR:CG2	1:A:192:GLN:HG2	2.36	0.56
1:C:33:PHE:HB2	12:C:832:HOH:O	2.05	0.56
3:I:6:ARG:NH1	4:M:58:LYS:HD3	2.20	0.56
1:A:150:ILE:HG23	12:A:940:HOH:O	2.06	0.56
1:C:120:ASN:ND2	1:C:122:GLU:OE1	2.35	0.56
1:C:129:LYS:HD2	1:C:129:LYS:N	2.21	0.56
2:D:53:GLY:HA2	2:D:69:ARG:HB3	1.87	0.56
1:A:14:GLU:OE2	1:A:81:HIS:HB3	2.05	0.56
3:I:124:ILE:HB	3:I:140:ALA:CB	2.34	0.56
3:I:185:PRO:CB	3:I:208:PHE:HB3	2.36	0.56
3:I:38:SER:HA	3:I:43:PRO:HB3	1.88	0.56
4:L:40:LEU:HD23	4:L:45:LYS:HA	1.86	0.56
4:M:11:SER:C	12:M:272:HOH:O	2.44	0.56
1:C:91:ALA:HB3	12:C:832:HOH:O	2.06	0.56
2:B:18:LYS:CD	2:B:80:GLU:HA	2.36	0.55
2:D:142:LYS:HD3	2:D:197:ARG:CZ	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:24:GLU:O	3:I:35:ARG:HA	2.06	0.55
3:I:96:GLN:CB	3:I:117:ALA:HB3	2.36	0.55
3:I:167:TRP:CD1	5:Q:1:GLU:HG2	2.40	0.55
1:C:118:ILE:HD11	1:C:147:ASP:OD2	2.06	0.55
2:D:37:GLN:CA	2:D:43:LEU:HA	2.37	0.55
1:C:140:LEU:HB2	1:C:182:ALA:O	2.05	0.55
2:D:105:THR:HG23	2:D:105:THR:O	2.07	0.55
3:I:58:GLU:O	3:I:62:ARG:HB2	2.06	0.55
4:L:21:ASN:HB3	4:L:70:PHE:CE1	2.41	0.55
2:B:31:ASN:HD22	2:B:50:TYR:HA	1.70	0.55
2:D:19:VAL:O	2:D:79:LEU:HD23	2.06	0.55
3:H:225:ILE:HG23	3:H:226:GLN:NE2	2.22	0.55
4:M:49:VAL:HA	4:M:68:THR:CG2	2.36	0.55
2:D:9:ARG:HA	2:D:112:THR:CG2	2.36	0.55
3:I:138:MET:O	3:I:141:LEU:HB2	2.06	0.55
3:I:140:ALA:O	3:I:144:LYS:N	2.40	0.55
1:A:186:GLN:HB3	1:A:189:PHE:HD2	1.71	0.55
3:I:23:MET:HB3	3:I:37:ASP:OD1	2.06	0.55
4:M:33:PRO:HB3	4:M:62:PHE:CE2	2.41	0.55
4:M:2:GLN:CB	4:M:32:PRO:HD3	2.37	0.55
2:D:186:ASN:ND2	2:D:186:ASN:O	2.40	0.55
3:H:202:ARG:HG3	3:H:246:SER:HB3	1.89	0.55
3:I:25:VAL:HG11	3:I:35:ARG:CZ	2.37	0.55
4:L:49:VAL:HG22	4:L:68:THR:CG2	2.37	0.55
3:H:192:HIS:CE1	4:L:98:ASP:HB3	2.42	0.55
4:M:69:GLU:O	4:M:70:PHE:HB3	2.06	0.55
5:Q:2:GLN:CA	5:Q:2:GLN:HE21	2.20	0.55
2:B:153:PHE:O	2:B:155:ASP:N	2.40	0.55
2:D:225:TRP:CZ3	2:D:232:PRO:HD2	2.42	0.55
3:I:170:ARG:HH11	3:I:170:ARG:HG2	1.71	0.55
10:B:810:NAG:H61	10:B:811:BMA:C3	2.33	0.55
1:C:170:MET:HG2	1:C:171:LYS:N	2.21	0.55
2:D:316:LEU:HG	2:D:117:GLU:H	1.72	0.55
1:C:106:PHE:CD1	2:D:43:LEU:HD23	2.42	0.55
3:H:21:ARG:HE	3:H:23:MET:HE2	1.72	0.55
3:I:135:ALA:HB1	3:I:137:ASP:CG	2.27	0.55
3:I:202:ARG:HG2	3:I:204:TRP:NE1	2.22	0.55
3:I:11:ALA:HA	3:I:21:ARG:O	2.07	0.55
2:D:143:ALA:HB3	2:D:198:VAL:HG23	1.88	0.54
4:L:37:ILE:HD12	4:L:51:MET:HE3	1.89	0.54
2:D:86:GLN:NE2	2:D:114:LEU:HD21	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:230:LEU:CD1	3:I:245:ALA:HB2	2.38	0.54
4:M:12:ARG:N	12:M:272:HOH:O	2.40	0.54
2:B:123:THR:O	2:B:152:PHE:HA	2.08	0.54
2:B:235:GLN:OE1	2:B:237:ILE:HD11	2.07	0.54
1:C:115:LEU:H	1:C:115:LEU:CD2	2.20	0.54
1:C:34:TRP:CH2	1:C:90:CYS:HB2	2.42	0.54
4:M:12:ARG:HE	4:M:13:HIS:HE1	1.54	0.54
1:A:158:SER:O	7:A:805:NAG:C8	2.56	0.54
1:A:17:SER:HA	1:A:78:ALA:O	2.06	0.54
3:I:35:ARG:HB3	3:I:48:ARG:HD3	1.89	0.54
2:D:164:ASN:HD22	2:D:164:ASN:N	2.04	0.54
2:D:35:TYR:CD2	2:D:43:LEU:HG	2.43	0.54
3:H:271:THR:O	3:H:271:THR:HG23	2.08	0.54
4:M:6:GLN:O	4:M:27:VAL:HA	2.07	0.54
4:L:97:ARG:HG2	4:L:97:ARG:HH11	1.72	0.54
2:D:123:THR:O	2:D:152:PHE:HB2	2.07	0.53
2:D:33:TYR:O	2:D:92:CYS:HA	2.08	0.53
3:H:220:ASN:ND2	3:H:222:GLU:OE1	2.41	0.53
3:I:127:ASN:N	3:I:127:ASN:HD22	2.05	0.53
3:I:141:LEU:HA	3:I:144:LYS:HB3	1.91	0.53
3:I:207:GLY:HA2	3:I:240:THR:HB	1.89	0.53
2:D:198:VAL:HG21	2:D:203:TRP:HB2	1.90	0.53
1:A:36:VAL:HG21	1:A:46:LEU:HD21	1.91	0.53
3:I:117:ALA:HB2	4:M:60:TRP:CE3	2.43	0.53
2:D:127:VAL:HG23	2:D:148:LEU:O	2.08	0.53
3:I:17:LEU:HD22	3:I:17:LEU:N	2.23	0.53
4:M:62:PHE:HD1	12:M:247:HOH:O	1.89	0.53
4:M:7:ILE:N	4:M:7:ILE:HD12	2.23	0.53
1:C:38:TYR:HB2	1:C:41:GLN:HB2	1.91	0.53
2:D:171:GLY:HA3	2:D:196:LEU:CD1	2.37	0.53
3:I:155:ARG:HG2	3:I:155:ARG:O	2.08	0.53
4:M:49:VAL:HA	4:M:68:THR:HG22	1.91	0.53
1:C:168:LEU:HD21	1:C:178:ASN:O	2.09	0.53
2:D:124:PRO:HG3	2:D:235:GLN:HE22	1.73	0.53
3:H:152:GLU:OE1	3:H:155:ARG:NH1	2.39	0.53
3:I:272:LEU:N	3:I:272:LEU:HD23	2.24	0.53
3:I:41:GLU:OE2	3:I:41:GLU:N	2.41	0.53
4:M:28:THR:HB	12:M:281:HOH:O	2.07	0.52
1:A:25:SER:O	1:A:26:TYR:HB2	2.09	0.52
1:C:115:LEU:HD22	1:C:115:LEU:N	2.24	0.52
2:D:145:LEU:HD23	2:D:145:LEU:N	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:185:PRO:HB3	3:I:208:PHE:CB	2.38	0.52
3:I:25:VAL:CG1	3:I:35:ARG:CZ	2.86	0.52
4:M:21:ASN:C	4:M:22:ILE:HD12	2.29	0.52
2:D:86:GLN:HE21	2:D:114:LEU:HD21	1.75	0.52
3:H:133:TRP:HH2	3:H:156:LEU:HD12	1.73	0.52
1:A:139:THR:O	1:A:140:LEU:HB2	2.09	0.52
1:A:38:TYR:HB3	1:A:39:PRO:HD2	1.90	0.52
3:H:135:ALA:HB1	3:H:140:ALA:CB	2.40	0.52
4:M:56:PHE:HB2	4:M:61:SER:O	2.09	0.52
1:C:151:ASN:ND2	1:C:151:ASN:O	2.42	0.52
2:D:150:ARG:C	2:D:150:ARG:HD2	2.30	0.52
3:I:127:ASN:HB2	3:I:129:ASP:OD1	2.10	0.52
3:I:232:GLU:HB2	12:I:950:HOH:O	2.10	0.52
2:D:121:ASN:OD1	2:D:122:VAL:N	2.42	0.52
3:I:237:GLY:HA3	12:M:248:HOH:O	2.09	0.52
2:D:83:THR:OG1	2:D:84:PRO:HD2	2.10	0.52
12:B:812:HOH:O	3:H:146:LYS:HG3	2.09	0.52
3:I:32:GLU:OE2	3:I:48:ARG:HG3	2.10	0.52
3:I:56:GLY:C	3:I:58:GLU:H	2.13	0.52
5:P:2:GLN:HE21	5:P:3:TYR:N	2.06	0.52
2:D:57:LYS:HD2	2:D:61:PRO:HB3	1.92	0.51
2:D:69:ARG:HH12	2:D:72:GLN:HA	1.74	0.51
3:H:145:HIS:O	3:H:149:GLN:HG3	2.11	0.51
1:A:36:VAL:CG2	1:A:46:LEU:HD21	2.41	0.51
2:B:159:LEU:HD12	2:B:160:SER:N	2.26	0.51
2:B:143:ALA:O	2:B:197:ARG:HA	2.10	0.51
1:C:18:LEU:HD12	1:C:19:GLN:H	1.75	0.51
2:D:51:GLY:O	2:D:69:ARG:CZ	2.59	0.51
3:I:94:THR:HG22	3:I:95:ILE:H	1.75	0.51
1:A:147:ASP:OD2	1:A:149:GLN:HB2	2.10	0.51
4:L:7:ILE:HD11	4:L:82:VAL:CG2	2.40	0.51
4:M:12:ARG:HH21	4:M:13:HIS:HE1	1.58	0.51
5:Q:2:GLN:HG3	5:Q:3:TYR:O	2.10	0.51
2:B:156:HIS:HB2	2:B:217:HIS:HB2	1.92	0.51
2:D:31:ASN:HB2	2:D:95:GLY:O	2.10	0.51
3:I:194:ARG:HH11	3:I:248:VAL:HG11	1.75	0.51
1:A:36:VAL:HG23	1:A:46:LEU:HG	1.92	0.51
1:C:50:TYR:HB3	3:I:158:ALA:HB1	1.92	0.51
1:A:42:GLY:HA2	2:B:91:PHE:CE2	2.46	0.51
2:B:69:ARG:HH12	2:B:72:GLN:C	2.14	0.51
3:H:111:ARG:CG	3:H:111:ARG:NH1	2.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:10:THR:HA	3:I:95:ILE:O	2.10	0.51
2:B:204:HIS:O	2:B:206:PRO:HD3	2.10	0.51
2:B:31:ASN:HA	2:B:49:SER:O	2.11	0.51
2:B:68:SER:O	2:B:70:PRO:HD3	2.11	0.51
4:L:40:LEU:HD21	4:L:81:ARG:NH2	2.20	0.51
3:I:196:GLU:HB3	12:I:992:HOH:O	2.11	0.51
3:I:155:ARG:HH22	5:Q:4:LYS:HB3	1.75	0.51
1:C:110:THR:O	1:C:110:THR:HG23	2.11	0.51
2:D:159:LEU:HD12	2:D:159:LEU:N	2.26	0.51
3:I:11:ALA:O	3:I:95:ILE:HG13	2.10	0.51
4:M:53:ASP:O	4:M:64:ILE:HD12	2.11	0.50
1:A:157:GLU:HG2	1:A:158:SER:O	2.11	0.50
1:A:168:LEU:O	1:A:176:LYS:HA	2.10	0.50
2:B:221:GLU:H	2:B:221:GLU:CD	2.15	0.50
1:C:168:LEU:HG	1:C:177:SER:HB3	1.93	0.50
2:D:77:LEU:HD23	2:D:79:LEU:HD22	1.92	0.50
3:H:218:GLN:NE2	3:H:260:HIS:CE1	2.79	0.50
1:A:140:LEU:HA	1:A:182:ALA:O	2.12	0.50
2:D:3:ALA:HA	2:D:108:PHE:O	2.12	0.50
3:I:242:GLN:HG2	12:I:912:HOH:O	2.11	0.50
1:A:173:MET:HG3	1:A:174:ASP:H	1.76	0.50
3:I:202:ARG:HD2	3:I:244:TRP:CD2	2.47	0.50
4:M:12:ARG:HB2	12:M:272:HOH:O	2.11	0.50
1:A:82:TRP:CZ2	1:A:167:VAL:HB	2.47	0.50
2:B:153:PHE:HB3	2:B:154:PRO:CD	2.41	0.50
1:C:93:SER:HB2	1:C:104:LEU:HD23	1.93	0.50
2:D:77:LEU:CD2	2:D:79:LEU:HD22	2.41	0.50
3:H:9:VAL:O	3:H:96:GLN:HA	2.11	0.50
3:I:170:ARG:O	3:I:173:LYS:HB3	2.11	0.50
1:A:54:PRO:O	1:A:65:GLU:HA	2.12	0.50
1:C:14:GLU:HG2	1:C:15:GLY:N	2.26	0.50
2:D:77:LEU:C	2:D:77:LEU:HD23	2.32	0.50
2:B:68:SER:C	2:B:70:PRO:HD3	2.32	0.50
1:C:128:LEU:C	1:C:129:LYS:HD2	2.32	0.50
1:C:3:VAL:CG1	1:C:107:GLY:N	2.75	0.50
2:D:210:PHE:HB2	2:D:241:ALA:HB3	1.93	0.50
3:I:96:GLN:HB3	4:M:56:PHE:CZ	2.47	0.50
2:D:152:PHE:CD1	2:D:152:PHE:N	2.80	0.50
2:D:6:GLN:HG2	2:D:110:ALA:HB3	1.93	0.50
3:H:202:ARG:HD3	3:H:244:TRP:CD2	2.46	0.50
3:H:248:VAL:O	3:H:248:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:12:ARG:CA	12:M:272:HOH:O	2.59	0.50
4:M:73:THR:HG22	4:M:74:GLU:N	2.27	0.50
2:D:140:LYS:CD	2:D:142:LYS:HB2	2.41	0.49
3:I:148:GLU:O	3:I:149:GLN:HG3	2.12	0.49
3:I:35:ARG:HB3	3:I:48:ARG:HE	1.76	0.49
4:M:2:GLN:CA	4:M:31:HIS:O	2.51	0.49
1:C:59:VAL:O	1:C:62:PHE:HD1	1.95	0.49
2:D:33:TYR:N	2:D:33:TYR:CD1	2.80	0.49
4:M:73:THR:CG2	4:M:74:GLU:N	2.75	0.49
1:C:60:ASN:HB2	1:C:62:PHE:HE1	1.77	0.49
2:D:125:PRO:HB2	2:D:214:VAL:HG11	1.92	0.49
4:L:49:VAL:HA	4:L:68:THR:HG22	1.93	0.49
4:M:28:THR:HG22	4:M:63:TYR:HB2	1.92	0.49
2:B:93:ALA:HA	2:B:107:TYR:O	2.12	0.49
2:D:169:HIS:O	2:D:170:SER:HB2	2.13	0.49
3:H:215:LEU:HD22	3:H:261:VAL:HG22	1.95	0.49
3:H:169:ARG:NH2	3:I:269:PRO:HD2	2.27	0.49
4:M:4:THR:HG23	4:M:86:SER:OG	2.12	0.49
1:A:156:MET:N	1:A:156:MET:SD	2.82	0.49
2:B:228:GLY:O	2:B:229:SER:C	2.50	0.49
2:D:11:LYS:HD2	2:D:12:VAL:H	1.77	0.49
3:I:56:GLY:O	3:I:59:TYR:HB3	2.12	0.49
3:I:116:TYR:OH	5:Q:5:PHE:HD2	1.95	0.49
3:I:9:VAL:HB	3:I:97:VAL:CG2	2.43	0.49
1:A:188:SER:O	1:A:189:PHE:HB2	2.12	0.49
1:A:179:GLY:HA3	2:B:195:ARG:NH1	2.27	0.49
2:B:78:ILE:N	2:B:78:ILE:HD12	2.28	0.49
1:C:160:THR:HG23	1:C:184:SER:HB3	1.94	0.49
2:D:146:VAL:HG22	2:D:147:CYS:N	2.27	0.49
2:D:150:ARG:HB2	2:D:191:CYS:HA	1.94	0.49
2:D:175:ASP:HB2	2:D:192:LEU:HD12	1.94	0.49
2:D:49:SER:OG	2:D:69:ARG:NE	2.45	0.49
1:C:82:TRP:CD1	1:C:116:PRO:HD3	2.48	0.49
2:D:14:VAL:HB	2:D:17:GLY:N	2.19	0.49
3:I:36:PHE:HB2	3:I:45:TYR:CD1	2.48	0.49
3:I:9:VAL:O	3:I:96:GLN:HA	2.12	0.49
4:L:48:LYS:O	4:L:48:LYS:HG3	2.12	0.49
2:B:152:PHE:CE1	2:B:190:TYR:HB2	2.48	0.49
1:A:170:MET:HB2	1:A:175:SER:CB	2.43	0.49
1:A:92:VAL:HG22	1:A:93:SER:N	2.28	0.49
2:B:66:LYS:NZ	2:B:80:GLU:OE2	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:37:ASP:C	3:I:39:ASP:H	2.16	0.49
3:I:35:ARG:HB3	3:I:48:ARG:NE	2.28	0.49
1:C:3:VAL:HG13	1:C:107:GLY:N	2.28	0.48
1:C:60:ASN:CB	1:C:62:PHE:HE1	2.26	0.48
2:D:199:SER:HB2	2:D:202:PHE:CD2	2.48	0.48
3:H:97:VAL:HA	3:H:115:GLN:O	2.13	0.48
2:B:87:THR:O	2:B:88:SER:HB2	2.12	0.48
1:C:142:LEU:HD22	1:C:143:PHE:H	1.78	0.48
3:H:6:ARG:NH1	3:H:113:TYR:OH	2.44	0.48
3:I:15:PRO:O	3:I:17:LEU:HD22	2.13	0.48
3:I:32:GLU:OE1	3:I:35:ARG:NH2	2.44	0.48
3:I:9:VAL:HG11	3:I:74:PHE:CE1	2.48	0.48
4:M:3:LYS:O	4:M:30:PHE:HA	2.14	0.48
4:M:20:PRO:HG3	4:M:71:THR:OG1	2.13	0.48
3:H:9:VAL:HB	3:H:97:VAL:CG1	2.24	0.48
3:I:191:HIS:HB2	3:I:274:TRP:CZ2	2.48	0.48
4:M:46:ILE:HG23	4:M:47:PRO:HD2	1.95	0.48
2:B:25:GLN:HG2	2:B:27:ASN:H	1.78	0.48
2:D:122:VAL:HG23	2:D:225:TRP:HZ3	1.77	0.48
2:D:143:ALA:HB3	2:D:198:VAL:CG2	2.42	0.48
3:H:113:TYR:CD2	3:H:113:TYR:N	2.80	0.48
3:I:217:TRP:HD1	3:I:228:MET:HE2	1.77	0.48
1:C:172:ALA:C	1:C:174:ASP:H	2.17	0.48
2:D:171:GLY:O	2:D:172:VAL:C	2.51	0.48
2:D:34:TRP:CD1	2:D:77:LEU:HB2	2.48	0.48
3:I:10:THR:HG22	3:I:23:MET:HG3	1.95	0.48
3:I:55:GLU:HB3	3:I:59:TYR:CD2	2.49	0.48
3:I:167:TRP:NE1	5:Q:1:GLU:OE2	2.46	0.48
2:B:316:LEU:N	2:B:316:LEU:HD12	2.29	0.48
1:C:55:VAL:O	1:C:55:VAL:HG23	2.14	0.48
2:D:173:SER:HB3	2:D:195:ARG:HG2	1.96	0.48
1:C:80:VAL:CG2	1:C:80:VAL:O	2.58	0.48
2:D:109:GLY:O	2:D:110:ALA:HB2	2.13	0.48
2:D:120:ARG:NH1	2:D:120:ARG:HB2	2.29	0.48
3:I:152:GLU:C	3:I:154:GLU:N	2.66	0.48
3:I:45:TYR:HB3	3:I:60:TRP:CZ3	2.49	0.48
3:H:194:ARG:HG2	3:H:195:PRO:HD2	1.95	0.48
3:H:249:VAL:HG23	3:H:254:GLU:HG3	1.95	0.48
3:I:207:GLY:HA2	3:I:240:THR:CB	2.44	0.48
2:D:216:PHE:HB3	2:D:235:GLN:O	2.13	0.48
2:D:79:LEU:HD23	2:D:79:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:199:VAL:HG21	3:H:251:LEU:HD13	1.95	0.48
3:I:14:ARG:NH2	3:I:21:ARG:HB2	2.29	0.47
1:C:14:GLU:HA	1:C:114:VAL:HG23	1.96	0.47
3:I:116:TYR:O	3:I:122:ASP:HA	2.14	0.47
2:D:18:LYS:HG3	2:D:80:GLU:OE2	2.14	0.47
2:D:142:LYS:HD3	2:D:197:ARG:NH1	2.29	0.47
2:D:31:ASN:O	2:D:94:SER:HA	2.14	0.47
3:I:132:THR:HG22	3:I:133:TRP:N	2.29	0.47
3:I:51:TRP:CZ3	3:I:52:MET:HG2	2.49	0.47
2:B:30:ASN:HA	2:B:72:GLN:HE22	1.79	0.47
3:H:218:GLN:NE2	3:H:260:HIS:ND1	2.62	0.47
3:I:130:LEU:N	3:I:130:LEU:CD2	2.77	0.47
4:L:17:ASN:HA	4:L:72:PRO:O	2.14	0.47
1:A:12:VAL:O	1:A:114:VAL:HA	2.14	0.47
2:D:46:ILE:HG22	2:D:47:HIS:CE1	2.49	0.47
5:Q:2:GLN:HA	5:Q:2:GLN:NE2	2.28	0.47
2:B:127:VAL:HG13	2:B:237:ILE:HG22	1.96	0.47
2:D:14:VAL:HG12	2:D:15:THR:H	1.78	0.47
3:I:155:ARG:HH22	5:Q:4:LYS:CB	2.27	0.47
1:A:128:LEU:HD12	1:A:128:LEU:N	2.30	0.47
1:A:45:LEU:HD11	1:A:47:LEU:O	2.15	0.47
2:D:214:VAL:O	2:D:216:PHE:N	2.47	0.47
2:D:125:PRO:HD3	2:D:216:PHE:CG	2.50	0.47
2:B:69:ARG:NH1	2:B:71:SER:O	2.48	0.47
1:C:91:ALA:HB2	1:C:106:PHE:HA	1.97	0.47
2:D:8:PRO:C	2:D:10:ASN:H	2.17	0.47
3:I:14:ARG:CZ	3:I:21:ARG:HB2	2.45	0.47
3:I:214:THR:HB	3:I:262:TYR:HB2	1.96	0.47
3:I:44:ARG:HG2	3:I:44:ARG:HH11	1.79	0.47
3:H:236:ALA:O	4:L:12:ARG:HD3	2.15	0.47
3:I:143:THR:HG21	5:Q:8:VAL:CB	2.45	0.47
2:D:6:GLN:OE1	2:D:6:GLN:HA	2.15	0.47
3:I:222:GLU:HG3	3:I:223:GLU:H	1.80	0.47
2:B:316:LEU:HD23	2:B:153:PHE:HE2	1.80	0.47
4:L:23:LEU:HD11	4:L:78:TYR:CB	2.45	0.47
4:L:23:LEU:HD11	4:L:78:TYR:HB3	1.97	0.47
4:M:30:PHE:O	4:M:31:HIS:HB2	2.14	0.47
1:C:196:LYS:HZ1	1:C:196:LYS:HB2	1.78	0.46
1:C:61:GLY:HA3	1:C:77:LYS:NZ	2.30	0.46
1:C:77:LYS:HE3	1:C:79:SER:H	1.81	0.46
1:C:93:SER:HB2	1:C:104:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:266:LEU:HD13	3:H:270:LEU:HG	1.95	0.46
1:C:50:TYR:HB3	3:I:158:ALA:CB	2.45	0.46
3:I:10:THR:CG2	3:I:23:MET:CG	2.93	0.46
3:I:79:ARG:HA	3:I:82:LEU:HD12	1.96	0.46
1:A:171:LYS:HG3	2:B:170:SER:HB2	1.97	0.46
1:C:1:GLN:OE1	1:C:100:PHE:N	2.47	0.46
3:I:143:THR:OG1	5:Q:8:VAL:HB	2.16	0.46
2:B:233:VAL:HG22	2:B:234:THR:N	2.30	0.46
3:H:191:HIS:NE2	3:H:199:VAL:HG11	2.30	0.46
3:I:143:THR:O	3:I:143:THR:HG22	2.14	0.46
3:I:74:PHE:CZ	3:I:97:VAL:HG21	2.50	0.46
3:I:147:TRP:HZ2	5:Q:8:VAL:HA	1.81	0.46
4:M:31:HIS:HD1	4:M:32:PRO:CA	2.19	0.46
1:A:129:LYS:NZ	1:A:129:LYS:HB2	2.30	0.46
1:C:137:ASP:CG	1:C:138:SER:H	2.18	0.46
1:C:5:GLN:HB3	1:C:7:ASP:OD2	2.15	0.46
2:D:136:GLU:HB2	2:D:140:LYS:NZ	2.31	0.46
2:D:15:THR:O	2:D:15:THR:HG22	2.14	0.46
3:H:206:LEU:HD23	3:H:242:GLN:HB3	1.97	0.46
3:I:88:SER:O	3:I:89:ALA:O	2.34	0.46
2:B:1:GLU:HB3	12:B:842:HOH:O	2.16	0.46
1:C:29:THR:HG21	12:C:853:HOH:O	2.15	0.46
3:H:180:LEU:O	3:H:181:ARG:C	2.53	0.46
3:I:152:GLU:O	3:I:154:GLU:N	2.49	0.46
3:I:27:TYR:HE2	3:I:32:GLU:HB2	1.80	0.46
4:L:7:ILE:HD11	4:L:82:VAL:HG21	1.98	0.46
1:C:20:LEU:HD13	1:C:88:TYR:CG	2.50	0.46
2:D:175:ASP:HB2	2:D:192:LEU:CD1	2.45	0.46
3:I:187:ALA:HA	3:I:204:TRP:O	2.16	0.46
4:M:24:ASN:OD1	4:M:65:LEU:HD21	2.16	0.46
1:A:195:PHE:O	1:A:198:THR:HG23	2.16	0.46
1:A:205:THR:O	1:A:205:THR:HG22	2.16	0.46
1:A:43:LEU:N	1:A:43:LEU:HD12	2.31	0.46
2:D:220:SER:C	2:D:222:GLU:H	2.19	0.46
3:H:191:HIS:HB2	3:H:274:TRP:CE2	2.51	0.46
3:I:221:GLY:O	3:I:222:GLU:HB2	2.16	0.46
3:I:94:THR:CG2	3:I:95:ILE:N	2.78	0.46
1:A:156:MET:HE3	12:A:956:HOH:O	2.16	0.46
1:C:155:THR:CG2	1:C:161:PHE:HA	2.38	0.46
1:C:38:TYR:HB2	1:C:41:GLN:CB	2.45	0.46
3:I:33:PHE:CA	3:I:48:ARG:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:ASN:HD21	10:B:809:NAG:H2	1.61	0.45
2:D:33:TYR:HB3	2:D:45:LEU:CD1	2.46	0.45
2:D:70:PRO:O	2:D:71:SER:CB	2.64	0.45
3:H:99:SER:HA	3:H:113:TYR:O	2.16	0.45
3:H:15:PRO:C	3:H:17:LEU:H	2.20	0.45
4:M:39:MET:O	4:M:46:ILE:HB	2.16	0.45
1:A:182:ALA:HB3	1:A:195:PHE:HE1	1.81	0.45
3:I:194:ARG:NH1	3:I:248:VAL:CG1	2.74	0.45
3:I:27:TYR:CE2	3:I:32:GLU:HB2	2.52	0.45
2:B:21:LEU:HD22	2:B:112:THR:HG21	1.97	0.45
2:B:30:ASN:HD21	3:H:146:LYS:HZ2	1.63	0.45
2:D:122:VAL:HA	2:D:154:PRO:HD3	1.98	0.45
2:D:32:MET:SD	2:D:75:PHE:HB2	2.56	0.45
2:B:23:CYS:O	2:B:74:ASN:HB2	2.17	0.45
1:C:24:TYR:OH	1:C:66:PHE:HE2	2.00	0.45
3:H:228:MET:HG2	3:H:246:SER:O	2.16	0.45
3:I:194:ARG:HB3	3:I:198:LYS:O	2.16	0.45
4:M:19:LYS:C	4:M:71:THR:HG23	2.37	0.45
1:C:167:VAL:O	2:D:173:SER:HB2	2.17	0.45
1:C:34:TRP:CZ3	1:C:90:CYS:HB2	2.51	0.45
1:A:70:ASN:OD1	1:A:70:ASN:N	2.49	0.45
1:A:85:SER:O	1:A:86:ALA:HB2	2.17	0.45
3:I:157:ARG:O	3:I:161:GLU:N	2.36	0.45
4:L:44:LYS:NZ	12:L:959:HOH:O	2.50	0.45
1:A:136:GLN:NE2	1:A:136:GLN:HA	2.32	0.45
2:D:148:LEU:N	2:D:148:LEU:HD12	2.32	0.45
2:D:45:LEU:O	2:D:59:ASP:HB3	2.17	0.45
3:H:220:ASN:O	3:H:220:ASN:ND2	2.46	0.45
3:I:14:ARG:HB3	3:I:17:LEU:HB2	1.98	0.45
4:M:40:LEU:N	4:M:40:LEU:CD1	2.80	0.45
1:A:168:LEU:HD11	2:B:171:GLY:O	2.17	0.45
1:C:1:GLN:HE21	1:C:105:THR:CG2	2.23	0.45
2:D:205:ASN:C	2:D:207:ARG:H	2.21	0.45
3:H:111:ARG:HD3	3:H:128:GLU:OE1	2.17	0.45
2:B:176:PRO:HG2	2:B:177:GLN:H	1.82	0.45
2:B:207:ARG:HA	2:B:207:ARG:HE	1.81	0.45
1:C:53:ASP:C	1:C:55:VAL:H	2.21	0.45
2:D:127:VAL:HG13	2:D:127:VAL:O	2.17	0.45
2:D:140:LYS:HG3	2:D:142:LYS:H	1.82	0.45
2:D:162:TRP:HE1	2:D:213:GLN:CB	2.29	0.45
3:I:114:GLN:O	3:I:115:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:14:ARG:O	3:H:17:LEU:HB2	2.17	0.44
3:I:191:HIS:HB2	3:I:274:TRP:CE2	2.52	0.44
4:L:56:PHE:HA	4:L:62:PHE:HA	1.98	0.44
2:D:13:ALA:CB	2:D:19:VAL:HG21	2.45	0.44
2:D:125:PRO:HG2	2:D:237:ILE:HB	1.99	0.44
3:H:133:TRP:CH2	3:H:156:LEU:HD12	2.50	0.44
12:C:826:HOH:O	3:H:220:ASN:HA	2.16	0.44
3:H:12:VAL:HA	3:H:93:HIS:O	2.17	0.44
2:D:175:ASP:O	2:D:192:LEU:HD11	2.17	0.44
3:I:108:ARG:HH11	3:I:108:ARG:HG3	1.82	0.44
3:I:166:GLU:HG2	12:I:999:HOH:O	2.17	0.44
3:I:47:PRO:CB	3:I:52:MET:HB3	2.48	0.44
3:I:80:THR:HG22	3:I:84:TYR:CE2	2.53	0.44
1:A:190:THR:HG23	1:A:192:GLN:HG2	1.99	0.44
3:H:105:SER:O	3:I:264:GLN:HA	2.18	0.44
3:I:5:LEU:HB2	3:I:168:LEU:HB2	1.98	0.44
1:C:51:SER:OG	1:C:52:GLY:N	2.50	0.44
3:H:29:ASP:O	3:H:30:ASP:HB2	2.18	0.44
3:I:33:PHE:O	3:I:52:MET:HG3	2.18	0.44
4:M:51:MET:CE	4:M:64:ILE:CD1	2.95	0.44
4:M:38:GLN:HE21	4:M:81:ARG:HB3	1.83	0.44
2:B:202:PHE:O	2:B:208:ASN:ND2	2.39	0.44
1:C:170:MET:CE	1:C:172:ALA:HB2	2.46	0.44
2:D:79:LEU:HD12	2:D:86:GLN:CD	2.37	0.44
4:M:28:THR:CA	12:M:281:HOH:O	2.66	0.44
5:P:2:GLN:HA	5:P:2:GLN:NE2	2.30	0.44
4:M:12:ARG:H	4:M:21:ASN:ND2	2.15	0.44
4:L:21:ASN:N	4:L:70:PHE:O	2.47	0.44
4:M:44:LYS:CG	4:M:44:LYS:O	2.65	0.44
1:A:160:THR:HG22	1:A:161:PHE:N	2.33	0.44
1:A:48:LYS:HD3	2:B:105:THR:HG23	2.00	0.44
2:D:72:GLN:HB2	2:D:72:GLN:HE21	1.54	0.44
3:H:103:VAL:HG13	3:H:168:LEU:HD23	2.00	0.44
1:C:114:VAL:O	1:C:114:VAL:HG13	2.17	0.43
1:C:82:TRP:CZ2	1:C:167:VAL:HG21	2.52	0.43
4:L:82:VAL:HG23	4:L:87:MET:HE1	1.99	0.43
4:M:59:ASP:O	4:M:60:TRP:CG	2.71	0.43
1:A:40:ARG:O	1:A:40:ARG:CD	2.66	0.43
2:B:33:TYR:N	2:B:33:TYR:CD1	2.86	0.43
1:C:128:LEU:HD12	2:D:130:PHE:HB2	2.00	0.43
10:C:814:NAG:HO3	10:C:815:NAG:H61	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLN:CG	2:D:110:ALA:HB3	2.48	0.43
2:D:18:LYS:CG	2:D:80:GLU:HG3	2.42	0.43
2:D:34:TRP:CH2	2:D:92:CYS:HB3	2.52	0.43
3:I:129:ASP:OD2	3:I:132:THR:N	2.51	0.43
4:L:1:ILE:HB	4:L:2:GLN:H	1.52	0.43
4:M:19:LYS:HD3	12:M:469:HOH:O	2.18	0.43
4:M:53:ASP:HB3	4:M:54:MET:H	1.59	0.43
4:M:84:HIS:ND1	4:M:86:SER:CB	2.81	0.43
1:A:32:LEU:CD1	1:A:66:PHE:HD2	2.31	0.43
2:B:153:PHE:CB	2:B:154:PRO:CD	2.96	0.43
2:B:127:VAL:HG13	2:B:237:ILE:CG2	2.48	0.43
2:B:55:THR:O	2:B:56:GLU:HG3	2.18	0.43
2:D:82:ALA:CB	2:D:116:VAL:HG11	2.48	0.43
3:H:3:HIS:HB3	3:H:29:ASP:OD1	2.18	0.43
3:H:85:TYR:O	3:H:86:ASN:C	2.56	0.43
1:C:151:ASN:N	1:C:151:ASN:HD22	2.15	0.43
3:H:121:CYS:O	3:H:122:ASP:C	2.56	0.43
3:H:187:ALA:HA	3:H:204:TRP:O	2.18	0.43
4:M:51:MET:CE	4:M:64:ILE:HD11	2.47	0.43
1:C:24:TYR:OH	1:C:71:SER:HA	2.19	0.43
2:D:164:ASN:HD22	2:D:164:ASN:H	1.66	0.43
2:D:163:VAL:HB	2:D:168:VAL:HG13	2.01	0.43
2:D:205:ASN:ND2	2:D:207:ARG:O	2.51	0.43
3:H:213:ILE:HG12	3:H:214:THR:H	1.83	0.43
3:I:214:THR:HA	12:I:983:HOH:O	2.17	0.43
4:L:96:ASP:HB3	4:L:99:MET:HB2	2.01	0.43
3:I:236:ALA:O	4:M:24:ASN:ND2	2.51	0.43
2:D:121:ASN:O	2:D:153:PHE:CB	2.67	0.43
2:D:199:SER:HB2	2:D:202:PHE:HD2	1.83	0.43
3:H:255:GLN:OE1	3:H:273:ARG:HD3	2.19	0.43
3:I:13:SER:HB3	3:I:78:LEU:CD1	2.48	0.43
3:I:143:THR:HG21	5:Q:8:VAL:HB	1.99	0.43
4:L:5:PRO:HB3	4:L:30:PHE:HB3	2.01	0.43
8:A:806:NAG:H3	8:A:807:BMA:O5	2.15	0.43
2:B:174:THR:O	2:B:175:ASP:C	2.57	0.43
2:D:118:ASP:O	2:D:121:ASN:ND2	2.51	0.43
2:D:147:CYS:C	2:D:148:LEU:HD12	2.39	0.43
2:D:244:ARG:HD2	2:D:244:ARG:H	1.82	0.43
3:I:127:ASN:N	3:I:127:ASN:ND2	2.67	0.43
3:I:209:TYR:HA	3:I:210:PRO:C	2.39	0.43
3:I:213:ILE:HG12	3:I:214:THR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:49:VAL:HG22	4:L:68:THR:HG21	2.00	0.43
1:C:117:TYR:CD1	1:C:118:ILE:N	2.87	0.43
2:D:194:SER:C	2:D:195:ARG:HE	2.22	0.43
2:D:221:GLU:N	2:D:221:GLU:CD	2.72	0.43
4:L:14:PRO:HA	4:L:15:PRO:HD2	1.81	0.43
4:L:37:ILE:HB	4:L:51:MET:HE1	1.99	0.43
4:L:80:CYS:O	4:L:92:THR:HA	2.18	0.43
3:I:143:THR:CG2	5:Q:8:VAL:HB	2.49	0.43
2:D:140:LYS:HD2	2:D:142:LYS:HB2	2.01	0.43
2:D:2:ALA:HA	2:D:26:THR:OG1	2.19	0.43
3:H:110:LEU:O	3:H:111:ARG:HG2	2.19	0.43
3:I:163:THR:O	3:I:166:GLU:HB2	2.18	0.43
3:I:190:THR:OG1	3:I:192:HIS:HE1	2.01	0.43
2:B:245:ALA:HA	12:B:880:HOH:O	2.19	0.43
1:C:142:LEU:C	1:C:142:LEU:HD13	2.39	0.43
2:D:219:LEU:HB2	2:D:231:LYS:HZ3	1.84	0.43
2:D:66:LYS:O	2:D:78:ILE:N	2.52	0.43
4:M:97:ARG:HG3	12:M:121:HOH:O	2.18	0.43
3:I:159:TYR:CZ	5:Q:3:TYR:HB2	2.53	0.43
1:C:149:GLN:HA	1:C:149:GLN:NE2	2.33	0.42
1:C:72:SER:HB3	1:C:74:HIS:CD2	2.54	0.42
2:D:94:SER:O	2:D:106:LEU:HD22	2.18	0.42
3:H:128:GLU:HG3	12:H:841:HOH:O	2.19	0.42
3:H:194:ARG:CG	3:H:195:PRO:HD2	2.49	0.42
3:H:272:LEU:N	3:H:272:LEU:HD12	2.34	0.42
2:B:159:LEU:C	2:B:159:LEU:HD12	2.39	0.42
1:C:170:MET:HB3	1:C:175:SER:OG	2.19	0.42
1:C:85:SER:OG	1:C:114:VAL:HG12	2.19	0.42
2:D:30:ASN:O	2:D:51:GLY:N	2.52	0.42
3:H:116:TYR:HB2	3:H:124:ILE:HG22	2.00	0.42
3:I:13:SER:C	3:I:15:PRO:HD3	2.39	0.42
3:I:199:VAL:HG23	3:I:200:THR:N	2.33	0.42
3:H:12:VAL:HG11	4:L:33:PRO:HG3	2.01	0.42
4:M:7:ILE:CB	4:M:93:VAL:HG21	2.43	0.42
2:D:127:VAL:HG11	2:D:238:SER:CA	2.49	0.42
2:D:61:PRO:CG	2:D:62:ASP:H	2.30	0.42
2:D:89:VAL:HG13	2:D:113:ARG:HB3	2.00	0.42
3:H:169:ARG:HE	3:I:268:GLU:HB3	1.84	0.42
3:I:25:VAL:HA	3:I:34:VAL:O	2.18	0.42
2:D:8:PRO:C	2:D:10:ASN:N	2.73	0.42
3:H:117:ALA:HB2	4:L:60:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:234:ARG:HD2	4:M:10:TYR:CE2	2.54	0.42
4:M:12:ARG:CB	12:M:272:HOH:O	2.68	0.42
3:I:234:ARG:HD3	4:M:8:GLN:HE22	1.83	0.42
2:B:137:ILE:HG21	2:B:204:HIS:NE2	2.35	0.42
2:B:65:TYR:CE2	2:B:79:LEU:HD21	2.54	0.42
1:C:167:VAL:C	1:C:168:LEU:HD23	2.39	0.42
1:C:59:VAL:O	1:C:62:PHE:CD1	2.72	0.42
2:D:121:ASN:OD1	2:D:153:PHE:CD2	2.72	0.42
2:D:18:LYS:HG3	2:D:80:GLU:CG	2.47	0.42
2:D:33:TYR:HB3	2:D:45:LEU:HD11	2.00	0.42
3:H:21:ARG:NE	3:H:23:MET:CE	2.82	0.42
3:H:21:ARG:NE	3:H:23:MET:HE2	2.35	0.42
3:H:128:GLU:CD	12:H:913:HOH:O	2.58	0.42
3:H:271:THR:C	3:H:272:LEU:HD12	2.39	0.42
1:C:114:VAL:O	1:C:114:VAL:HG22	2.19	0.42
2:D:193:SER:OG	2:D:195:ARG:NH2	2.52	0.42
2:D:31:ASN:HB3	2:D:33:TYR:OH	2.20	0.42
2:D:88:SER:OG	2:D:89:VAL:N	2.51	0.42
3:H:21:ARG:HE	3:H:23:MET:CE	2.31	0.42
3:I:263:HIS:HD2	3:I:265:GLY:N	2.15	0.42
4:M:12:ARG:H	4:M:21:ASN:HD21	1.65	0.42
2:B:142:LYS:CG	12:B:906:HOH:O	2.67	0.42
2:B:69:ARG:NH1	2:B:72:GLN:O	2.41	0.42
3:H:170:ARG:NH1	12:H:832:HOH:O	2.53	0.42
3:H:6:ARG:HG2	3:H:113:TYR:OH	2.20	0.42
3:I:80:THR:HG22	3:I:84:TYR:CZ	2.55	0.42
3:I:81:LEU:O	3:I:84:TYR:HB2	2.20	0.42
1:A:203:ASN:HB3	1:A:204:ALA:H	1.59	0.42
1:C:133:PRO:HB2	1:C:134:ARG:NH1	2.35	0.42
1:C:155:THR:HG21	1:C:160:THR:O	2.19	0.42
1:C:191:CYS:C	1:C:192:GLN:HG3	2.41	0.42
1:C:48:LYS:C	12:C:827:HOH:O	2.58	0.42
2:D:235:GLN:OE1	2:D:237:ILE:HD11	2.19	0.42
3:H:192:HIS:HB2	3:H:200:THR:HB	2.02	0.42
3:H:215:LEU:CD2	3:H:261:VAL:HG13	2.50	0.42
4:L:36:GLU:HB3	4:L:83:LYS:HB3	2.02	0.42
1:A:55:VAL:CG2	1:A:55:VAL:O	2.67	0.42
1:C:144:THR:HA	1:C:178:ASN:O	2.19	0.42
1:C:16:ALA:HB1	12:C:829:HOH:O	2.20	0.42
2:D:121:ASN:O	2:D:153:PHE:HB2	2.20	0.42
2:D:182:SER:HB2	2:D:189:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:219:LEU:HD13	2:D:223:ASP:OD1	2.20	0.42
2:D:6:GLN:NE2	2:D:112:THR:HG23	2.35	0.42
3:I:4:SER:C	12:I:954:HOH:O	2.57	0.42
4:L:7:ILE:HD11	4:L:82:VAL:HG22	2.02	0.42
1:A:11:THR:HA	1:A:113:ILE:O	2.20	0.41
2:B:2:ALA:HB2	12:H:871:HOH:O	2.19	0.41
1:C:106:PHE:CE1	2:D:43:LEU:HD23	2.55	0.41
3:H:230:LEU:HD23	3:H:230:LEU:O	2.19	0.41
3:I:230:LEU:HG	3:I:243:LYS:HE3	2.02	0.41
3:I:48:ARG:HA	3:I:48:ARG:HH11	1.85	0.41
1:A:123:PRO:HG2	1:A:203:ASN:HB2	2.02	0.41
1:A:154:LYS:C	1:A:162:ILE:HD12	2.40	0.41
1:A:191:CYS:HA	1:A:194:ILE:CG2	2.48	0.41
2:B:27:ASN:CB	2:B:29:HIS:ND1	2.81	0.41
1:C:1:GLN:HG3	1:C:105:THR:HG21	2.02	0.41
1:C:7:ASP:CG	1:C:110:THR:HB	2.40	0.41
2:D:152:PHE:HD2	2:D:154:PRO:HD2	1.84	0.41
3:I:234:ARG:HD3	4:M:8:GLN:NE2	2.34	0.41
3:I:25:VAL:HG12	3:I:35:ARG:NE	2.35	0.41
4:M:21:ASN:N	4:M:70:PHE:O	2.48	0.41
1:A:207:PRO:C	1:A:209:SER:H	2.23	0.41
1:C:161:PHE:O	1:C:162:ILE:HD13	2.21	0.41
3:H:36:PHE:HB2	3:H:45:TYR:CD1	2.55	0.41
3:I:164:CYS:O	3:I:165:VAL:C	2.58	0.41
3:I:25:VAL:O	3:I:25:VAL:HG23	2.21	0.41
1:A:188:SER:O	1:A:189:PHE:CB	2.68	0.41
2:B:73:GLU:CD	2:B:73:GLU:H	2.24	0.41
1:C:8:ALA:O	1:C:9:ARG:HB3	2.20	0.41
2:D:14:VAL:C	2:D:16:GLY:H	2.23	0.41
2:D:162:TRP:O	2:D:211:ARG:HB2	2.20	0.41
3:I:190:THR:OG1	3:I:202:ARG:HB3	2.21	0.41
1:A:191:CYS:O	1:A:194:ILE:HG22	2.21	0.41
1:A:40:ARG:O	1:A:40:ARG:HD2	2.20	0.41
1:C:146:PHE:C	1:C:146:PHE:CD1	2.93	0.41
2:D:162:TRP:HB2	2:D:211:ARG:HB2	2.02	0.41
2:D:74:ASN:HA	2:D:74:ASN:HD22	1.58	0.41
3:H:214:THR:HB	3:H:262:TYR:HB2	2.01	0.41
3:H:218:GLN:HB2	3:H:258:THR:OG1	2.20	0.41
3:I:33:PHE:HA	3:I:48:ARG:HB2	2.03	0.41
1:C:47:LEU:C	1:C:47:LEU:HD12	2.41	0.41
2:D:120:ARG:CZ	2:D:120:ARG:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:SER:O	2:D:202:PHE:HB2	2.21	0.41
3:I:45:TYR:HB3	3:I:60:TRP:HE3	1.85	0.41
3:I:8:PHE:CD1	3:I:27:TYR:CD1	3.04	0.41
4:M:84:HIS:ND1	4:M:86:SER:HB3	2.35	0.41
1:C:144:THR:O	1:C:145:ASP:HB2	2.21	0.41
1:C:77:LYS:HD2	1:C:78:ALA:N	2.33	0.41
2:D:198:VAL:HG21	2:D:203:TRP:CB	2.50	0.41
2:D:154:PRO:HG2	2:D:216:PHE:CZ	2.56	0.41
3:H:4:SER:HA	3:H:101:CYS:O	2.21	0.41
4:L:37:ILE:HD12	4:L:51:MET:CE	2.51	0.41
4:M:40:LEU:N	4:M:40:LEU:HD12	2.35	0.41
2:B:152:PHE:CE1	2:B:190:TYR:CB	3.04	0.41
2:D:120:ARG:CB	2:D:120:ARG:NH1	2.84	0.41
3:I:96:GLN:OE1	4:M:56:PHE:CD1	2.74	0.41
4:L:46:ILE:HG23	4:L:47:PRO:HD2	2.03	0.41
4:M:28:THR:CB	12:M:281:HOH:O	2.65	0.41
1:A:186:GLN:HG2	12:A:976:HOH:O	2.21	0.41
2:D:137:ILE:HG13	2:D:204:HIS:NE2	2.36	0.41
2:D:153:PHE:H	2:D:154:PRO:CD	2.34	0.41
2:D:177:GLN:HA	2:D:177:GLN:OE1	2.20	0.41
3:H:249:VAL:HG12	3:H:257:TYR:CE2	2.55	0.41
3:H:271:THR:O	3:H:271:THR:CG2	2.69	0.41
3:I:124:ILE:HD12	3:I:135:ALA:HB2	2.01	0.41
3:I:222:GLU:HG3	3:I:223:GLU:N	2.35	0.41
3:H:176:ASN:OD1	3:H:177:ALA:N	2.54	0.41
3:I:194:ARG:NH1	3:I:248:VAL:CG2	2.83	0.41
3:I:262:TYR:CD1	3:I:269:PRO:HB3	2.56	0.41
3:I:72:GLN:O	3:I:73:SER:C	2.57	0.41
3:I:78:LEU:O	3:I:82:LEU:HG	2.21	0.41
4:M:37:ILE:HD11	4:M:51:MET:HE1	2.03	0.41
4:M:8:GLN:HG2	12:M:426:HOH:O	2.19	0.41
2:B:211:ARG:NH1	12:B:869:HOH:O	2.43	0.41
2:B:6:GLN:OE1	2:B:91:PHE:HA	2.20	0.41
2:B:88:SER:OG	2:B:89:VAL:N	2.54	0.41
1:C:14:GLU:HA	1:C:114:VAL:CG2	2.50	0.41
1:C:196:LYS:NZ	1:C:196:LYS:CB	2.84	0.41
1:C:57:GLN:HE22	3:H:256:TYR:HD1	1.65	0.41
2:D:6:GLN:HE21	2:D:111:GLY:C	2.25	0.41
3:H:201:LEU:HD11	3:H:254:GLU:HB3	2.03	0.41
3:H:71:GLU:OE2	3:H:75:ARG:NH2	2.53	0.41
3:I:156:LEU:HD23	3:I:156:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:194:ARG:CG	3:I:195:PRO:CD	2.97	0.41
3:I:81:LEU:O	3:I:82:LEU:C	2.58	0.41
1:A:188:SER:HB3	1:A:189:PHE:H	1.70	0.40
2:B:139:ASN:HD22	2:B:140:LYS:HG3	1.86	0.40
2:B:153:PHE:HB3	2:B:154:PRO:HD2	2.03	0.40
2:B:30:ASN:HB2	5:P:6:TYR:CE1	2.56	0.40
1:C:142:LEU:HD11	2:D:144:THR:CB	2.46	0.40
2:D:146:VAL:CG2	2:D:147:CYS:N	2.84	0.40
3:H:187:ALA:O	3:H:188:HIS:HB3	2.21	0.40
3:I:94:THR:CG2	3:I:95:ILE:H	2.33	0.40
5:Q:2:GLN:HG3	5:Q:3:TYR:N	2.36	0.40
1:A:192:GLN:HG3	1:A:193:ASP:N	2.35	0.40
2:B:60:ILE:HG13	2:B:60:ILE:O	2.21	0.40
1:C:109:GLY:O	1:C:110:THR:HB	2.21	0.40
1:C:32:LEU:HD13	1:C:73:PHE:CD1	2.56	0.40
2:D:54:SER:H	2:D:69:ARG:CB	2.34	0.40
3:I:75:ARG:NH1	12:I:951:HOH:O	2.53	0.40
4:L:59:ASP:O	4:L:60:TRP:HB2	2.22	0.40
1:C:128:LEU:CD2	1:C:140:LEU:HG	2.49	0.40
1:C:19:GLN:HE22	1:C:74:HIS:HB3	1.86	0.40
2:D:142:LYS:HZ2	2:D:197:ARG:HD3	1.86	0.40
3:H:102:GLU:HG3	3:H:113:TYR:HE2	1.85	0.40
3:I:201:LEU:O	3:I:246:SER:CB	2.69	0.40
3:I:36:PHE:HB2	3:I:45:TYR:HA	2.03	0.40
4:L:41:LYS:O	4:L:42:ASN:C	2.59	0.40
1:A:206:TYR:CB	2:B:135:ALA:HB1	2.50	0.40
2:B:6:GLN:HG2	2:B:92:CYS:SG	2.61	0.40
1:C:82:TRP:HH2	1:C:167:VAL:HG21	1.83	0.40
2:D:121:ASN:CG	2:D:153:PHE:CE2	2.93	0.40
2:D:205:ASN:O	2:D:207:ARG:N	2.54	0.40
2:D:33:TYR:CD2	2:D:48:TYR:CB	3.05	0.40
2:D:36:ARG:O	2:D:36:ARG:HG2	2.20	0.40
3:H:141:LEU:O	3:H:145:HIS:CD2	2.75	0.40
3:H:185:PRO:HA	3:H:206:LEU:O	2.22	0.40
4:L:17:ASN:OD1	4:L:73:THR:O	2.39	0.40
1:A:81:HIS:O	1:A:114:VAL:HG11	2.21	0.40
2:B:142:LYS:HG2	12:B:906:HOH:O	2.21	0.40
1:C:140:LEU:HD23	1:C:140:LEU:N	2.36	0.40
2:D:34:TRP:CZ3	2:D:92:CYS:HB3	2.57	0.40
3:H:133:TRP:O	3:H:144:LYS:NZ	2.46	0.40
3:H:230:LEU:H	3:H:230:LEU:HD23	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:132:THR:HG22	3:I:133:TRP:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:SER:CB	12:B:859:HOH:O[4_555]	1.98	0.22

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	200/202 (99%)	169 (84%)	24 (12%)	7 (4%)	4	3
1	C	200/202 (99%)	134 (67%)	43 (22%)	23 (12%)	0	0
2	B	235/237 (99%)	214 (91%)	17 (7%)	4 (2%)	11	13
2	D	235/237 (99%)	154 (66%)	62 (26%)	19 (8%)	1	0
3	H	272/275 (99%)	246 (90%)	23 (8%)	3 (1%)	17	23
3	I	272/275 (99%)	226 (83%)	34 (12%)	12 (4%)	3	2
4	L	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
4	M	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	0
5	P	6/8 (75%)	5 (83%)	0	1 (17%)	0	0
5	Q	6/8 (75%)	5 (83%)	0	1 (17%)	0	0
All	All	1620/1642 (99%)	1319 (81%)	223 (14%)	78 (5%)	2	1

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	PRO

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Mol	Chain	Res	Type
1	A	140	LEU
1	C	7	ASP
2	B	153	PHE
2	B	226	PRO
2	D	13	ALA
2	D	75	PHE
2	D	172	VAL
3	H	226	GLN
3	I	89	ALA
4	M	41	LYS
1	C	50	TYR
1	C	73	PHE
1	C	82	TRP
1	C	83	SER
1	C	174	ASP
1	C	190	THR
1	C	203	ASN
2	D	61	PRO
2	D	71	SER
2	D	149	ALA
2	D	199	SER
2	D	215	GLN
4	M	60	TRP
5	P	7	SER
5	Q	7	SER
1	C	101	ALA
1	C	144	THR
1	C	154	LYS
1	C	158	SER
1	C	159	GLY
1	C	209	SER
2	D	16	GLY
2	D	121	ASN
2	D	155	ASP
3	I	139	ALA
3	I	153	ALA
3	I	164	CYS
3	I	176	ASN
3	I	222	GLU
4	M	47	PRO
4	M	50	GLU
4	M	57	SER

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Mol	Chain	Res	Type
1	A	69	SER
1	A	203	ASN
1	C	110	THR
1	C	137	ASP
1	C	187	THR
2	B	155	ASP
2	D	110	ALA
2	D	138	ALA
2	D	206	PRO
2	D	233	VAL
3	I	55	GLU
3	I	82	LEU
3	I	148	GLU
4	M	40	LEU
1	A	198	THR
1	C	86	ALA
1	C	173	MET
1	C	192	GLN
2	D	153	PHE
3	H	227	ASP
3	H	255	GLN
3	I	38	SER
3	I	119	ASP
4	M	31	HIS
4	M	90	PRO
1	A	123	PRO
1	A	189	PHE
1	C	80	VAL
1	C	99	GLY
2	D	98	GLY
2	B	176	PRO
2	D	109	GLY
3	I	43	PRO
1	C	125	VAL
2	D	232	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/176 (100%)	165 (94%)	11 (6%)	21	33
1	C	176/176 (100%)	161 (92%)	15 (8%)	12	19
2	B	200/200 (100%)	194 (97%)	6 (3%)	46	67
2	D	200/200 (100%)	185 (92%)	15 (8%)	16	24
3	H	231/232 (100%)	215 (93%)	16 (7%)	18	28
3	I	230/232 (99%)	210 (91%)	20 (9%)	12	18
4	L	94/94 (100%)	89 (95%)	5 (5%)	26	42
4	M	94/94 (100%)	89 (95%)	5 (5%)	26	42
5	P	8/8 (100%)	7 (88%)	1 (12%)	5	6
5	Q	8/8 (100%)	6 (75%)	2 (25%)	1	0
All	All	1417/1420 (100%)	1321 (93%)	96 (7%)	18	29

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	3	VAL
1	A	30	PRO
1	A	39	PRO
1	A	56	VAL
1	A	114	VAL
1	A	129	LYS
1	A	155	THR
1	A	156	MET
1	A	157	GLU
1	A	161	PHE
1	C	7	ASP
1	C	9	ARG
1	C	19	GLN
1	C	20	LEU
1	C	30	PRO
1	C	62	PHE
1	C	71	SER
1	C	100	PHE
1	C	102	SER
1	C	120	ASN
1	C	128	LEU
1	C	139	THR

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Mol	Chain	Res	Type
1	C	141	CYS
1	C	151	ASN
1	C	168	LEU
2	B	25	GLN
2	B	49	SER
2	B	139	ASN
2	B	159	LEU
2	B	242	TRP
2	B	244	ARG
2	D	37	GLN
2	D	38	ASP
2	D	44	ARG
2	D	72	GLN
2	D	74	ASN
2	D	78	ILE
2	D	106	LEU
2	D	145	LEU
2	D	152	PHE
2	D	162	TRP
2	D	186	ASN
2	D	202	PHE
2	D	207	ARG
2	D	242	TRP
2	D	244	ARG
3	H	5	LEU
3	H	12	VAL
3	H	14	ARG
3	H	19	GLU
3	H	21	ARG
3	H	45	TYR
3	H	46	GLU
3	H	97	VAL
3	H	99	SER
3	H	103	VAL
3	H	111	ARG
3	H	156	LEU
3	H	212	ASP
3	H	220	ASN
3	H	227	ASP
3	H	230	LEU
3	I	33	PHE
3	I	39	ASP

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Mol	Chain	Res	Type
3	I	45	TYR
3	I	48	ARG
3	I	50	ARG
3	I	52	MET
3	I	70	ASN
3	I	85	TYR
3	I	87	GLN
3	I	88	SER
3	I	99	SER
3	I	113	TYR
3	I	114	GLN
3	I	137	ASP
3	I	138	MET
3	I	145	HIS
3	I	229	GLU
3	I	231	VAL
3	I	251	LEU
3	I	272	LEU
4	L	12	ARG
4	L	23	LEU
4	L	70	PHE
4	L	92	THR
4	L	97	ARG
4	M	7	ILE
4	M	53	ASP
4	M	70	PHE
4	M	74	GLU
4	M	87	MET
5	P	2	GLN
5	Q	2	GLN
5	Q	8	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	136	GLN
1	A	185	ASN
1	A	186	GLN
1	A	203	ASN
1	C	5	GLN
1	C	19	GLN

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Mol	Chain	Res	Type
1	C	74	HIS
1	C	81	HIS
1	C	149	GLN
1	C	151	ASN
1	C	203	ASN
2	B	30	ASN
2	B	31	ASN
2	B	37	GLN
2	B	72	GLN
2	B	121	ASN
2	B	139	ASN
2	B	236	ASN
2	D	6	GLN
2	D	10	ASN
2	D	25	GLN
2	D	37	GLN
2	D	74	ASN
2	D	86	GLN
2	D	139	ASN
2	D	164	ASN
2	D	186	ASN
2	D	235	GLN
3	H	54	GLN
3	H	115	GLN
3	H	127	ASN
3	H	145	HIS
3	H	174	ASN
3	H	218	GLN
3	H	220	ASN
3	H	226	GLN
3	H	263	HIS
3	I	42	ASN
3	I	54	GLN
3	I	70	ASN
3	I	72	GLN
3	I	86	ASN
3	I	87	GLN
3	I	96	GLN
3	I	114	GLN
3	I	127	ASN
3	I	149	GLN
3	I	192	HIS

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Mol	Chain	Res	Type
3	I	255	GLN
3	I	263	HIS
4	L	29	GLN
4	M	8	GLN
4	M	13	HIS
4	M	21	ASN
4	M	29	GLN
4	M	38	GLN
5	P	2	GLN
5	Q	2	GLN

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 ⓘ

10 carbohydrates 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$
6	NAG	A	803	1,6	14,14,15	1.05	0	15,19,21	2.12	2 (13%)
6	NAG	A	804	6	14,14,15	1.05	1 (7%)	15,19,21	1.68	3 (20%)
8	NAG	A	806	8,7	14,14,15	0.61	0	15,19,21	1.17	1 (6%)
8	BMA	A	807	8	11,11,12	1.49	3 (27%)	13,15,17	2.98	6 (46%)
10	NAG	B	809	10,2	14,14,15	0.98	0	15,19,21	1.90	3 (20%)
10	NAG	B	810	10	14,14,15	1.15	2 (14%)	15,19,21	2.02	2 (13%)
10	BMA	B	811	10	11,11,12	0.77	1 (9%)	13,15,17	2.00	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	C	814	1,10	14,14,15	1.06	1 (7%)	15,19,21	1.84	3 (20%)
10	NAG	C	815	10	14,14,15	1.11	2 (14%)	15,19,21	2.53	3 (20%)
10	BMA	C	816	10	11,11,12	1.20	1 (9%)	13,15,17	1.03	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
6	NAG	A	803	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	804	6	-	0/6/23/26	0/1/1/1
8	NAG	A	806	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	807	8	-	0/2/19/22	0/1/1/1
10	NAG	B	809	10,2	-	0/6/23/26	0/1/1/1
10	NAG	B	810	10	-	0/6/23/26	0/1/1/1
10	BMA	B	811	10	-	0/2/19/22	0/1/1/1
10	NAG	C	814	1,10	-	0/6/23/26	0/1/1/1
10	NAG	C	815	10	-	0/6/23/26	0/1/1/1
10	BMA	C	816	10	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	807	BMA	O5-C5	-3.31	1.36	1.43
10	C	816	BMA	O5-C1	-3.22	1.38	1.43
10	B	810	NAG	O5-C1	-2.81	1.39	1.43
10	C	815	NAG	O5-C1	-2.71	1.39	1.43
6	A	804	NAG	O5-C1	-2.69	1.39	1.43
10	B	810	NAG	O4-C4	-2.53	1.37	1.43
10	C	815	NAG	C1-C2	-2.40	1.49	1.52
8	A	807	BMA	O5-C1	-2.25	1.40	1.43
10	B	811	BMA	O5-C1	-2.12	1.40	1.43
10	C	814	NAG	C2-N2	-2.08	1.42	1.46
8	A	807	BMA	O2-C2	-2.01	1.38	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	815	NAG	O5-C1-C2	-7.96	100.39	111.47
6	A	803	NAG	O5-C1-C2	-7.05	101.67	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	809	NAG	O5-C1-C2	-5.76	103.46	111.47
10	C	814	NAG	O5-C1-C2	-5.34	104.05	111.47
10	B	811	BMA	O5-C1-C2	-5.18	102.67	110.79
8	A	807	BMA	O2-C2-C1	-4.42	100.19	109.18
10	B	810	NAG	O4-C4-C3	-4.15	101.33	110.36
10	C	815	NAG	O6-C6-C5	-3.98	97.95	111.34
10	B	809	NAG	O4-C4-C5	-3.34	100.86	109.28
8	A	807	BMA	O5-C1-C2	-3.25	105.69	110.79
10	C	815	NAG	O4-C4-C3	-3.24	103.30	110.36
8	A	806	NAG	O5-C1-C2	-2.86	107.49	111.47
10	C	814	NAG	C4-C3-C2	-2.29	107.66	111.02
10	B	811	BMA	C6-C5-C4	-2.19	107.89	113.00
8	A	807	BMA	O4-C4-C5	-2.08	104.04	109.28
10	B	809	NAG	O4-C4-C3	2.19	115.13	110.36
8	A	807	BMA	C1-C2-C3	2.58	112.92	109.65
6	A	804	NAG	C1-C2-N2	2.78	115.23	110.49
10	C	814	NAG	C3-C4-C5	2.90	115.32	110.22
6	A	804	NAG	C1-O5-C5	2.92	116.19	112.17
6	A	803	NAG	O4-C4-C3	3.42	117.79	110.36
10	B	811	BMA	C1-C2-C3	3.50	114.08	109.65
6	A	804	NAG	O5-C1-C2	3.94	116.95	111.47
8	A	807	BMA	O2-C2-C3	5.12	120.22	110.17
10	B	810	NAG	O5-C1-C2	6.03	119.86	111.47
8	A	807	BMA	C1-O5-C5	6.66	121.34	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	803	NAG	1	0
8	A	806	NAG	5	0
8	A	807	BMA	4	0
10	B	809	NAG	8	0
10	B	810	NAG	5	0
10	B	811	BMA	5	0
10	C	814	NAG	4	0
10	C	815	NAG	3	0

5.6 Ligand geometry

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$
7	NAG	A	805	1,8	14,14,15	0.88	0	15,19,21	1.60	1 (6%)
9	GOL	A	902	-	5,5,5	0.29	0	5,5,5	0.63	0
7	NAG	B	808	2	14,14,15	0.88	1 (7%)	15,19,21	2.01	1 (6%)
7	NAG	H	812	3,7	14,14,15	1.02	0	15,19,21	2.22	1 (6%)
7	NAG	H	813	7	14,14,15	0.61	0	15,19,21	1.04	2 (13%)
9	GOL	I	903	-	5,5,5	0.64	0	5,5,5	0.78	0
9	GOL	L	901	-	5,5,5	0.34	0	5,5,5	0.62	0
11	ACY	P	1001	-	1,3,3	1.95	0	0,3,3	0.00	-

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
7	NAG	A	805	1,8	-	0/6/23/26	0/1/1/1
9	GOL	A	902	-	-	0/4/4/4	0/0/0/0
7	NAG	B	808	2	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	H	812	3,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	H	813	7	-	0/6/23/26	0/1/1/1
9	GOL	I	903	-	-	0/4/4/4	0/0/0/0
9	GOL	L	901	-	-	0/4/4/4	0/0/0/0
11	ACY	P	1001	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	808	NAG	C2-N2	-2.10	1.42	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	812	NAG	O5-C1-C2	-7.97	100.38	111.47
7	B	808	NAG	O5-C1-C2	-6.78	102.03	111.47
7	A	805	NAG	O5-C1-C2	-5.27	104.14	111.47
7	H	813	NAG	O5-C1-C2	-2.51	107.97	111.47
7	H	813	NAG	C4-C3-C2	-2.01	108.06	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	808	NAG	C1
7	H	812	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	805	NAG	11	0
7	H	812	NAG	2	0
7	H	813	NAG	5	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, 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	202/202 (100%)	0.44	13 (6%) 20 18	4, 25, 74, 98	0
1	C	202/202 (100%)	2.33	89 (44%) 0 0	52, 82, 127, 136	0
2	B	237/237 (100%)	0.10	2 (0%) 86 84	14, 27, 47, 74	0
2	D	237/237 (100%)	3.22	143 (60%) 0 0	59, 113, 124, 141	0
3	H	274/275 (99%)	0.12	3 (1%) 80 79	7, 23, 43, 54	0
3	I	274/275 (99%)	0.57	24 (8%) 11 9	15, 47, 70, 77	0
4	L	99/99 (100%)	-0.11	0 100 100	9, 21, 36, 44	0
4	M	99/99 (100%)	0.57	2 (2%) 65 63	32, 47, 61, 65	0
5	P	8/8 (100%)	0.28	0 100 100	10, 14, 19, 19	0
5	Q	8/8 (100%)	3.45	6 (75%) 0 0	81, 84, 89, 91	0
All	All	1640/1642 (99%)	0.98	282 (17%) 2 1	4, 39, 122, 141	0

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	145	LEU	15.6
1	C	211	VAL	14.2
2	D	218	GLY	13.1
2	D	214	VAL	12.7
1	C	127	ALA	11.6
2	D	143	ALA	11.3
2	D	219	LEU	11.0
2	D	129	LEU	10.5
2	D	196	LEU	10.3
2	D	159	LEU	10.3
1	C	207	PRO	10.2
2	D	154	PRO	10.2
2	D	127	VAL	10.2

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Mol	Chain	Res	Type	RSRZ
5	Q	8	VAL	10.1
2	D	144	THR	10.0
2	D	241	ALA	9.6
1	C	140	LEU	9.3
2	D	146	VAL	8.9
2	D	179	TYR	8.4
1	C	128	LEU	8.4
2	D	242	TRP	8.2
2	D	244	ARG	8.1
2	D	210	PHE	8.0
2	D	142	LYS	8.0
1	C	188	SER	7.9
2	D	153	PHE	7.9
1	C	208	SER	7.8
2	D	148	LEU	7.5
1	C	141	CYS	7.5
2	D	92	CYS	7.4
2	D	21	LEU	7.3
1	C	125	VAL	7.3
2	D	231	LYS	7.2
2	D	192	LEU	7.2
2	D	233	VAL	6.8
2	D	14	VAL	6.7
1	C	209	SER	6.7
2	D	93	ALA	6.6
2	D	114	LEU	6.5
1	C	142	LEU	6.5
1	C	184	SER	6.4
1	C	91	ALA	6.3
2	D	228	GLY	6.3
1	C	152	VAL	6.2
1	C	179	GLY	6.2
2	D	232	PRO	6.2
1	C	162	ILE	6.1
1	C	183	TRP	6.0
1	C	158	SER	6.0
2	D	122	VAL	6.0
2	D	182	SER	5.9
2	D	131	GLU	5.9
1	C	159	GLY	5.8
2	D	198	VAL	5.8
2	D	190	TYR	5.8

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Mol	Chain	Res	Type	RSRZ
2	D	193	SER	5.7
3	I	123	TYR	5.7
2	D	7	SER	5.5
2	D	220	SER	5.5
1	C	126	TYR	5.5
1	C	206	TYR	5.4
2	D	195	ARG	5.3
2	D	316	LEU	5.3
1	C	156	MET	5.3
2	D	245	ALA	5.3
1	A	206	TYR	5.2
2	D	178	ALA	5.2
1	C	181	ILE	5.2
2	D	75	PHE	5.2
2	D	149	ALA	5.1
2	D	128	SER	5.1
1	C	161	PHE	5.1
2	D	165	GLY	5.0
2	D	77	LEU	4.9
2	D	162	TRP	4.9
2	D	226	PRO	4.8
1	C	163	THR	4.8
1	C	147	ASP	4.8
2	D	132	PRO	4.8
2	D	133	SER	4.8
1	C	123	PRO	4.8
1	C	187	THR	4.7
2	D	91	PHE	4.7
2	B	2	ALA	4.6
2	D	81	LEU	4.6
2	D	202	PHE	4.6
1	C	180	ALA	4.6
1	A	213	CYS	4.5
2	D	119	LEU	4.5
2	D	197	ARG	4.5
1	C	146	PHE	4.5
1	C	153	PRO	4.5
1	C	182	ALA	4.4
2	D	98	GLY	4.4
2	D	137	ILE	4.4
2	D	130	PHE	4.3
2	D	111	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	243	GLY	4.3
1	C	176	LYS	4.3
2	D	213	GLN	4.3
1	C	88	TYR	4.2
2	D	164	ASN	4.2
2	D	224	LYS	4.1
2	D	223	ASP	4.1
2	D	163	VAL	4.1
2	D	168	VAL	4.1
2	D	87	THR	4.1
2	D	85	SER	4.1
1	C	129	LYS	4.1
1	C	198	THR	4.0
1	C	92	VAL	4.0
1	C	157	GLU	4.0
2	D	204	HIS	4.0
1	C	212	PRO	4.0
2	D	79	LEU	4.0
2	D	189	SER	4.0
2	D	208	ASN	4.0
1	C	210	ASP	4.0
2	D	160	SER	4.0
2	D	4	VAL	3.9
1	C	168	LEU	3.9
1	C	135	SER	3.9
2	D	180	LYS	3.9
1	A	189	PHE	3.9
1	C	205	THR	3.8
2	D	203	TRP	3.8
2	D	134	LYS	3.7
1	C	213	CYS	3.7
1	C	47	LEU	3.7
2	D	229	SER	3.7
1	C	155	THR	3.7
2	D	215	GLN	3.6
2	D	227	GLU	3.6
1	C	121	PRO	3.6
3	I	116	TYR	3.6
2	D	157	VAL	3.6
2	D	225	TRP	3.6
2	D	158	GLU	3.5
2	D	161	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	209	HIS	3.5
2	D	6	GLN	3.5
1	C	38	TYR	3.4
2	D	125	PRO	3.4
2	D	107	TYR	3.3
3	I	12	VAL	3.3
2	D	45	LEU	3.3
2	D	230	PRO	3.3
2	D	174	THR	3.3
1	A	156	MET	3.3
1	C	102	SER	3.3
1	C	82	TRP	3.3
5	Q	1	GLU	3.2
2	D	147	CYS	3.2
3	I	84	TYR	3.2
1	C	204	ALA	3.2
1	C	166	THR	3.2
1	C	194	ILE	3.2
2	D	60	ILE	3.2
2	D	207	ARG	3.1
1	C	144	THR	3.1
5	Q	4	LYS	3.1
3	I	22	TYR	3.1
1	C	167	VAL	3.1
2	D	235	GLN	3.0
5	Q	3	TYR	3.0
2	D	94	SER	3.0
1	C	193	ASP	3.0
2	D	187	TYR	3.0
1	C	46	LEU	3.0
2	D	234	THR	3.0
3	I	17	LEU	3.0
1	C	137	ASP	2.9
2	D	97	GLY	2.9
1	C	139	THR	2.9
2	D	2	ALA	2.9
1	C	148	SER	2.9
2	D	136	GLU	2.9
1	C	48	LYS	2.9
2	D	1	GLU	2.8
2	D	118	ASP	2.8
2	D	120	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	192	GLN	2.8
3	I	92	SER	2.8
2	D	124	PRO	2.8
2	D	173	SER	2.8
2	D	80	GLU	2.8
2	D	156	HIS	2.8
2	D	19	VAL	2.8
2	D	176	PRO	2.8
2	D	212	CYS	2.8
1	C	165	ALA	2.8
2	D	247	CYS	2.7
2	D	237	ILE	2.7
3	I	95	ILE	2.7
5	Q	6	TYR	2.7
1	C	115	LEU	2.7
1	C	186	GLN	2.7
1	C	189	PHE	2.7
5	Q	5	PHE	2.7
1	C	143	PHE	2.7
3	H	225	ILE	2.7
1	A	212	PRO	2.7
2	B	1	GLU	2.7
1	A	194	ILE	2.7
1	C	100	PHE	2.7
1	C	62	PHE	2.7
1	A	195	PHE	2.6
1	A	207	PRO	2.6
2	D	181	GLU	2.6
2	D	113	ARG	2.6
2	D	13	ALA	2.6
3	I	42	ASN	2.6
1	C	196	LYS	2.6
2	D	48	TYR	2.6
2	D	106	LEU	2.5
2	D	205	ASN	2.5
1	A	155	THR	2.5
1	C	118	ILE	2.5
1	C	44	GLN	2.5
2	D	222	GLU	2.5
3	I	142	ILE	2.5
2	D	200	ALA	2.5
2	D	33	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	145	ASP	2.5
1	C	170	MET	2.5
1	C	64	ALA	2.5
2	D	8	PRO	2.5
2	D	141	GLN	2.5
2	D	88	SER	2.4
2	D	108	PHE	2.4
3	I	82	LEU	2.4
1	A	209	SER	2.4
1	C	138	SER	2.4
3	I	140	ALA	2.4
1	C	32	LEU	2.4
2	D	216	PHE	2.4
1	C	112	VAL	2.4
3	I	8	PHE	2.4
2	D	177	GLN	2.4
2	D	109	GLY	2.3
3	I	28	VAL	2.3
3	I	85	TYR	2.3
1	C	43	LEU	2.3
1	C	72	SER	2.3
2	D	22	SER	2.3
3	I	64	THR	2.3
2	D	211	ARG	2.3
2	D	56	GLU	2.3
2	D	90	TYR	2.3
2	D	126	LYS	2.3
1	A	198	THR	2.2
3	I	51	TRP	2.2
1	C	150	ILE	2.2
2	D	3	ALA	2.2
3	I	136	ALA	2.2
1	C	90	CYS	2.2
1	A	159	GLY	2.1
3	I	98	ILE	2.1
1	C	39	PRO	2.1
3	H	251	LEU	2.1
3	I	89	ALA	2.1
2	D	140	LYS	2.1
3	I	124	ILE	2.1
2	D	10	ASN	2.1
3	H	138	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	22	CYS	2.1
1	A	208	SER	2.1
4	M	51	MET	2.1
4	M	82	VAL	2.1
2	D	201	THR	2.1
1	C	40	ARG	2.1
1	C	151	ASN	2.1
1	C	116	PRO	2.1
1	C	132	ASP	2.1
2	D	155	ASP	2.1
2	D	121	ASN	2.0
2	D	84	PRO	2.0
1	C	190	THR	2.0
2	D	152	PHE	2.0
3	I	57	PRO	2.0
3	I	151	GLY	2.0
3	I	114	GLN	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](#)

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(Å ²)	Q<0.9
10	NAG	B	809	14/15	0.81	0.36	16.10	101,103,106,108	0
6	NAG	A	803	14/15	0.88	0.30	3.47	80,88,98,103	0
10	NAG	C	814	14/15	0.75	0.19	-0.35	115,122,124,125	0
10	BMA	C	816	11/12	0.83	0.25	-	131,132,132,133	0
6	NAG	A	804	14/15	0.82	0.26	-	109,114,116,116	0
10	NAG	B	810	14/15	0.87	0.27	-	112,115,117,119	0
10	NAG	C	815	14/15	0.53	0.29	-	125,127,128,130	0
8	NAG	A	806	14/15	0.71	0.39	-	130,130,130,131	0
8	BMA	A	807	11/12	0.73	0.23	-	129,130,130,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	BMA	B	811	11/12	0.78	0.20	-	121,123,124,124	0

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
11	ACY	P	1001	4/4	0.69	0.56	17.52	84,84,84,85	0
9	GOL	A	902	6/6	0.82	0.53	14.71	112,112,112,112	0
9	GOL	L	901	6/6	0.81	0.34	7.03	101,101,101,101	0
7	NAG	A	805	14/15	0.49	0.32	2.43	128,129,130,130	0
7	NAG	B	808	14/15	0.59	0.29	-	91,103,104,105	0
7	NAG	H	813	14/15	0.81	0.33	-	125,126,126,126	0
7	NAG	H	812	14/15	0.67	0.20	-	102,113,115,115	0
9	GOL	I	903	6/6	0.62	0.27	-	101,102,102,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.