Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:01 PM GMT

PDB ID	:	4E36
Title	:	Crystal structure of the human Endoplasmic Reticulum Aminopeptidase 2 variant N392K
Authors	:	Birtley, J.R.; Saridakis, E.; Pegias, P.; Stratikos, E.; Mavridis, I.M.
Deposited on	:	2012-03-09
Resolution	:	3.22 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:

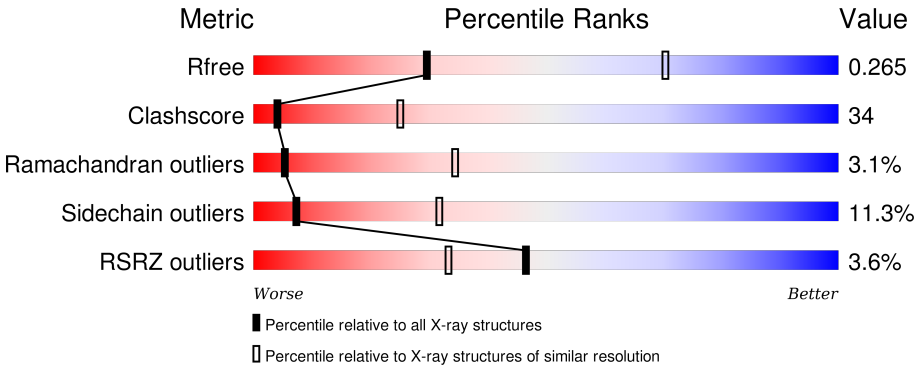
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.22 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	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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	967	39% 44% 7% 10%
1	B	967	6% 36% 45% 7% 11%

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	LYS	A	1001	-	-	-	X
2	LYS	B	1005	-	-	-	X
5	MES	A	1009	-	-	-	X
5	MES	B	1010	-	-	-	X
7	MAN	B	1001	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14341 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.

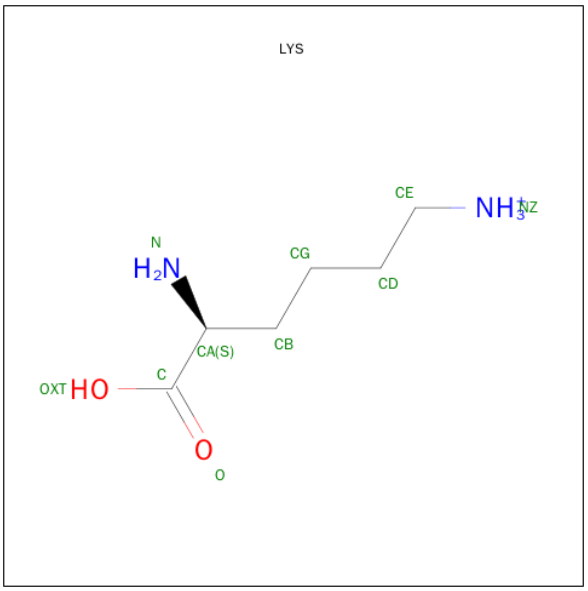
- Molecule 1 is a protein called Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	869	Total	C	N	O	S	2	2	0
			7030	4537	1167	1299	27			
1	B	859	Total	C	N	O	S	0	0	0
			6969	4501	1157	1284	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	PHE	SEE REMARK 999	UNP Q6P179
A	961	ARG	-	EXPRESSION TAG	UNP Q6P179
A	962	HIS	-	EXPRESSION TAG	UNP Q6P179
A	963	HIS	-	EXPRESSION TAG	UNP Q6P179
A	964	HIS	-	EXPRESSION TAG	UNP Q6P179
A	965	HIS	-	EXPRESSION TAG	UNP Q6P179
A	966	HIS	-	EXPRESSION TAG	UNP Q6P179
A	967	HIS	-	EXPRESSION TAG	UNP Q6P179
B	2	VAL	PHE	SEE REMARK 999	UNP Q6P179
B	961	ARG	-	EXPRESSION TAG	UNP Q6P179
B	962	HIS	-	EXPRESSION TAG	UNP Q6P179
B	963	HIS	-	EXPRESSION TAG	UNP Q6P179
B	964	HIS	-	EXPRESSION TAG	UNP Q6P179
B	965	HIS	-	EXPRESSION TAG	UNP Q6P179
B	966	HIS	-	EXPRESSION TAG	UNP Q6P179
B	967	HIS	-	EXPRESSION TAG	UNP Q6P179

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).

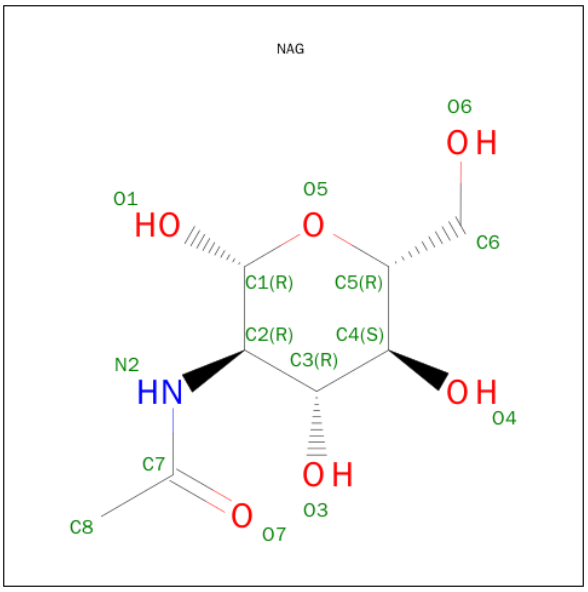


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

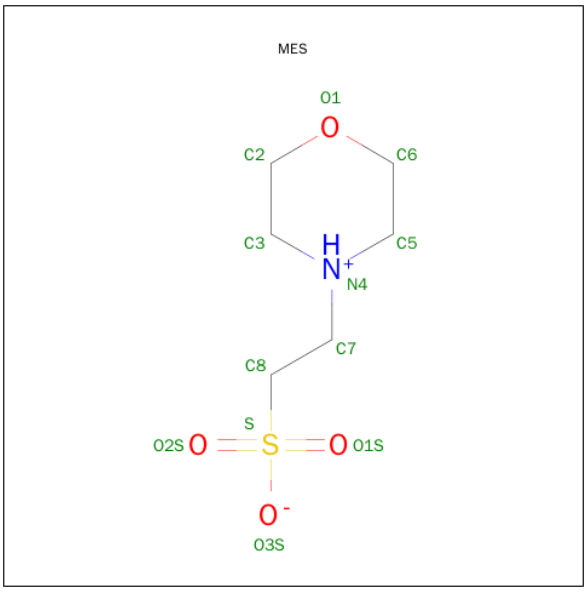
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 12 6 1 4 1	0	0
5	B	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Zn 1 1	0	0
6	A	1	Total Zn 1 1	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	4	Total C N O 50 28 2 20	0	0

- Molecule 8 is water.

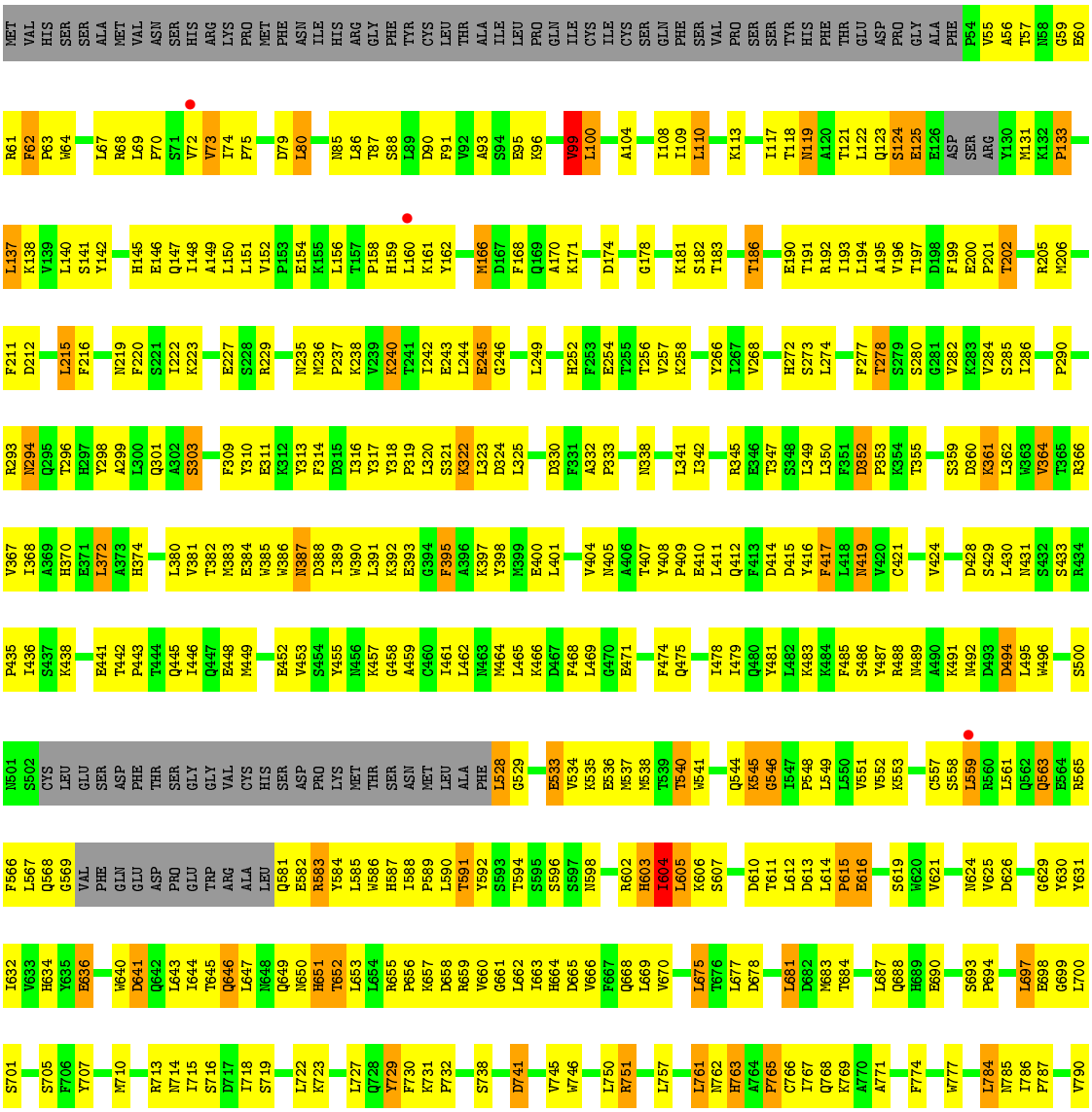
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	66	Total O 66 66	0	0
8	B	40	Total O 40 40	0	0

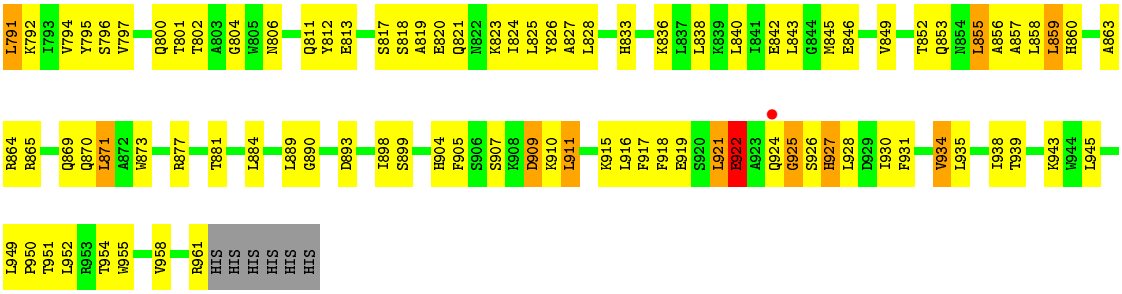
3 Residue-property plots (i)

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

- Molecule 1: Endoplasmic reticulum aminopeptidase 2

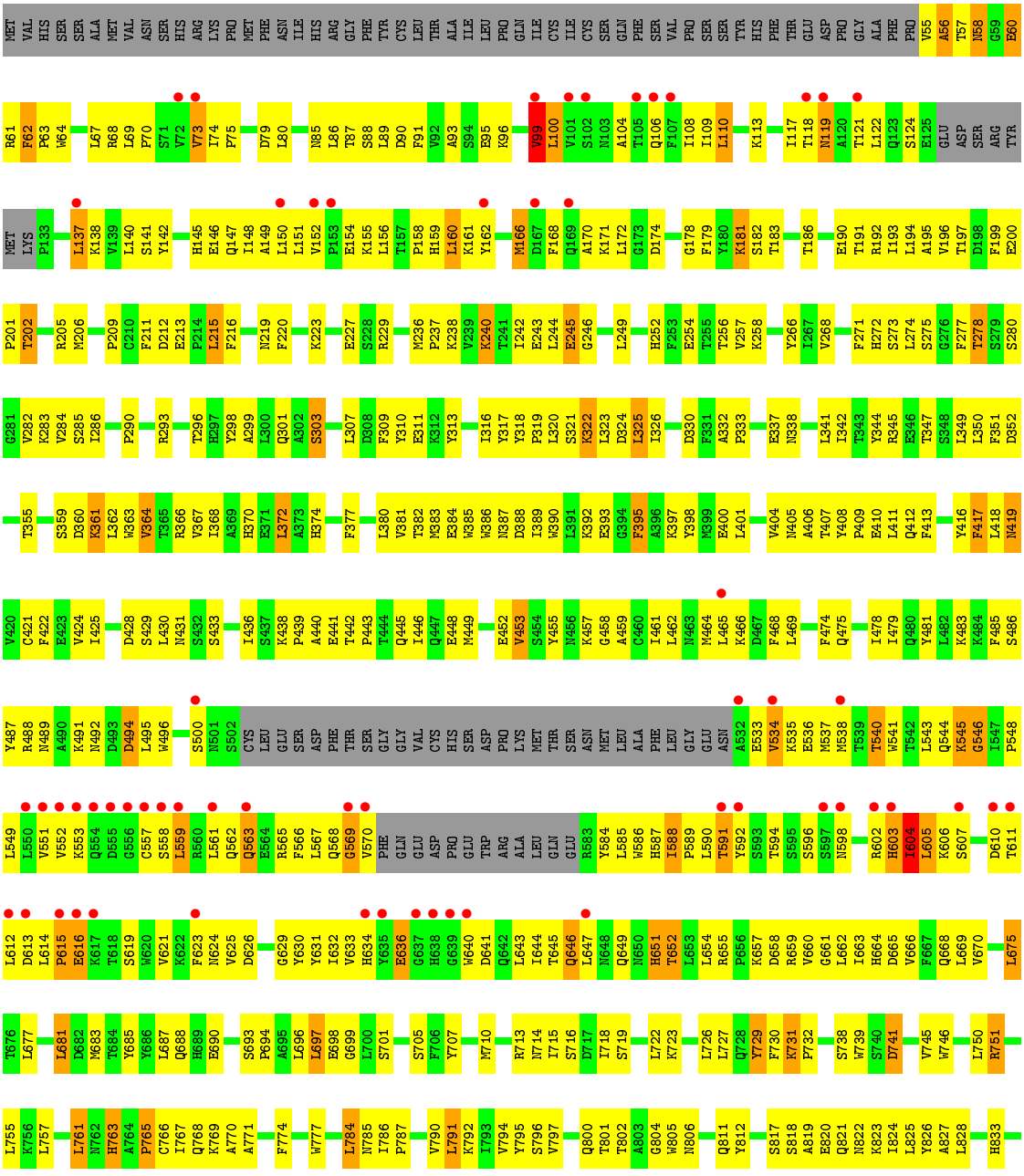
Chain A:

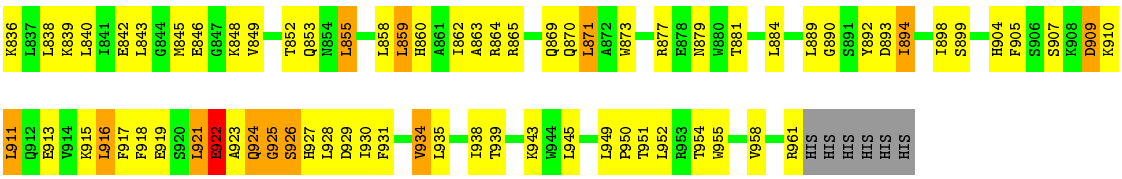




• Molecule 1: Endoplasmic reticulum aminopeptidase 2

Chain B:




K836
L837
L838
K839
L840
T841
E842
L843
G844
M845
E846
G847
K848
V849
T852
Q853
N854
L855
L858
L859
H860
A861
I862
A863
R864
R865
Q869
Q870
L871
A872
W873
R877
E878
N879
W880
T881
L884
L889
G890
S891
Y892
D893
T894
I898
S899
H904
F905
S906
S907
K908
D909
K910
L911
Q912
E913
V914
K915
L916
F917
F918
E919
S920
L921
E922
A923
Q924
G925
S926
H927
L928
D929
I930
F931
V934
L935
I938
T939
K943
W944
L945
L949
P950
T951
L952
R953
T954
W955
V958
R961
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.34Å 134.45Å 127.37Å 90.00° 90.85° 90.00°	Depositor
Resolution (Å)	11.00 – 3.22 59.45 – 3.22	Depositor EDS
% Data completeness (in resolution range)	89.4 (11.00-3.22) 99.1 (59.45-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.209 , 0.261 0.211 , 0.265	Depositor DCC
R_{free} test set	1965 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	69.6	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 65.1	EDS
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 40288 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14341	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.37	0/7207	0.54	0/9769
1	B	0.39	0/7139	0.54	0/9674
All	All	0.38	0/14346	0.54	0/19443

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	922	GLU	Peptide

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	7030	0	6950	459	1
1	B	6969	0	6937	495	1
2	A	10	0	12	0	0
2	B	10	0	12	4	0
3	A	56	0	50	7	0
3	B	28	0	25	2	0
4	A	42	0	39	2	0
4	B	14	0	13	0	0
5	A	12	0	12	1	0
5	B	12	0	12	4	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	50	0	43	6	0
8	A	66	0	0	5	0
8	B	40	0	0	8	0
All	All	14341	0	14105	961	2

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 34.

All (961) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:HG3	3:A:1002:NAG:H82	1.27	1.07
1:A:227:GLU:HG3	3:A:1002:NAG:C8	1.84	1.07
1:A:56:ALA:HB1	1:A:57:THR:HA	1.40	1.02
1:B:488:ARG:HG2	1:B:489:ASN:H	1.24	1.00
1:B:741:ASP:OD2	1:B:787:PRO:HB3	1.61	0.99
1:A:741:ASP:OD2	1:A:787:PRO:HB3	1.63	0.97
1:A:205:ARG:HH21	1:A:212:ASP:HB3	1.30	0.97
1:A:488:ARG:HG2	1:A:489:ASN:H	1.26	0.97
1:B:604:ILE:H	1:B:604:ILE:HD12	1.30	0.96
1:B:205:ARG:HH21	1:B:212:ASP:HB3	1.24	0.96
7:B:1001:MAN:O3	7:B:1002:MAN:H5	1.66	0.94
1:A:355:THR:HG21	1:A:820:GLU:HB2	1.50	0.94
1:B:355:THR:HG21	1:B:820:GLU:HB2	1.47	0.94
1:B:56:ALA:HB2	1:B:62:PHE:H	1.34	0.92
1:A:551:VAL:HG12	1:A:634:HIS:HB3	1.53	0.91
1:A:533:GLU:HA	8:A:1132:HOH:O	1.68	0.90
1:B:551:VAL:HG12	1:B:634:HIS:HB3	1.53	0.90
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.54	0.90
1:A:604:ILE:HD12	1:A:604:ILE:H	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.53	0.89
1:B:56:ALA:HB1	1:B:61:ARG:HA	1.54	0.88
1:A:528:LEU:HD23	1:A:529:GLY:HA2	1.56	0.88
1:A:73:VAL:HG11	1:A:108:ILE:HG12	1.55	0.87
1:A:666:VAL:HG21	1:A:683:MET:SD	2.15	0.87
7:B:1001:MAN:C3	7:B:1002:MAN:H5	2.07	0.85
1:B:801:THR:HG23	1:B:804:GLY:H	1.41	0.84
1:B:56:ALA:CB	1:B:61:ARG:HA	2.07	0.84
1:B:104:ALA:HB2	1:B:158:PRO:HD3	1.58	0.84
1:B:75:PRO:HG3	1:B:211:PHE:CD1	2.12	0.84
1:A:75:PRO:HG3	1:A:211:PHE:CD1	2.13	0.83
1:B:73:VAL:HG11	1:B:108:ILE:HG12	1.58	0.83
1:B:666:VAL:HG21	1:B:683:MET:SD	2.18	0.83
1:A:191:THR:H	1:B:191:THR:HB	1.42	0.82
1:A:801:THR:HG23	1:A:804:GLY:H	1.44	0.81
1:A:537:MET:O	1:A:540:THR:HG23	1.79	0.81
1:A:104:ALA:HB2	1:A:158:PRO:HD3	1.61	0.80
1:B:533:GLU:HB3	8:B:1134:HOH:O	1.82	0.80
1:B:278:THR:CG2	1:B:282:VAL:HB	2.12	0.79
1:B:56:ALA:HB2	1:B:62:PHE:N	1.97	0.79
1:A:681:LEU:HB3	1:A:955:TRP:CE2	2.18	0.79
1:B:537:MET:O	1:B:540:THR:HG23	1.82	0.78
1:B:594:THR:HG22	1:B:621:VAL:HG12	1.64	0.78
1:A:278:THR:CG2	1:A:282:VAL:HB	2.13	0.78
1:A:594:THR:HG22	1:A:621:VAL:HG12	1.65	0.78
1:B:57:THR:HB	1:B:58:ASN:CG	2.04	0.78
1:A:152:VAL:HG12	1:A:154:GLU:H	1.50	0.77
1:B:488:ARG:HG2	1:B:489:ASN:N	2.00	0.77
1:B:429:SER:O	1:B:430:LEU:HD23	1.85	0.77
1:B:446:ILE:O	1:B:449:MET:HB2	1.84	0.77
1:B:681:LEU:HB3	1:B:955:TRP:CE2	2.19	0.77
1:B:710:MET:HB3	1:B:719:SER:HB3	1.67	0.77
1:A:429:SER:O	1:A:430:LEU:HD23	1.85	0.76
1:A:56:ALA:CB	1:A:57:THR:HA	2.15	0.76
1:A:125:GLU:OE1	1:A:125:GLU:HA	1.84	0.76
1:B:548:PRO:HG3	1:B:586:TRP:CD2	2.22	0.75
1:A:548:PRO:HG3	1:A:586:TRP:CD2	2.21	0.75
1:A:57:THR:HG23	1:A:141:SER:O	1.86	0.75
1:A:138:LYS:HB3	1:A:151:LEU:HB2	1.68	0.75
1:A:278:THR:HG21	1:A:282:VAL:HB	1.69	0.75
1:B:278:THR:HG21	1:B:282:VAL:HB	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ILE:O	1:A:449:MET:HB2	1.88	0.74
1:A:528:LEU:CD2	1:A:529:GLY:HA2	2.18	0.74
1:B:160:LEU:HA	8:B:1127:HOH:O	1.87	0.74
1:B:338:ASN:HB2	1:B:341:LEU:O	1.86	0.74
1:A:710:MET:HB3	1:A:719:SER:HB3	1.69	0.74
1:B:384:GLU:HA	1:B:489:ASN:HD22	1.51	0.73
1:A:227:GLU:CG	3:A:1002:NAG:H82	2.12	0.73
1:B:540:THR:O	1:B:544:GLN:HG2	1.88	0.73
1:B:138:LYS:HB3	1:B:151:LEU:HB2	1.68	0.73
1:B:488:ARG:CG	1:B:489:ASN:H	2.02	0.73
1:B:152:VAL:HG12	1:B:154:GLU:H	1.53	0.73
1:B:537:MET:CE	1:B:589:PRO:HG3	2.19	0.73
1:B:56:ALA:CB	1:B:62:PHE:N	2.51	0.73
1:B:677:LEU:HG	1:B:681:LEU:CD2	2.19	0.73
1:B:817:SER:O	1:B:821:GLN:HG3	1.89	0.73
1:A:488:ARG:HG2	1:A:489:ASN:N	2.01	0.73
1:A:677:LEU:HG	1:A:681:LEU:CD2	2.18	0.72
1:A:662:LEU:O	1:A:666:VAL:HG23	1.89	0.72
1:B:388:ASP:OD2	1:B:492:ASN:HB2	1.89	0.72
1:B:784:LEU:HD22	1:B:785:ASN:N	2.04	0.72
1:A:118:THR:O	1:A:119:ASN:HB2	1.89	0.71
1:B:688:GLN:HB3	1:B:729:TYR:HE2	1.55	0.71
1:A:540:THR:O	1:A:544:GLN:HG2	1.89	0.71
1:B:408:TYR:HB3	1:B:411:LEU:HG	1.72	0.71
1:B:333:PRO:HG3	2:B:1005:LYS:HE3	1.70	0.71
1:B:954:THR:O	1:B:958:VAL:HG23	1.90	0.71
1:B:57:THR:HB	1:B:58:ASN:ND2	2.06	0.71
1:A:528:LEU:CB	1:A:529:GLY:HA2	2.20	0.71
1:B:602:ARG:O	1:B:603:HIS:HB2	1.91	0.71
1:B:605:LEU:HD12	1:B:606:LYS:N	2.05	0.70
1:A:605:LEU:HD12	1:A:606:LYS:N	2.06	0.70
1:A:954:THR:O	1:A:958:VAL:HG23	1.91	0.70
1:A:433:SER:O	1:A:545:LYS:HD3	1.91	0.70
1:B:311:GLU:HG2	1:B:317:TYR:HA	1.73	0.70
1:A:784:LEU:HD22	1:A:785:ASN:N	2.05	0.70
1:B:662:LEU:O	1:B:666:VAL:HG23	1.91	0.70
1:B:918:PHE:CE2	1:B:931:PHE:HA	2.26	0.70
1:A:537:MET:CE	1:A:589:PRO:HG3	2.21	0.70
1:A:615:PRO:O	1:A:616:GLU:HB2	1.91	0.70
1:A:401:LEU:HD12	1:A:417:PHE:CD2	2.27	0.70
1:B:797:VAL:O	1:B:800:GLN:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:TRP:HD1	1:B:387:ASN:ND2	1.90	0.69
1:A:488:ARG:CG	1:A:489:ASN:H	2.03	0.69
1:B:828:LEU:HD23	1:B:840:LEU:HD21	1.74	0.69
1:A:688:GLN:HB3	1:A:729:TYR:HE2	1.55	0.69
1:A:465:LEU:HD13	1:A:538:MET:SD	2.32	0.69
1:A:338:ASN:HB2	1:A:341:LEU:O	1.93	0.69
1:B:924:GLN:O	1:B:926:SER:N	2.26	0.68
1:B:545:LYS:CG	1:B:546:GLY:H	2.06	0.68
1:B:615:PRO:O	1:B:616:GLU:HB2	1.91	0.68
1:A:828:LEU:HD23	1:A:840:LEU:HD21	1.76	0.68
1:A:727:LEU:HD11	1:A:763:HIS:HB2	1.75	0.68
1:A:602:ARG:O	1:A:603:HIS:HB2	1.93	0.68
1:B:873:TRP:CZ2	1:B:877:ARG:HD3	2.29	0.68
1:A:364:VAL:O	1:A:368:ILE:HG13	1.94	0.68
1:A:382:THR:O	1:A:489:ASN:HA	1.94	0.68
1:B:442:THR:HG23	1:B:445:GLN:H	1.59	0.68
1:A:385:TRP:HD1	1:A:387:ASN:ND2	1.92	0.68
1:A:918:PHE:CE2	1:A:931:PHE:HA	2.28	0.68
1:B:563:GLN:O	1:B:563:GLN:HG3	1.94	0.68
1:A:442:THR:HG23	1:A:445:GLN:H	1.58	0.67
1:B:67:LEU:HA	1:B:145:HIS:HD2	1.59	0.67
1:A:67:LEU:HA	1:A:145:HIS:HD2	1.60	0.67
1:B:468:PHE:CD2	1:B:469:LEU:HG	2.29	0.67
1:A:311:GLU:HG2	1:A:317:TYR:HA	1.77	0.67
1:B:918:PHE:CE2	1:B:934:VAL:HG11	2.30	0.67
1:A:195:ALA:HB3	1:A:268:VAL:HG22	1.76	0.67
1:A:388:ASP:OD2	1:A:492:ASN:HB2	1.95	0.67
1:B:419:ASN:HD22	1:B:419:ASN:N	1.93	0.67
1:B:56:ALA:HB1	1:B:61:ARG:CA	2.23	0.66
1:B:441:GLU:HB2	1:B:445:GLN:OE1	1.96	0.66
1:B:626:ASP:OD1	1:B:655:ARG:HD3	1.95	0.66
1:A:419:ASN:N	1:A:419:ASN:HD22	1.94	0.66
1:B:677:LEU:HB3	1:B:951:THR:HG21	1.75	0.66
1:B:626:ASP:HA	1:B:657:LYS:HB2	1.78	0.66
1:B:727:LEU:HD21	1:B:761:LEU:HB3	1.78	0.66
1:B:118:THR:O	1:B:119:ASN:HB2	1.93	0.66
1:A:533:GLU:HG2	1:A:533:GLU:O	1.95	0.65
1:B:718:ILE:HD12	1:B:949:LEU:HD11	1.77	0.65
1:B:298:TYR:CZ	1:B:361:LYS:HD2	2.31	0.65
1:A:384:GLU:HA	1:A:489:ASN:HD22	1.59	0.65
1:A:408:TYR:HB3	1:A:411:LEU:HG	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:HG3	3:A:1002:NAG:H83	1.78	0.65
1:A:545:LYS:CG	1:A:546:GLY:H	2.10	0.65
1:A:918:PHE:CE2	1:A:934:VAL:HG11	2.31	0.65
1:B:382:THR:O	1:B:489:ASN:HA	1.96	0.65
1:A:468:PHE:CD2	1:A:469:LEU:HG	2.32	0.65
1:B:466:LYS:HB2	1:B:474:PHE:CD2	2.32	0.65
1:B:784:LEU:HD22	1:B:785:ASN:H	1.62	0.65
1:B:433:SER:O	1:B:545:LYS:HD3	1.97	0.65
1:A:461:ILE:HG13	1:A:462:LEU:N	2.11	0.65
1:A:626:ASP:HA	1:A:657:LYS:HB2	1.78	0.65
1:A:905:PHE:HB2	1:A:938:ILE:HD13	1.78	0.64
1:A:197:THR:HG23	1:A:266:TYR:O	1.97	0.64
1:A:784:LEU:HD22	1:A:785:ASN:H	1.61	0.64
1:A:626:ASP:OD1	1:A:655:ARG:HD3	1.96	0.64
1:B:69:LEU:HD23	1:B:147:GLN:HE21	1.63	0.64
1:B:236:MET:HB3	1:B:254:GLU:HB3	1.80	0.64
1:A:677:LEU:HB3	1:A:951:THR:HG21	1.80	0.64
1:B:152:VAL:HG21	1:B:156:LEU:HD21	1.79	0.64
1:A:386:TRP:CD1	1:A:446:ILE:HD13	2.33	0.64
1:A:441:GLU:HB2	1:A:445:GLN:OE1	1.98	0.64
7:B:1001:MAN:H3	7:B:1002:MAN:H5	1.78	0.64
1:B:659:ARG:HD2	1:B:690:GLU:OE1	1.98	0.64
1:B:777:TRP:HB2	1:B:786:ILE:HD11	1.79	0.64
1:B:195:ALA:HB3	1:B:268:VAL:HG22	1.79	0.64
1:B:401:LEU:HD12	1:B:417:PHE:CD2	2.33	0.64
1:B:457:LYS:HE3	1:B:630:TYR:CE2	2.33	0.64
1:A:457:LYS:HE3	1:A:630:TYR:CE2	2.33	0.64
1:B:727:LEU:HD11	1:B:763:HIS:HB2	1.79	0.64
1:B:86:LEU:HD21	1:B:268:VAL:HG23	1.80	0.64
1:B:863:ALA:HB1	1:B:904:HIS:HE1	1.62	0.64
1:B:75:PRO:HG2	1:B:216:PHE:HB3	1.80	0.64
1:B:461:ILE:HG13	1:B:462:LEU:N	2.11	0.64
1:B:386:TRP:CD1	1:B:446:ILE:HD13	2.33	0.64
1:A:777:TRP:HB2	1:A:786:ILE:HD11	1.80	0.64
1:A:797:VAL:O	1:A:800:GLN:HG2	1.97	0.64
1:B:833:HIS:HB2	1:B:836:LYS:HG3	1.79	0.63
1:B:452:GLU:H	1:B:452:GLU:CD	2.01	0.63
1:B:122:LEU:CB	1:B:137:LEU:HD21	2.28	0.63
1:A:817:SER:O	1:A:821:GLN:HG3	1.99	0.63
1:A:299:ALA:O	1:A:303:SER:OG	2.16	0.63
1:B:323:LEU:HD11	1:B:342:ILE:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ILE:HD12	1:A:949:LEU:HD11	1.79	0.63
1:B:915:LYS:O	1:B:919:GLU:HG2	1.97	0.63
1:A:563:GLN:HG3	1:A:563:GLN:O	1.98	0.63
1:B:605:LEU:HD12	1:B:606:LYS:H	1.63	0.63
1:B:677:LEU:HB3	1:B:951:THR:CG2	2.29	0.63
1:B:364:VAL:O	1:B:368:ILE:HG13	1.98	0.63
1:B:56:ALA:O	1:B:57:THR:HG23	1.98	0.62
1:A:122:LEU:CB	1:A:137:LEU:HD21	2.29	0.62
1:B:332:ALA:HB3	1:B:333:PRO:HD3	1.81	0.62
1:B:905:PHE:HB2	1:B:938:ILE:HD13	1.81	0.62
1:A:410:GLU:O	1:A:412:GLN:HG3	1.99	0.62
1:A:582:GLU:O	1:A:583:ARG:CB	2.47	0.62
1:A:915:LYS:O	1:A:919:GLU:HG2	1.98	0.62
1:B:141:SER:HA	1:B:148:ILE:HG22	1.81	0.62
1:A:457:LYS:HE3	1:A:630:TYR:HE2	1.63	0.62
1:B:812:TYR:CE1	1:B:821:GLN:HB3	2.35	0.62
1:B:122:LEU:HB3	1:B:137:LEU:HD21	1.82	0.62
1:B:412:GLN:OE1	1:B:746:TRP:HD1	1.82	0.62
1:B:481:TYR:O	1:B:485:PHE:HD2	1.83	0.61
1:B:465:LEU:HD13	1:B:538:MET:SD	2.38	0.61
1:B:646:GLN:HA	1:B:646:GLN:HE21	1.63	0.61
1:A:400:GLU:O	1:A:404:VAL:HG23	2.01	0.61
1:B:299:ALA:O	1:B:303:SER:OG	2.17	0.61
1:A:945:LEU:HD22	1:A:949:LEU:HD22	1.81	0.61
1:B:777:TRP:HB2	1:B:786:ILE:CD1	2.30	0.61
1:B:457:LYS:HE3	1:B:630:TYR:HE2	1.63	0.61
1:B:475:GLN:O	1:B:479:ILE:HG12	2.01	0.61
1:B:448:GLU:OE2	1:B:928:LEU:HA	2.00	0.61
1:A:727:LEU:HD21	1:A:761:LEU:HB3	1.82	0.61
1:B:400:GLU:O	1:B:404:VAL:HG23	2.00	0.61
1:A:152:VAL:HG21	1:A:156:LEU:HD21	1.81	0.61
1:A:873:TRP:CZ2	1:A:877:ARG:HD3	2.35	0.61
1:A:448:GLU:OE2	1:A:928:LEU:HA	2.01	0.61
1:A:69:LEU:HD23	1:A:147:GLN:HE21	1.65	0.61
1:B:945:LEU:HD22	1:B:949:LEU:HD22	1.83	0.61
1:A:236:MET:HB3	1:A:254:GLU:HB3	1.83	0.61
1:B:205:ARG:NH2	1:B:212:ASP:HB3	2.07	0.61
1:A:442:THR:HG22	1:A:445:GLN:NE2	2.16	0.61
1:A:298:TYR:CZ	1:A:361:LYS:HD2	2.36	0.61
1:A:452:GLU:CD	1:A:452:GLU:H	2.03	0.61
1:A:323:LEU:HD11	1:A:342:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:LEU:HD12	1:B:325:LEU:N	2.16	0.60
1:A:99:VAL:HG12	1:A:100:LEU:H	1.65	0.60
1:A:220:PHE:O	1:A:256:THR:HG23	2.01	0.60
1:A:838:LEU:HD23	1:A:871:LEU:HD21	1.83	0.60
1:B:313:TYR:HE2	1:B:478:ILE:HD11	1.66	0.60
1:A:605:LEU:HD12	1:A:606:LYS:H	1.66	0.60
1:B:442:THR:HG22	1:B:445:GLN:NE2	2.17	0.60
1:A:860:HIS:O	1:A:860:HIS:HD2	1.83	0.60
1:A:205:ARG:NH2	1:A:212:ASP:HB3	2.11	0.60
1:B:99:VAL:HG12	1:B:100:LEU:H	1.66	0.60
1:A:528:LEU:HB3	1:A:529:GLY:CA	2.31	0.60
1:B:545:LYS:CG	1:B:546:GLY:N	2.65	0.60
1:A:86:LEU:HD21	1:A:268:VAL:HG23	1.83	0.60
1:A:863:ALA:HB1	1:A:904:HIS:HE1	1.66	0.60
1:A:227:GLU:HB3	1:A:229:ARG:HG2	1.84	0.60
1:A:141:SER:HA	1:A:148:ILE:HG22	1.84	0.60
1:A:156:LEU:HD12	1:A:162:TYR:CE1	2.37	0.60
1:B:464:MET:HG3	1:B:629:GLY:HA2	1.83	0.60
1:A:122:LEU:HB3	1:A:137:LEU:HD21	1.82	0.60
1:B:332:ALA:O	1:B:345:ARG:NH1	2.34	0.60
1:B:763:HIS:O	1:B:767:ILE:HG22	2.01	0.60
1:B:62:PHE:CE1	1:B:142:TYR:HB2	2.37	0.59
1:B:158:PRO:HB2	1:B:159:HIS:HD2	1.67	0.59
1:A:286:ILE:CG2	1:A:296:THR:HB	2.32	0.59
1:A:442:THR:O	1:A:446:ILE:HG13	2.03	0.59
1:B:431:ASN:HA	1:B:565:ARG:HH22	1.67	0.59
1:B:624:ASN:HD21	1:B:629:GLY:H	1.50	0.59
1:A:183:THR:HA	1:A:192:ARG:O	2.03	0.59
1:A:158:PRO:HB2	1:A:159:HIS:HD2	1.67	0.59
1:B:552:VAL:HG12	1:B:561:LEU:HD23	1.85	0.59
1:A:56:ALA:HB1	1:A:57:THR:CA	2.27	0.59
1:A:763:HIS:O	1:A:767:ILE:HG22	2.02	0.59
1:A:833:HIS:HB2	1:A:836:LYS:HG3	1.83	0.59
1:A:731:LYS:N	1:A:732:PRO:HD2	2.16	0.59
1:A:545:LYS:CG	1:A:546:GLY:N	2.66	0.59
1:A:412:GLN:OE1	1:A:746:TRP:HD1	1.85	0.59
1:B:286:ILE:CG2	1:B:296:THR:HB	2.32	0.59
1:A:325:LEU:HD12	1:A:325:LEU:N	2.17	0.59
1:B:714:ASN:O	1:B:716:SER:N	2.36	0.59
1:A:486:SER:HB3	1:A:487:TYR:CD2	2.38	0.59
1:A:475:GLN:O	1:A:479:ILE:HG12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ALA:HA	1:B:62:PHE:HB2	1.84	0.59
1:A:659:ARG:HD2	1:A:690:GLU:OE1	2.01	0.59
1:A:442:THR:OG1	1:A:443:PRO:HD2	2.01	0.59
1:A:398:TYR:OH	1:A:466:LYS:HD3	2.03	0.59
1:B:918:PHE:CZ	1:B:934:VAL:HG11	2.38	0.59
1:B:855:LEU:HD22	1:B:859:LEU:HD22	1.83	0.59
1:B:604:ILE:CD1	1:B:604:ILE:H	2.06	0.58
1:B:410:GLU:O	1:B:412:GLN:HG3	2.03	0.58
1:A:566:PHE:CE2	1:A:632:ILE:HD12	2.38	0.58
1:A:855:LEU:HD22	1:A:859:LEU:HD22	1.86	0.58
1:A:646:GLN:HE21	1:A:646:GLN:HA	1.67	0.58
1:A:466:LYS:HB2	1:A:474:PHE:CD2	2.38	0.58
1:B:466:LYS:HG3	1:B:466:LYS:O	2.04	0.58
1:A:313:TYR:HE2	1:A:478:ILE:HD11	1.69	0.58
1:B:355:THR:HG21	1:B:820:GLU:CB	2.29	0.58
1:A:481:TYR:O	1:A:485:PHE:HD2	1.87	0.58
1:B:889:LEU:HD21	1:B:925:GLY:HA2	1.86	0.58
1:B:220:PHE:O	1:B:256:THR:HG23	2.04	0.58
1:B:156:LEU:HD12	1:B:162:TYR:CE1	2.38	0.57
1:A:431:ASN:HA	1:A:565:ARG:HH22	1.68	0.57
1:B:731:LYS:N	1:B:732:PRO:HD2	2.18	0.57
1:A:889:LEU:HD13	1:A:928:LEU:HD21	1.85	0.57
1:B:486:SER:HB3	1:B:487:TYR:CD2	2.38	0.57
1:A:60:GLU:HB3	8:A:1153:HOH:O	2.04	0.57
1:A:918:PHE:CZ	1:A:934:VAL:HG11	2.39	0.57
1:B:106:GLN:HE21	1:B:155:LYS:NZ	2.02	0.57
1:A:604:ILE:CD1	1:A:604:ILE:H	2.12	0.57
1:B:710:MET:O	1:B:713:ARG:O	2.22	0.57
1:B:442:THR:O	1:B:446:ILE:HG13	2.04	0.57
1:A:75:PRO:HG2	1:A:216:PHE:HB3	1.86	0.57
1:A:567:LEU:HD11	1:A:581:GLN:N	2.20	0.57
1:B:85:ASN:HB3	1:B:88:SER:HB3	1.86	0.57
1:A:666:VAL:O	1:A:670:VAL:HG23	2.05	0.57
1:B:727:LEU:O	1:B:731:LYS:HB2	2.03	0.57
1:A:466:LYS:HG3	1:A:466:LYS:O	2.04	0.57
1:B:566:PHE:CE2	1:B:632:ILE:HD12	2.40	0.57
1:B:272:HIS:CE1	1:B:290:PRO:HB3	2.40	0.57
1:B:544:GLN:NE2	1:B:584:TYR:HD1	2.03	0.57
1:A:677:LEU:HB3	1:A:951:THR:CG2	2.35	0.57
1:B:282:VAL:HG21	1:B:318:TYR:HD2	1.68	0.56
1:B:333:PRO:CG	2:B:1005:LYS:HE3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ILE:HG21	1:A:791:LEU:HA	1.87	0.56
1:A:828:LEU:HB3	1:A:840:LEU:HD11	1.87	0.56
1:B:398:TYR:OH	1:B:466:LYS:HD3	2.05	0.56
1:B:924:GLN:O	1:B:926:SER:HA	2.06	0.56
1:B:889:LEU:HD13	1:B:928:LEU:HD21	1.87	0.56
1:A:272:HIS:CE1	1:A:290:PRO:HB3	2.39	0.56
1:A:528:LEU:HB3	1:A:529:GLY:HA2	1.86	0.56
1:B:442:THR:OG1	1:B:443:PRO:HD2	2.06	0.56
1:A:777:TRP:HB2	1:A:786:ILE:CD1	2.35	0.56
1:A:332:ALA:O	1:A:345:ARG:NH1	2.37	0.56
1:A:714:ASN:O	1:A:716:SER:N	2.38	0.56
1:A:309:PHE:CD2	1:A:309:PHE:C	2.79	0.56
1:A:693:SER:N	1:A:694:PRO:HD2	2.21	0.56
1:A:419:ASN:HD22	1:A:419:ASN:H	1.54	0.56
1:B:792:LYS:HG2	1:B:826:TYR:CD2	2.40	0.56
1:B:421:CYS:O	1:B:424:VAL:HG12	2.04	0.56
1:A:67:LEU:HA	1:A:145:HIS:CD2	2.40	0.56
1:A:792:LYS:HG2	1:A:826:TYR:CD2	2.40	0.56
1:B:929:ASP:HA	8:B:1106:HOH:O	2.05	0.56
1:B:666:VAL:O	1:B:670:VAL:HG23	2.05	0.56
1:B:828:LEU:HB3	1:B:840:LEU:HD11	1.88	0.56
1:B:928:LEU:HB2	1:B:930:ILE:HG22	1.87	0.56
1:A:731:LYS:N	1:A:732:PRO:CD	2.68	0.56
1:A:332:ALA:HB3	1:A:333:PRO:HD3	1.88	0.56
1:B:182:SER:HB2	1:B:330:ASP:HB2	1.87	0.55
1:A:257:VAL:HG23	1:A:258:LYS:O	2.06	0.55
1:A:812:TYR:CE1	1:A:821:GLN:HB3	2.42	0.55
1:B:838:LEU:HD23	1:B:871:LEU:HD21	1.88	0.55
1:A:548:PRO:HG3	1:A:586:TRP:CE3	2.41	0.55
1:B:197:THR:HG23	1:B:266:TYR:O	2.07	0.55
1:B:731:LYS:HE2	1:B:763:HIS:CE1	2.42	0.55
1:A:877:ARG:HG3	1:A:917:PHE:CD1	2.41	0.55
1:A:819:ALA:O	1:A:823:LYS:HG3	2.06	0.55
1:B:693:SER:N	1:B:694:PRO:HD2	2.22	0.55
1:A:581:GLN:HG3	1:A:582:GLU:H	1.71	0.55
1:B:892:TYR:CE1	5:B:1010:MES:H52	2.42	0.55
1:A:407:THR:C	1:A:409:PRO:HD3	2.27	0.55
1:A:421:CYS:O	1:A:424:VAL:HG12	2.06	0.55
1:B:89:LEU:HD13	1:B:181:LYS:HD3	1.87	0.55
1:A:533:GLU:CG	1:A:533:GLU:O	2.54	0.55
1:A:811:GLN:HA	1:A:811:GLN:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:921:LEU:O	1:B:922:GLU:HB2	2.07	0.55
1:A:124:SER:HB2	1:A:131:MET:O	2.07	0.55
1:B:67:LEU:HA	1:B:145:HIS:CD2	2.39	0.55
1:B:309:PHE:CD2	1:B:309:PHE:C	2.79	0.55
1:B:236:MET:CE	1:B:256:THR:HA	2.37	0.55
1:B:424:VAL:HG21	1:B:457:LYS:HB2	1.88	0.55
1:B:777:TRP:HB2	1:B:784:LEU:HD12	1.89	0.54
1:A:552:VAL:HG12	1:A:561:LEU:HD23	1.89	0.54
1:B:819:ALA:O	1:B:823:LYS:HG3	2.08	0.54
1:B:257:VAL:HG23	1:B:258:LYS:O	2.07	0.54
1:B:227:GLU:HB3	1:B:229:ARG:HG2	1.90	0.54
1:A:229:ARG:NH2	1:B:190:GLU:OE2	2.34	0.54
1:A:710:MET:CB	1:A:719:SER:HB3	2.37	0.54
1:A:113:LYS:HG2	1:A:206:MET:HG2	1.90	0.54
1:B:624:ASN:HB2	1:B:631:TYR:CE2	2.42	0.54
1:A:624:ASN:HD21	1:A:629:GLY:H	1.56	0.54
1:A:624:ASN:HB2	1:A:631:TYR:CE2	2.42	0.54
1:B:786:ILE:HG21	1:B:791:LEU:HA	1.89	0.54
1:B:183:THR:HA	1:B:192:ARG:O	2.07	0.54
1:B:407:THR:C	1:B:409:PRO:HD3	2.28	0.54
1:B:838:LEU:O	1:B:842:GLU:HG3	2.08	0.54
1:A:258:LYS:HG2	3:A:1004:NAG:O6	2.07	0.54
1:A:581:GLN:HB3	1:A:584:TYR:HE2	1.72	0.54
1:B:877:ARG:HG3	1:B:917:PHE:CD1	2.42	0.54
1:B:487:TYR:HA	8:B:1104:HOH:O	2.08	0.54
1:A:738:SER:O	1:A:751:ARG:CD	2.56	0.54
1:B:496:TRP:CE3	1:B:496:TRP:HA	2.43	0.54
1:A:566:PHE:CD2	1:A:632:ILE:HD12	2.43	0.54
1:B:811:GLN:NE2	1:B:811:GLN:HA	2.22	0.54
1:A:435:PRO:HA	8:A:1143:HOH:O	2.08	0.54
1:A:62:PHE:CE1	1:A:142:TYR:HB2	2.42	0.54
1:A:182:SER:HB2	1:A:330:ASP:HB2	1.89	0.54
1:B:56:ALA:CB	1:B:61:ARG:CA	2.81	0.53
1:A:537:MET:HE2	1:A:589:PRO:HG3	1.90	0.53
1:B:731:LYS:N	1:B:732:PRO:CD	2.70	0.53
1:A:928:LEU:HB2	1:A:930:ILE:HG22	1.90	0.53
1:A:85:ASN:HB3	1:A:88:SER:HB3	1.91	0.53
1:A:650:ASN:OD1	4:A:1007:NAG:N2	2.41	0.53
1:B:62:PHE:CD1	1:B:142:TYR:HB2	2.43	0.53
1:B:634:HIS:HE1	1:B:675:LEU:CD1	2.22	0.53
1:A:123:GLN:HG2	1:A:133:PRO:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:MET:O	1:A:713:ARG:O	2.27	0.53
1:B:640:TRP:CZ3	1:B:666:VAL:HG22	2.44	0.53
1:B:405:ASN:O	1:B:409:PRO:HG3	2.09	0.53
1:B:738:SER:O	1:B:751:ARG:CD	2.57	0.53
1:A:245:GLU:HG2	1:A:246:GLY:N	2.23	0.53
1:B:710:MET:CB	1:B:719:SER:HB3	2.37	0.53
1:A:286:ILE:HG21	1:A:296:THR:HB	1.91	0.53
1:B:934:VAL:O	1:B:938:ILE:HG13	2.08	0.53
1:A:838:LEU:O	1:A:842:GLU:HG3	2.09	0.52
3:B:1007:NAG:H61	3:B:1008:NAG:H82	1.89	0.52
1:B:615:PRO:O	1:B:616:GLU:CB	2.58	0.52
1:B:285:SER:HB2	1:B:324:ASP:OD1	2.10	0.52
1:B:56:ALA:CB	1:B:62:PHE:H	2.10	0.52
1:A:186:THR:HG23	1:A:190:GLU:O	2.08	0.52
1:A:528:LEU:CB	1:A:529:GLY:CA	2.87	0.52
1:B:557:CYS:O	1:B:613:ASP:HA	2.10	0.52
1:A:118:THR:O	1:A:119:ASN:CB	2.58	0.52
1:B:805:TRP:HH2	1:B:839:LYS:HD3	1.75	0.52
1:B:100:LEU:HD13	1:B:161:LYS:HG2	1.90	0.52
1:A:123:GLN:NE2	1:A:133:PRO:HB3	2.25	0.52
1:A:634:HIS:HE1	1:A:675:LEU:CD1	2.23	0.52
1:A:109:ILE:HD11	1:A:149:ALA:HB2	1.91	0.52
1:B:363:TRP:O	1:B:366:ARG:HB2	2.09	0.52
1:A:202:THR:OG1	1:A:202:THR:O	2.27	0.52
1:B:860:HIS:O	1:B:860:HIS:HD2	1.93	0.52
1:B:923:ALA:O	1:B:924:GLN:HB2	2.10	0.51
1:B:730:PHE:C	1:B:732:PRO:HD2	2.31	0.51
1:B:605:LEU:HD12	1:B:607:SER:H	1.75	0.51
1:A:355:THR:HG21	1:A:820:GLU:CB	2.33	0.51
1:A:730:PHE:C	1:A:732:PRO:HD2	2.30	0.51
1:B:665:ASP:O	1:B:669:LEU:HG	2.10	0.51
1:B:56:ALA:HB1	1:B:62:PHE:N	2.25	0.51
1:A:528:LEU:HD23	1:A:529:GLY:CA	2.34	0.51
1:B:186:THR:HG23	1:B:190:GLU:O	2.10	0.51
1:B:419:ASN:HD22	1:B:419:ASN:H	1.55	0.51
1:B:677:LEU:HG	1:B:681:LEU:HD23	1.90	0.51
1:B:545:LYS:HG2	1:B:546:GLY:N	2.26	0.51
1:A:677:LEU:HG	1:A:681:LEU:HD23	1.93	0.51
1:A:282:VAL:HG21	1:A:318:TYR:HD2	1.75	0.51
1:A:615:PRO:O	1:A:616:GLU:CB	2.58	0.51
1:B:863:ALA:HA	1:B:869:GLN:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ASN:HA	1:B:565:ARG:NH2	2.25	0.51
1:A:293:ARG:NH2	7:B:1001:MAN:O2	2.40	0.51
1:B:777:TRP:HH2	1:B:811:GLN:HG2	1.76	0.51
1:A:934:VAL:O	1:A:938:ILE:HG13	2.11	0.51
2:B:1005:LYS:HB3	5:B:1010:MES:O1S	2.11	0.51
1:A:496:TRP:CE3	1:A:496:TRP:HA	2.46	0.51
1:B:924:GLN:O	1:B:925:GLY:C	2.48	0.51
1:A:345:ARG:NH2	1:A:853:GLN:HB2	2.26	0.51
1:A:919:GLU:O	1:A:922:GLU:HB2	2.11	0.50
1:B:553:LYS:HB2	1:B:636:GLU:OE2	2.11	0.50
1:B:681:LEU:HB3	1:B:955:TRP:CZ2	2.46	0.50
1:B:479:ILE:O	1:B:483:LYS:HG3	2.11	0.50
1:B:349:LEU:C	1:B:350:LEU:HD23	2.30	0.50
1:B:892:TYR:CD1	5:B:1010:MES:H71	2.47	0.50
1:B:545:LYS:HG3	1:B:546:GLY:H	1.75	0.50
1:B:428:ASP:OD2	1:B:457:LYS:HD2	2.11	0.50
1:A:431:ASN:HA	1:A:565:ARG:NH2	2.26	0.50
1:A:442:THR:CG2	1:A:445:GLN:HG3	2.41	0.50
1:A:777:TRP:HB2	1:A:784:LEU:HD12	1.92	0.50
1:A:935:LEU:O	1:A:939:THR:HG23	2.10	0.50
1:B:537:MET:HE1	1:B:589:PRO:HG3	1.91	0.50
1:B:537:MET:HE2	1:B:589:PRO:HG3	1.93	0.50
1:A:191:THR:HB	1:B:191:THR:H	1.76	0.50
1:A:405:ASN:O	1:A:409:PRO:HG3	2.12	0.50
1:A:69:LEU:HD22	1:A:109:ILE:HG22	1.92	0.50
1:A:860:HIS:O	1:A:860:HIS:CD2	2.65	0.50
1:B:924:GLN:O	1:B:926:SER:CA	2.60	0.50
1:A:911:LEU:O	1:A:915:LYS:HB2	2.12	0.50
1:A:662:LEU:HB3	1:A:683:MET:CE	2.41	0.50
1:B:411:LEU:HA	1:B:745:VAL:HG21	1.93	0.50
1:A:917:PHE:CE2	1:A:921:LEU:HD11	2.46	0.50
1:B:845:MET:SD	1:B:855:LEU:HD11	2.52	0.50
1:A:219:ASN:OD1	1:A:258:LYS:HD3	2.11	0.50
1:B:442:THR:CG2	1:B:445:GLN:HG3	2.41	0.49
1:B:566:PHE:CD2	1:B:632:ILE:HD12	2.46	0.49
1:A:681:LEU:HB3	1:A:955:TRP:CZ2	2.46	0.49
1:A:557:CYS:O	1:A:613:ASP:HA	2.12	0.49
1:B:362:LEU:HD13	1:B:411:LEU:HB3	1.94	0.49
1:B:479:ILE:HG22	1:B:483:LYS:HE3	1.94	0.49
1:A:863:ALA:HA	1:A:869:GLN:HA	1.95	0.49
1:A:500:SER:HB3	1:A:534:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ILE:HD11	1:B:458:GLY:N	2.27	0.49
1:B:113:LYS:HG2	1:B:206:MET:HG2	1.94	0.49
1:B:548:PRO:HG3	1:B:586:TRP:CE3	2.47	0.49
1:A:545:LYS:HG3	1:A:546:GLY:H	1.76	0.49
1:A:464:MET:HG3	1:A:629:GLY:HA2	1.93	0.49
1:B:898:ILE:HG22	1:B:899:SER:N	2.26	0.49
1:B:654:LEU:HA	8:B:1121:HOH:O	2.13	0.49
1:A:75:PRO:CG	1:A:211:PHE:CD1	2.92	0.49
1:B:918:PHE:CE2	1:B:934:VAL:CG1	2.95	0.49
1:B:917:PHE:CE2	1:B:921:LEU:HD11	2.47	0.49
1:B:67:LEU:HB3	1:B:145:HIS:CD2	2.47	0.49
1:A:693:SER:OG	1:A:750:LEU:HD22	2.13	0.49
1:B:245:GLU:HG2	1:B:246:GLY:N	2.27	0.49
1:A:372:LEU:HD23	1:A:372:LEU:N	2.27	0.49
1:A:414:ASP:O	8:A:1101:HOH:O	2.19	0.49
1:A:235:ASN:O	1:A:322:LYS:HE3	2.13	0.49
1:B:741:ASP:OD2	1:B:787:PRO:CB	2.48	0.49
1:B:56:ALA:HB1	1:B:61:ARG:C	2.32	0.49
1:B:889:LEU:HD21	1:B:925:GLY:CA	2.42	0.49
1:A:236:MET:CE	1:A:256:THR:HA	2.42	0.49
1:A:349:LEU:C	1:A:350:LEU:HD23	2.33	0.49
1:B:877:ARG:HA	1:B:917:PHE:CE1	2.48	0.49
1:B:440:ALA:HA	8:B:1117:HOH:O	2.11	0.49
1:B:873:TRP:CE2	1:B:877:ARG:HD3	2.47	0.49
1:B:108:ILE:HB	1:B:150:LEU:HB2	1.94	0.49
1:B:640:TRP:CH2	1:B:666:VAL:HG22	2.47	0.49
1:B:388:ASP:CG	1:B:492:ASN:HB2	2.33	0.49
1:B:634:HIS:CE1	1:B:675:LEU:HD13	2.48	0.48
1:B:286:ILE:HG21	1:B:296:THR:HB	1.94	0.48
1:B:397:LYS:HB3	1:B:459:ALA:HB2	1.95	0.48
1:B:347:THR:HG22	1:B:818:SER:HB2	1.94	0.48
1:A:362:LEU:HD13	1:A:411:LEU:HB3	1.94	0.48
1:B:223:LYS:HD3	1:B:252:HIS:CE1	2.48	0.48
1:B:537:MET:HA	1:B:587:HIS:HB2	1.96	0.48
1:A:108:ILE:HB	1:A:150:LEU:HB2	1.94	0.48
1:B:707:TYR:HE1	1:B:723:LYS:HB2	1.78	0.48
1:B:118:THR:O	1:B:119:ASN:CB	2.62	0.48
1:A:407:THR:O	1:A:409:PRO:HD3	2.14	0.48
1:B:69:LEU:HD22	1:B:109:ILE:HG22	1.94	0.48
1:B:565:ARG:O	1:B:567:LEU:HD12	2.14	0.48
1:A:544:GLN:NE2	1:A:584:TYR:HD1	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LEU:HA	1:A:745:VAL:HG21	1.96	0.48
1:A:877:ARG:HA	1:A:917:PHE:CE1	2.48	0.48
1:A:926:SER:HA	1:A:927:HIS:HA	1.60	0.48
1:A:479:ILE:O	1:A:483:LYS:HG3	2.13	0.48
1:A:347:THR:HG22	1:A:818:SER:HB2	1.94	0.48
1:B:243:GLU:HA	1:B:249:LEU:HD23	1.94	0.48
1:B:491:LYS:O	1:B:494:ASP:HB2	2.14	0.48
1:A:319:PRO:HB2	1:A:320:LEU:HD23	1.96	0.48
1:A:777:TRP:HH2	1:A:811:GLN:HG2	1.79	0.48
1:B:109:ILE:HD11	1:B:149:ALA:HB2	1.96	0.48
1:A:870:GLN:O	1:A:871:LEU:C	2.51	0.48
1:A:245:GLU:CG	1:A:246:GLY:N	2.75	0.48
1:B:395:PHE:HE2	1:B:495:LEU:HD21	1.78	0.48
1:A:565:ARG:HD2	1:A:584:TYR:CE2	2.48	0.48
1:B:757:LEU:CD1	1:B:761:LEU:HD22	2.44	0.48
1:A:537:MET:HE1	1:A:589:PRO:HG3	1.96	0.48
1:B:911:LEU:O	1:B:915:LYS:HB2	2.13	0.48
1:A:653:LEU:HD21	4:A:1007:NAG:H82	1.94	0.48
1:A:380:LEU:HG	1:A:486:SER:HA	1.95	0.48
1:A:845:MET:SD	1:A:855:LEU:HD11	2.53	0.48
1:A:62:PHE:CD1	1:A:142:TYR:HB2	2.49	0.48
1:A:491:LYS:HB2	1:A:491:LYS:HE3	1.61	0.48
1:B:552:VAL:HG12	1:B:561:LEU:CD2	2.42	0.48
1:B:380:LEU:HG	1:B:486:SER:HA	1.95	0.48
1:B:75:PRO:CG	1:B:211:PHE:CD1	2.92	0.47
1:A:538:MET:HA	1:A:541:TRP:HD1	1.79	0.47
1:A:285:SER:HB2	1:A:324:ASP:OD1	2.14	0.47
1:B:790:VAL:O	1:B:794:VAL:HG23	2.14	0.47
1:B:604:ILE:HD12	1:B:604:ILE:N	2.14	0.47
1:B:634:HIS:HE1	1:B:675:LEU:HD13	1.80	0.47
1:A:429:SER:C	1:A:430:LEU:HD23	2.33	0.47
1:B:935:LEU:O	1:B:939:THR:HG23	2.14	0.47
1:B:500:SER:HB3	1:B:534:VAL:HB	1.96	0.47
1:B:182:SER:CB	1:B:330:ASP:HB2	2.44	0.47
1:A:56:ALA:CB	1:A:57:THR:CA	2.89	0.47
1:A:401:LEU:C	1:A:401:LEU:HD23	2.35	0.47
1:B:668:GLN:OE1	1:B:668:GLN:HA	2.14	0.47
1:A:605:LEU:HD12	1:A:607:SER:H	1.79	0.47
1:B:119:ASN:O	1:B:166:MET:HA	2.13	0.47
1:A:925:GLY:O	1:A:926:SER:C	2.53	0.47
1:B:496:TRP:HA	1:B:496:TRP:HE3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD13	1:A:161:LYS:HG2	1.96	0.47
3:A:1004:NAG:H62	3:A:1005:NAG:O5	2.15	0.47
1:B:245:GLU:CG	1:B:246:GLY:N	2.78	0.47
1:B:243:GLU:O	1:B:244:LEU:HD23	2.14	0.47
1:A:559:LEU:HD12	1:A:612:LEU:O	2.14	0.47
1:B:662:LEU:HB3	1:B:683:MET:CE	2.44	0.47
1:A:545:LYS:HG2	1:A:546:GLY:N	2.29	0.47
1:B:655:ARG:HB2	1:B:658:ASP:OD2	2.14	0.47
1:A:407:THR:OG1	1:A:408:TYR:HD2	1.98	0.47
1:B:342:ILE:HG22	1:B:344:TYR:CE1	2.48	0.47
1:B:661:GLY:O	1:B:664:HIS:HB3	2.14	0.47
1:B:587:HIS:CE1	1:B:606:LYS:HD2	2.49	0.47
1:A:640:TRP:CZ3	1:A:666:VAL:HG22	2.50	0.47
1:B:345:ARG:NH2	1:B:853:GLN:HB2	2.29	0.47
1:A:791:LEU:HD11	1:A:795:TYR:CZ	2.50	0.47
1:B:538:MET:HA	1:B:541:TRP:HD1	1.79	0.47
1:B:178:GLY:O	1:B:197:THR:HA	2.15	0.47
1:B:309:PHE:HD2	1:B:310:TYR:N	2.13	0.47
1:A:898:ILE:HG22	1:A:899:SER:N	2.29	0.47
1:A:110:LEU:HD12	1:A:148:ILE:HG13	1.97	0.47
1:A:146:GLU:OE1	1:A:205:ARG:HD2	2.15	0.47
1:A:274:LEU:HD21	1:A:293:ARG:HE	1.79	0.47
1:B:949:LEU:N	1:B:950:PRO:HD2	2.30	0.47
1:B:791:LEU:HD11	1:B:795:TYR:CZ	2.50	0.47
1:A:792:LYS:HB2	8:A:1144:HOH:O	2.15	0.47
1:B:693:SER:O	1:B:697:LEU:HB2	2.15	0.47
1:A:922:GLU:HG2	1:A:926:SER:OG	2.14	0.47
1:B:205:ARG:HH21	1:B:212:ASP:CB	2.11	0.47
1:B:309:PHE:CD2	1:B:310:TYR:N	2.84	0.46
1:A:90:ASP:CB	1:A:171:LYS:HA	2.46	0.46
1:A:949:LEU:N	1:A:950:PRO:HD2	2.29	0.46
1:B:905:PHE:O	1:B:938:ILE:HG23	2.14	0.46
1:A:763:HIS:NE2	1:A:765:PRO:HG2	2.30	0.46
1:B:763:HIS:NE2	1:B:765:PRO:HG2	2.29	0.46
1:B:643:LEU:O	1:B:646:GLN:HB3	2.15	0.46
1:A:313:TYR:O	1:A:479:ILE:HD11	2.14	0.46
1:B:659:ARG:O	1:B:663:ILE:HG13	2.16	0.46
1:A:119:ASN:O	1:A:166:MET:HA	2.15	0.46
1:B:407:THR:OG1	1:B:408:TYR:HD2	1.97	0.46
1:B:939:THR:O	1:B:943:LYS:HG3	2.16	0.46
1:A:67:LEU:HB3	1:A:145:HIS:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:HA	1:A:75:PRO:HD3	1.74	0.46
1:B:429:SER:C	1:B:430:LEU:HD23	2.36	0.46
1:B:280:SER:HB2	1:B:317:TYR:HE1	1.80	0.46
1:B:911:LEU:HD11	1:B:939:THR:HG22	1.97	0.46
1:A:313:TYR:CE2	1:A:478:ILE:HD11	2.50	0.46
1:B:723:LYS:O	1:B:727:LEU:HD23	2.15	0.46
1:B:110:LEU:HD12	1:B:148:ILE:HG13	1.96	0.46
1:A:485:PHE:O	1:A:486:SER:C	2.52	0.46
1:A:389:ILE:HD12	1:A:392:LYS:HE3	1.98	0.46
1:B:122:LEU:HD11	1:B:162:TYR:CB	2.37	0.46
1:B:594:THR:HG21	1:B:614:LEU:HD11	1.98	0.46
1:A:723:LYS:O	1:A:727:LEU:HD23	2.16	0.46
1:A:812:TYR:HB2	1:A:824:ILE:HG21	1.98	0.46
1:B:843:LEU:HD22	1:B:849:VAL:HB	1.98	0.46
1:A:428:ASP:OD2	1:A:457:LYS:HD2	2.15	0.46
1:A:436:ILE:HD11	1:A:458:GLY:N	2.31	0.46
1:A:651:HIS:CD2	1:A:652:THR:N	2.84	0.46
7:B:1001:MAN:H3	7:B:1002:MAN:C5	2.43	0.46
1:A:589:PRO:C	1:A:590:LEU:HD23	2.36	0.46
1:B:924:GLN:HA	1:B:924:GLN:OE1	2.15	0.46
1:B:313:TYR:CE2	1:B:478:ILE:HD11	2.48	0.46
1:B:696:LEU:HD23	1:B:750:LEU:HD21	1.98	0.46
1:B:387:ASN:HB3	1:B:438:LYS:O	2.15	0.46
1:B:591:THR:O	1:B:592:TYR:HB3	2.16	0.46
1:B:64:TRP:CD2	1:B:70:PRO:HG3	2.51	0.46
1:A:604:ILE:O	1:A:605:LEU:CB	2.63	0.46
1:A:934:VAL:CG1	1:A:935:LEU:N	2.77	0.46
1:A:182:SER:CB	1:A:330:ASP:HB2	2.46	0.46
1:A:395:PHE:HE2	1:A:495:LEU:HD21	1.80	0.46
1:A:238:LYS:HB3	1:A:238:LYS:HE2	1.76	0.46
1:B:421:CYS:HA	1:B:424:VAL:HG12	1.97	0.45
1:A:921:LEU:O	1:A:922:GLU:HB2	2.16	0.45
1:A:884:LEU:HD21	1:A:889:LEU:HD23	1.98	0.45
1:A:479:ILE:HG22	1:A:483:LYS:HE3	1.97	0.45
1:A:634:HIS:CE1	1:A:675:LEU:HD13	2.51	0.45
1:A:536:GLU:O	1:A:540:THR:HG22	2.15	0.45
1:B:351:PHE:CE1	1:B:361:LYS:HB2	2.51	0.45
1:A:424:VAL:HG21	1:A:457:LYS:HB2	1.98	0.45
1:A:860:HIS:C	1:A:860:HIS:CD2	2.89	0.45
1:A:661:GLY:O	1:A:664:HIS:HB3	2.16	0.45
1:B:200:GLU:HA	1:B:201:PRO:HA	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ILE:HD12	1:B:392:LYS:HE3	1.99	0.45
1:B:568:GLN:O	1:B:569:GLY:O	2.34	0.45
7:B:1001:MAN:HO3	7:B:1002:MAN:H5	1.77	0.45
1:B:386:TRP:HB3	1:B:446:ILE:HG23	1.99	0.45
1:B:545:LYS:HG2	1:B:546:GLY:H	1.77	0.45
1:A:873:TRP:CE2	1:A:877:ARG:HD3	2.51	0.45
1:B:140:LEU:O	1:B:148:ILE:HA	2.16	0.45
1:A:651:HIS:CD2	1:A:651:HIS:C	2.89	0.45
1:A:668:GLN:OE1	1:A:668:GLN:HA	2.16	0.45
1:B:662:LEU:HB3	1:B:683:MET:HE1	1.98	0.45
1:A:388:ASP:CG	1:A:492:ASN:HB2	2.37	0.45
1:B:313:TYR:O	1:B:479:ILE:HD11	2.16	0.45
1:B:549:LEU:HB2	1:B:566:PHE:HD2	1.82	0.45
1:B:726:LEU:HA	1:B:726:LEU:HD23	1.84	0.45
1:A:581:GLN:HB3	1:A:584:TYR:CE2	2.51	0.45
1:B:67:LEU:CA	1:B:145:HIS:CD2	2.99	0.45
1:B:693:SER:OG	1:B:750:LEU:HD22	2.16	0.45
1:A:393:GLU:OE1	1:A:455:TYR:CE2	2.70	0.45
1:B:274:LEU:HD21	1:B:293:ARG:HE	1.81	0.45
1:B:240:LYS:HB2	1:B:240:LYS:HE3	1.60	0.45
1:B:536:GLU:O	1:B:540:THR:HG22	2.17	0.45
1:B:60:GLU:HB2	1:B:61:ARG:HA	1.97	0.45
1:A:860:HIS:O	1:A:864:ARG:HG3	2.17	0.45
1:A:697:LEU:HD12	1:A:697:LEU:HA	1.73	0.45
1:B:491:LYS:HB2	1:B:491:LYS:HE3	1.61	0.45
1:A:591:THR:O	1:A:592:TYR:HB3	2.17	0.45
1:B:393:GLU:OE1	1:B:455:TYR:CE2	2.69	0.45
1:A:64:TRP:CD2	1:A:70:PRO:HG3	2.52	0.45
1:A:243:GLU:HA	1:A:249:LEU:HD23	1.98	0.45
1:B:138:LYS:HD2	1:B:151:LEU:HD12	1.99	0.45
1:B:777:TRP:HA	1:B:784:LEU:HB3	1.99	0.45
1:B:784:LEU:HD13	1:B:786:ILE:HD12	1.98	0.45
1:B:934:VAL:CG1	1:B:935:LEU:N	2.80	0.45
1:B:647:LEU:O	1:B:651:HIS:HB3	2.17	0.45
1:A:91:PHE:CE2	1:A:170:ALA:HB3	2.52	0.45
1:B:60:GLU:HB2	1:B:61:ARG:CA	2.47	0.45
1:B:104:ALA:CB	1:B:158:PRO:HD3	2.39	0.45
1:A:594:THR:HG21	1:A:614:LEU:HD11	1.99	0.45
1:A:655:ARG:O	1:A:658:ASP:HB2	2.16	0.45
1:A:884:LEU:HD12	1:A:884:LEU:HA	1.67	0.45
1:B:273:SER:HA	1:B:286:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:O	1:A:478:ILE:HG12	2.17	0.45
1:A:643:LEU:O	1:A:646:GLN:HB3	2.17	0.45
1:B:651:HIS:CD2	1:B:652:THR:N	2.85	0.45
1:A:223:LYS:HD3	1:A:252:HIS:CE1	2.51	0.45
1:A:140:LEU:O	1:A:148:ILE:HA	2.17	0.45
1:B:158:PRO:CB	1:B:159:HIS:HD2	2.30	0.45
1:A:565:ARG:O	1:A:567:LEU:HD12	2.16	0.45
1:A:537:MET:HA	1:A:587:HIS:HB2	1.99	0.45
1:A:589:PRO:O	1:A:590:LEU:HD23	2.17	0.45
1:B:922:GLU:HA	1:B:922:GLU:OE2	2.17	0.45
1:B:889:LEU:O	1:B:889:LEU:HD12	2.17	0.45
1:A:301:GLN:NE2	1:A:408:TYR:OH	2.50	0.45
1:A:62:PHE:HA	1:A:63:PRO:HD3	1.67	0.45
1:B:436:ILE:HA	1:B:453:VAL:CG1	2.47	0.45
1:A:243:GLU:O	1:A:244:LEU:HD23	2.17	0.45
1:A:907:SER:HB2	1:A:909:ASP:OD2	2.17	0.45
1:A:843:LEU:HD22	1:A:849:VAL:HB	1.97	0.45
5:A:1009:MES:H32	5:A:1009:MES:H82	1.70	0.45
1:A:294:ASN:HA	1:A:294:ASN:HD22	1.64	0.45
1:B:146:GLU:OE1	1:B:205:ARG:HD2	2.17	0.44
1:B:366:ARG:HD2	1:B:413:PHE:CE1	2.52	0.44
1:B:592:TYR:OH	1:B:612:LEU:HD21	2.17	0.44
1:A:568:GLN:O	1:A:569:GLY:O	2.35	0.44
1:B:894:ILE:HD13	1:B:894:ILE:HA	1.79	0.44
1:A:939:THR:O	1:A:943:LYS:HG3	2.17	0.44
1:A:873:TRP:O	1:A:877:ARG:HB2	2.18	0.44
1:B:275:SER:HB3	1:B:283:LYS:HE2	1.99	0.44
1:A:138:LYS:HD2	1:A:151:LEU:HD12	1.99	0.44
1:B:812:TYR:HB2	1:B:824:ILE:HG21	2.00	0.44
1:A:387:ASN:HB3	1:A:438:LYS:O	2.18	0.44
1:A:196:VAL:HG22	1:A:197:THR:N	2.33	0.44
1:A:491:LYS:O	1:A:494:ASP:HB2	2.17	0.44
1:B:355:THR:O	1:B:355:THR:HG22	2.17	0.44
1:A:918:PHE:CE2	1:A:934:VAL:CG1	2.98	0.44
1:A:421:CYS:HA	1:A:424:VAL:HG12	1.99	0.44
1:B:863:ALA:HB1	1:B:904:HIS:CE1	2.48	0.44
1:A:922:GLU:HA	1:A:926:SER:HB2	1.98	0.44
1:B:860:HIS:CD2	1:B:860:HIS:C	2.90	0.44
1:A:796:SER:HA	1:A:827:ALA:HB1	1.98	0.44
1:A:168:PHE:CD1	1:A:168:PHE:N	2.85	0.44
1:B:55:VAL:O	1:B:56:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:CYS:O	1:A:614:LEU:N	2.48	0.44
1:B:821:GLN:O	1:B:822:ASN:C	2.55	0.44
1:A:496:TRP:HA	1:A:496:TRP:HE3	1.83	0.44
1:B:106:GLN:HG3	1:B:155:LYS:HD3	1.99	0.44
1:A:693:SER:O	1:A:697:LEU:HB2	2.18	0.44
3:A:1002:NAG:H62	3:A:1003:NAG:C1	2.48	0.44
1:B:337:GLU:OE2	2:B:1005:LYS:N	2.51	0.44
1:A:124:SER:CB	1:A:131:MET:H	2.30	0.44
1:A:910:LYS:HD3	1:A:910:LYS:HA	1.83	0.44
1:A:655:ARG:HB2	1:A:658:ASP:OD2	2.18	0.44
1:A:366[B]:ARG:HE	1:A:400:GLU:CD	2.20	0.44
1:A:397:LYS:O	1:A:400:GLU:HB2	2.18	0.44
1:A:316:ILE:HG12	1:A:483:LYS:HE2	2.00	0.44
1:A:309:PHE:CD2	1:A:310:TYR:N	2.86	0.44
1:B:553:LYS:O	1:B:559:LEU:HA	2.17	0.44
1:B:646:GLN:HE21	1:B:646:GLN:CA	2.28	0.44
1:A:663:ILE:N	1:A:683:MET:HE1	2.33	0.44
1:A:763:HIS:CG	1:A:765:PRO:HD2	2.53	0.44
1:A:611:THR:HG22	1:A:612:LEU:N	2.33	0.44
1:B:90:ASP:HA	1:B:172:LEU:H	1.83	0.44
1:B:62:PHE:HA	1:B:63:PRO:HD3	1.68	0.43
1:B:74:ILE:HA	1:B:75:PRO:HD3	1.76	0.43
1:A:67:LEU:HD12	1:A:68:ARG:N	2.33	0.43
1:B:401:LEU:HD23	1:B:401:LEU:C	2.38	0.43
1:A:922:GLU:OE2	1:A:926:SER:HB2	2.17	0.43
1:A:553:LYS:HB2	1:A:636:GLU:OE2	2.18	0.43
1:A:665:ASP:O	1:A:669:LEU:HG	2.18	0.43
1:A:390:TRP:CZ2	1:A:391:LEU:HD23	2.53	0.43
1:A:858:LEU:HD12	1:A:858:LEU:O	2.18	0.43
1:A:158:PRO:CB	1:A:159:HIS:HD2	2.30	0.43
1:B:624:ASN:HD21	1:B:629:GLY:N	2.13	0.43
1:A:553:LYS:O	1:A:559:LEU:HA	2.18	0.43
1:B:907:SER:HB2	1:B:909:ASP:OD2	2.18	0.43
1:A:205:ARG:HH21	1:A:212:ASP:CB	2.16	0.43
1:B:551:VAL:CG1	1:B:634:HIS:HB3	2.37	0.43
1:A:662:LEU:HB3	1:A:683:MET:HE1	2.00	0.43
1:A:565:ARG:HD3	1:A:581:GLN:HB2	1.99	0.43
1:B:884:LEU:HD12	1:B:884:LEU:HA	1.70	0.43
1:B:774:PHE:HB2	1:B:794:VAL:CG1	2.48	0.43
1:B:69:LEU:CD2	1:B:147:GLN:HE21	2.31	0.43
1:A:757:LEU:CD1	1:A:761:LEU:HD22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:PHE:CE1	1:B:421:CYS:SG	3.11	0.43
1:B:197:THR:HB	1:B:199:PHE:CZ	2.54	0.43
1:B:664:HIS:O	1:B:668:GLN:HG2	2.17	0.43
1:B:90:ASP:CB	1:B:171:LYS:HA	2.48	0.43
1:B:623:PHE:HB2	1:B:633:VAL:HG11	2.01	0.43
1:B:796:SER:HA	1:B:827:ALA:HB1	2.01	0.43
1:A:240:LYS:HE3	1:A:240:LYS:HB2	1.61	0.43
1:B:884:LEU:HD21	1:B:889:LEU:HD23	2.01	0.43
1:B:416:TYR:O	1:B:418:LEU:N	2.52	0.43
1:A:534:VAL:O	1:A:535:LYS:C	2.56	0.43
1:B:271:PHE:CD2	1:B:326:ILE:HD11	2.53	0.43
1:A:641:ASP:N	1:A:641:ASP:OD1	2.51	0.43
1:B:168:PHE:CD1	1:B:168:PHE:N	2.86	0.43
1:B:237:PRO:HG3	1:B:322:LYS:CG	2.49	0.43
1:B:589:PRO:C	1:B:590:LEU:HD23	2.38	0.43
1:B:640:TRP:O	1:B:644:ILE:HG13	2.19	0.43
1:B:710:MET:HG3	1:B:718:ILE:HB	1.99	0.43
1:A:934:VAL:HG12	1:A:935:LEU:N	2.34	0.43
1:B:870:GLN:O	1:B:871:LEU:C	2.56	0.43
1:B:860:HIS:O	1:B:864:ARG:HG3	2.18	0.43
1:B:909:ASP:O	1:B:913:GLU:HG3	2.19	0.43
1:A:122:LEU:HD11	1:A:162:TYR:CB	2.38	0.43
1:A:318:TYR:HA	1:A:319:PRO:HD3	1.75	0.43
1:B:359:SER:O	1:B:360:ASP:C	2.56	0.43
1:B:833:HIS:O	1:B:836:LYS:HB2	2.19	0.43
1:B:836:LYS:O	1:B:839:LYS:HB3	2.19	0.43
1:A:845:MET:O	1:A:846:GLU:C	2.57	0.43
1:B:179:PHE:CD1	1:B:197:THR:HG22	2.54	0.43
1:B:227:GLU:OE1	1:B:229:ARG:HD3	2.19	0.43
1:B:91:PHE:CE2	1:B:170:ALA:HB3	2.53	0.43
1:A:640:TRP:O	1:A:644:ILE:HG13	2.19	0.43
1:A:197:THR:HB	1:A:199:PHE:CZ	2.53	0.43
1:B:422:PHE:HA	1:B:425:ILE:HD12	2.00	0.43
1:A:355:THR:O	1:A:355:THR:HG22	2.17	0.43
1:B:777:TRP:CH2	1:B:811:GLN:HG2	2.53	0.43
1:B:802:THR:HG22	1:B:806:ASN:ND2	2.34	0.43
1:B:588:ILE:HD11	1:B:631:TYR:CG	2.53	0.43
1:A:552:VAL:HG12	1:A:561:LEU:CD2	2.49	0.43
1:B:491:LYS:H	1:B:494:ASP:HB2	1.84	0.43
1:B:419:ASN:ND2	1:B:419:ASN:N	2.64	0.42
1:A:398:TYR:C	1:A:398:TYR:CD2	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:HB2	1:A:566:PHE:HD2	1.84	0.42
1:B:687:LEU:HD11	1:B:699:GLY:HA3	2.01	0.42
1:A:178:GLY:O	1:A:197:THR:HA	2.19	0.42
1:B:452:GLU:CD	1:B:452:GLU:N	2.71	0.42
1:A:273:SER:HA	1:A:286:ILE:O	2.19	0.42
1:A:237:PRO:HG3	1:A:322:LYS:CG	2.50	0.42
1:A:707:TYR:HE1	1:A:723:LYS:HB2	1.84	0.42
1:B:731:LYS:HG2	1:B:731:LYS:HZ3	1.75	0.42
1:A:196:VAL:CG2	1:A:197:THR:N	2.82	0.42
1:A:646:GLN:CA	1:A:646:GLN:HE21	2.31	0.42
1:B:377:PHE:CZ	1:B:395:PHE:CD1	3.08	0.42
1:A:592:TYR:OH	1:A:612:LEU:HD21	2.19	0.42
1:B:651:HIS:CD2	1:B:651:HIS:C	2.92	0.42
1:A:790:VAL:O	1:A:794:VAL:HG23	2.19	0.42
1:B:604:ILE:O	1:B:605:LEU:CB	2.66	0.42
1:A:710:MET:HG3	1:A:718:ILE:HB	2.01	0.42
1:B:845:MET:O	1:B:846:GLU:C	2.57	0.42
1:B:196:VAL:HG22	1:B:197:THR:N	2.34	0.42
1:B:442:THR:HG22	1:B:445:GLN:CD	2.40	0.42
1:A:419:ASN:ND2	1:A:419:ASN:N	2.65	0.42
1:B:325:LEU:HB3	1:B:344:TYR:CE1	2.54	0.42
1:B:475:GLN:O	1:B:478:ILE:HG12	2.19	0.42
1:A:452:GLU:CD	1:A:452:GLU:N	2.72	0.42
1:B:219:ASN:OD1	1:B:258:LYS:HD3	2.18	0.42
1:A:93:ALA:HB3	1:A:168:PHE:CE2	2.55	0.42
1:A:768:GLN:O	1:A:771:ALA:HB3	2.20	0.42
1:B:79:ASP:HB2	1:B:96:LYS:HB3	2.02	0.42
1:A:104:ALA:CB	1:A:158:PRO:HD3	2.43	0.42
1:B:360:ASP:O	1:B:361:LYS:C	2.58	0.42
1:A:863:ALA:HB1	1:A:904:HIS:CE1	2.51	0.42
1:A:693:SER:N	1:A:694:PRO:CD	2.82	0.42
1:B:559:LEU:HD12	1:B:612:LEU:O	2.19	0.42
1:A:774:PHE:HB2	1:A:794:VAL:CG1	2.50	0.42
1:A:227:GLU:OE1	1:A:229:ARG:HD3	2.20	0.42
1:B:438:LYS:HG3	1:B:439:PRO:HD2	2.02	0.42
1:A:284:VAL:HG11	1:A:303:SER:HB2	2.01	0.42
1:B:397:LYS:O	1:B:400:GLU:HB2	2.20	0.42
1:B:860:HIS:O	1:B:860:HIS:CD2	2.73	0.42
1:B:534:VAL:O	1:B:535:LYS:C	2.58	0.42
1:B:319:PRO:HB2	1:B:320:LEU:HD23	2.00	0.42
1:B:565:ARG:HD2	1:B:584:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ASN:CB	1:B:438:LYS:O	2.68	0.42
1:B:919:GLU:O	1:B:922:GLU:HB2	2.20	0.42
1:B:889:LEU:HA	1:B:890:GLY:HA2	1.62	0.42
1:B:496:TRP:CZ2	1:B:538:MET:HB3	2.55	0.42
1:B:870:GLN:HE22	1:B:910:LYS:HE3	1.85	0.42
1:A:79:ASP:HB2	1:A:96:LYS:HB3	2.02	0.42
1:A:634:HIS:HE1	1:A:675:LEU:HD13	1.84	0.42
1:A:496:TRP:CZ2	1:A:538:MET:HB3	2.55	0.42
1:A:67:LEU:CA	1:A:145:HIS:CD2	3.01	0.42
1:B:468:PHE:CE2	1:B:469:LEU:HG	2.55	0.42
1:B:284:VAL:HG11	1:B:303:SER:HB2	2.00	0.42
1:A:889:LEU:HA	1:A:890:GLY:HA2	1.60	0.42
1:B:636:GLU:H	1:B:636:GLU:HG3	1.62	0.42
1:A:79:ASP:O	1:A:95:GLU:HA	2.20	0.42
1:A:687:LEU:HD11	1:A:699:GLY:HA3	2.01	0.42
1:B:370:HIS:CD2	1:B:370:HIS:C	2.93	0.42
1:B:858:LEU:O	1:B:858:LEU:HD12	2.19	0.42
1:B:104:ALA:H	1:B:158:PRO:HG3	1.85	0.42
1:B:757:LEU:HD11	1:B:761:LEU:HD22	2.02	0.42
1:A:852:THR:O	1:A:855:LEU:HB2	2.20	0.42
1:B:106:GLN:HE21	1:B:155:LYS:HZ2	1.68	0.42
1:A:856:ALA:O	1:A:857:ALA:C	2.58	0.42
1:B:916:LEU:HD22	1:B:916:LEU:HA	1.85	0.42
1:B:768:GLN:O	1:B:771:ALA:HB3	2.20	0.42
1:A:784:LEU:HD13	1:A:786:ILE:HD12	2.02	0.41
1:B:655:ARG:O	1:B:658:ASP:HB2	2.20	0.41
1:A:889:LEU:HD12	1:A:889:LEU:O	2.20	0.41
1:B:390:TRP:CB	1:B:436:ILE:HG23	2.50	0.41
1:B:95:GLU:OE1	1:B:209:PRO:HD2	2.21	0.41
1:B:238:LYS:HB3	1:B:238:LYS:HE2	1.72	0.41
1:B:372:LEU:N	1:B:372:LEU:HD23	2.34	0.41
1:A:741:ASP:OD2	1:A:787:PRO:CB	2.51	0.41
1:A:442:THR:HG22	1:A:445:GLN:CD	2.40	0.41
1:B:817:SER:O	1:B:821:GLN:CG	2.65	0.41
1:A:433:SER:HB3	1:A:545:LYS:HG3	2.02	0.41
1:B:201:PRO:HD2	1:B:202:THR:HG23	2.01	0.41
1:B:213:GLU:HB2	1:B:216:PHE:CD2	2.54	0.41
1:B:386:TRP:CB	1:B:446:ILE:HG23	2.50	0.41
1:A:386:TRP:HB3	1:A:446:ILE:HG23	2.02	0.41
1:A:761:LEU:O	1:A:762:ASN:HB2	2.21	0.41
1:A:397:LYS:HB3	1:A:459:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:HIS:CE1	1:A:392:LYS:HG2	2.56	0.41
1:A:647:LEU:O	1:A:651:HIS:HB3	2.19	0.41
1:B:79:ASP:O	1:B:95:GLU:HA	2.20	0.41
1:A:370:HIS:C	1:A:370:HIS:CD2	2.93	0.41
1:B:923:ALA:O	1:B:924:GLN:CB	2.67	0.41
1:B:67:LEU:HD12	1:B:68:ARG:N	2.35	0.41
1:B:763:HIS:CG	1:B:765:PRO:HD2	2.55	0.41
1:B:398:TYR:CD2	1:B:398:TYR:C	2.94	0.41
1:A:359:SER:O	1:A:360:ASP:C	2.58	0.41
1:A:381:VAL:HG13	1:A:485:PHE:CB	2.50	0.41
1:A:314:PHE:O	1:A:316:ILE:HG13	2.21	0.41
1:A:309:PHE:HD2	1:A:310:TYR:N	2.17	0.41
1:B:183:THR:HG22	1:B:193:ILE:HG12	2.02	0.41
1:A:215:LEU:HA	1:A:489:ASN:ND2	2.35	0.41
1:B:551:VAL:CG2	1:B:562:GLN:HB2	2.50	0.41
1:B:805:TRP:CH2	1:B:839:LYS:HD3	2.54	0.41
1:A:436:ILE:HA	1:A:453:VAL:CG1	2.50	0.41
1:A:200:GLU:HA	1:A:201:PRO:HA	1.69	0.41
1:A:700:LEU:HD23	1:A:700:LEU:HA	1.90	0.41
1:B:589:PRO:O	1:B:590:LEU:HD23	2.20	0.41
1:B:407:THR:O	1:B:409:PRO:HD3	2.21	0.41
1:B:559:LEU:HD12	1:B:612:LEU:HB3	2.02	0.41
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.92	0.41
1:A:777:TRP:CH2	1:A:811:GLN:HG2	2.56	0.41
1:A:416:TYR:O	1:A:417:PHE:C	2.59	0.41
1:B:770:ALA:CB	1:B:797:VAL:HG21	2.51	0.41
1:A:280:SER:HB2	1:A:317:TYR:HE1	1.85	0.41
1:B:802:THR:HG23	1:B:836:LYS:CE	2.50	0.41
1:A:219:ASN:OD1	1:A:258:LYS:CD	2.68	0.41
1:B:374:HIS:CE1	1:B:392:LYS:HG2	2.55	0.41
1:B:93:ALA:HB3	1:B:168:PHE:CE2	2.55	0.41
1:B:385:TRP:CG	1:B:386:TRP:N	2.88	0.41
1:A:442:THR:OG1	1:A:443:PRO:CD	2.68	0.41
1:A:366[A]:ARG:HD3	1:A:400:GLU:OE1	2.21	0.41
1:B:611:THR:HG22	1:B:612:LEU:N	2.36	0.41
1:B:662:LEU:O	1:B:663:ILE:C	2.59	0.41
1:B:277:PHE:HA	1:B:282:VAL:O	2.21	0.41
1:B:385:TRP:CD1	1:B:387:ASN:ND2	2.80	0.41
1:B:301:GLN:NE2	1:B:408:TYR:OH	2.53	0.41
1:A:688:GLN:HB3	1:A:729:TYR:CE2	2.46	0.41
1:A:802:THR:HG23	1:A:836:LYS:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:CG2	1:B:197:THR:N	2.84	0.41
1:B:257:VAL:HB	3:B:1007:NAG:O6	2.21	0.41
1:B:543:LEU:HB3	8:B:1101:HOH:O	2.20	0.41
1:B:660:VAL:HG13	1:B:698:GLU:OE1	2.21	0.41
1:B:215:LEU:HA	1:B:489:ASN:HD21	1.86	0.41
1:B:215:LEU:HA	1:B:489:ASN:ND2	2.36	0.41
1:A:551:VAL:CG1	1:A:634:HIS:HB3	2.37	0.41
1:B:236:MET:HG2	1:B:256:THR:HG22	2.03	0.41
1:B:381:VAL:HG13	1:B:485:PHE:CB	2.51	0.41
1:B:739:TRP:CZ2	1:B:755:LEU:HD22	2.56	0.41
1:A:659:ARG:O	1:A:663:ILE:HG13	2.21	0.40
1:A:441:GLU:HA	1:A:441:GLU:OE2	2.21	0.40
1:A:415:ASP:HB2	1:A:746:TRP:CZ2	2.56	0.40
1:B:543:LEU:HD22	8:B:1101:HOH:O	2.20	0.40
1:B:307:LEU:HA	1:B:307:LEU:HD12	1.91	0.40
1:B:685:TYR:O	1:B:688:GLN:HG2	2.21	0.40
5:B:1010:MES:H32	5:B:1010:MES:H81	1.47	0.40
1:B:416:TYR:O	1:B:417:PHE:C	2.60	0.40
1:A:660:VAL:HG13	1:A:698:GLU:OE1	2.21	0.40
1:B:879:ASN:N	1:B:879:ASN:HD22	2.20	0.40
1:A:528:LEU:CG	1:A:529:GLY:HA2	2.51	0.40
1:B:873:TRP:O	1:B:877:ARG:HB2	2.21	0.40
1:B:763:HIS:C	1:B:765:PRO:HD2	2.42	0.40
1:A:655:ARG:HA	1:A:656:PRO:HD3	1.86	0.40
1:A:802:THR:HG22	1:A:806:ASN:ND2	2.35	0.40
1:B:309:PHE:CE1	1:B:406:ALA:CB	3.04	0.40
1:A:245:GLU:CD	1:A:246:GLY:H	2.25	0.40
1:A:640:TRP:CH2	1:A:666:VAL:HG22	2.56	0.40
1:B:801:THR:HG23	1:B:804:GLY:N	2.21	0.40
1:A:777:TRP:HA	1:A:784:LEU:HB3	2.03	0.40
1:B:727:LEU:HD12	1:B:731:LYS:HE3	2.04	0.40
1:A:360:ASP:O	1:A:361:LYS:C	2.59	0.40
1:A:90:ASP:HB3	1:A:171:LYS:HA	2.04	0.40
1:B:858:LEU:HD11	1:B:862:ILE:HD11	2.04	0.40
1:A:277:PHE:HA	1:A:282:VAL:O	2.21	0.40
1:A:905:PHE:O	1:A:938:ILE:HG23	2.22	0.40
1:B:316:ILE:HG12	1:B:483:LYS:HE2	2.04	0.40
1:A:486:SER:HB3	1:A:487:TYR:HD2	1.83	0.40
1:A:813:GLU:OE1	1:B:848:LYS:NZ	2.52	0.40
1:A:80:LEU:O	1:A:222:ILE:HA	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:SER:O	1:A:961:ARG:NH2[2_655]	2.11	0.09
1:B:320:LEU:O	1:B:961:ARG:NH1[2_556]	2.19	0.01

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	863/967 (89%)	729 (84%)	108 (12%)	26 (3%)	5	36
1	B	851/967 (88%)	710 (83%)	114 (13%)	27 (3%)	5	33
All	All	1714/1934 (89%)	1439 (84%)	222 (13%)	53 (3%)	5	34

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	119	ASN
1	A	583	ARG
1	A	596	SER
1	A	603	HIS
1	A	604	ILE
1	A	605	LEU
1	A	616	GLU
1	A	715	ILE
1	A	922	GLU
1	B	119	ASN
1	B	569	GLY
1	B	596	SER
1	B	603	HIS
1	B	604	ILE
1	B	605	LEU
1	B	616	GLU

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Mol	Chain	Res	Type
1	B	715	ILE
1	B	922	GLU
1	B	924	GLN
1	B	925	GLY
1	B	926	SER
1	A	546	GLY
1	B	417	PHE
1	B	534	VAL
1	B	546	GLY
1	A	100	LEU
1	A	417	PHE
1	A	545	LYS
1	A	619	SER
1	A	763	HIS
1	B	60	GLU
1	B	100	LEU
1	B	763	HIS
1	A	921	LEU
1	B	545	LYS
1	B	619	SER
1	B	765	PRO
1	A	59	GLY
1	A	471	GLU
1	A	649	GLN
1	A	765	PRO
1	B	56	ALA
1	B	649	GLN
1	B	921	LEU
1	B	615	PRO
1	A	615	PRO
1	A	99	VAL
1	A	133	PRO
1	B	99	VAL
1	B	453	VAL
1	A	72	VAL
1	A	925	GLY

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	768/870 (88%)	679 (88%)	89 (12%)	7 30
1	B	768/870 (88%)	684 (89%)	84 (11%)	8 33
All	All	1536/1740 (88%)	1363 (89%)	173 (11%)	7 32

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	62	PHE
1	A	73	VAL
1	A	80	LEU
1	A	87	THR
1	A	99	VAL
1	A	110	LEU
1	A	117	ILE
1	A	121	THR
1	A	124	SER
1	A	125	GLU
1	A	137	LEU
1	A	160	LEU
1	A	166	MET
1	A	174	ASP
1	A	181	LYS
1	A	186	THR
1	A	193	ILE
1	A	194	LEU
1	A	202	THR
1	A	215	LEU
1	A	240	LYS
1	A	242	ILE
1	A	245	GLU
1	A	278	THR
1	A	294	ASN
1	A	303	SER
1	A	321	SER
1	A	322	LYS
1	A	352	ASP
1	A	361	LYS
1	A	364	VAL
1	A	367	VAL

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Mol	Chain	Res	Type
1	A	372	LEU
1	A	383	MET
1	A	387	ASN
1	A	395	PHE
1	A	419	ASN
1	A	494	ASP
1	A	528	LEU
1	A	533	GLU
1	A	540	THR
1	A	558	SER
1	A	559	LEU
1	A	563	GLN
1	A	585	LEU
1	A	588	ILE
1	A	591	THR
1	A	598	ASN
1	A	604	ILE
1	A	610	ASP
1	A	625	VAL
1	A	636	GLU
1	A	641	ASP
1	A	645	THR
1	A	646	GLN
1	A	651	HIS
1	A	652	THR
1	A	675	LEU
1	A	678	ASP
1	A	681	LEU
1	A	684	THR
1	A	697	LEU
1	A	701	SER
1	A	705	SER
1	A	722	LEU
1	A	729	TYR
1	A	741	ASP
1	A	751	ARG
1	A	761	LEU
1	A	766	CYS
1	A	769	LYS
1	A	784	LEU
1	A	791	LEU
1	A	825	LEU

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Mol	Chain	Res	Type
1	A	855	LEU
1	A	859	LEU
1	A	865	ARG
1	A	871	LEU
1	A	881	THR
1	A	893	ASP
1	A	909	ASP
1	A	911	LEU
1	A	916	LEU
1	A	922	GLU
1	A	924	GLN
1	A	927	HIS
1	A	934	VAL
1	A	952	LEU
1	B	58	ASN
1	B	62	PHE
1	B	73	VAL
1	B	80	LEU
1	B	87	THR
1	B	99	VAL
1	B	110	LEU
1	B	117	ILE
1	B	121	THR
1	B	124	SER
1	B	137	LEU
1	B	160	LEU
1	B	166	MET
1	B	174	ASP
1	B	181	LYS
1	B	194	LEU
1	B	202	THR
1	B	215	LEU
1	B	240	LYS
1	B	242	ILE
1	B	245	GLU
1	B	278	THR
1	B	303	SER
1	B	321	SER
1	B	322	LYS
1	B	325	LEU
1	B	352	ASP
1	B	361	LYS

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Mol	Chain	Res	Type
1	B	364	VAL
1	B	367	VAL
1	B	372	LEU
1	B	383	MET
1	B	395	PHE
1	B	419	ASN
1	B	494	ASP
1	B	540	THR
1	B	558	SER
1	B	559	LEU
1	B	563	GLN
1	B	570	VAL
1	B	585	LEU
1	B	588	ILE
1	B	591	THR
1	B	598	ASN
1	B	604	ILE
1	B	610	ASP
1	B	625	VAL
1	B	636	GLU
1	B	641	ASP
1	B	645	THR
1	B	646	GLN
1	B	651	HIS
1	B	652	THR
1	B	675	LEU
1	B	681	LEU
1	B	697	LEU
1	B	701	SER
1	B	705	SER
1	B	722	LEU
1	B	729	TYR
1	B	731	LYS
1	B	741	ASP
1	B	751	ARG
1	B	761	LEU
1	B	766	CYS
1	B	769	LYS
1	B	784	LEU
1	B	791	LEU
1	B	825	LEU
1	B	852	THR

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Mol	Chain	Res	Type
1	B	855	LEU
1	B	859	LEU
1	B	865	ARG
1	B	871	LEU
1	B	881	THR
1	B	893	ASP
1	B	894	ILE
1	B	909	ASP
1	B	911	LEU
1	B	916	LEU
1	B	922	GLU
1	B	927	HIS
1	B	934	VAL
1	B	952	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	123	GLN
1	A	145	HIS
1	A	147	GLN
1	A	159	HIS
1	A	252	HIS
1	A	294	ASN
1	A	301	GLN
1	A	419	ASN
1	A	489	ASN
1	A	544	GLN
1	A	624	ASN
1	A	646	GLN
1	A	651	HIS
1	A	806	ASN
1	A	811	GLN
1	A	860	HIS
1	A	869	GLN
1	A	870	GLN
1	A	879	ASN
1	A	904	HIS
1	A	924	GLN
1	A	927	HIS
1	A	959	ASN

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Mol	Chain	Res	Type
1	B	58	ASN
1	B	106	GLN
1	B	145	HIS
1	B	147	GLN
1	B	159	HIS
1	B	294	ASN
1	B	301	GLN
1	B	419	ASN
1	B	489	ASN
1	B	544	GLN
1	B	624	ASN
1	B	646	GLN
1	B	651	HIS
1	B	664	HIS
1	B	806	ASN
1	B	811	GLN
1	B	860	HIS
1	B	869	GLN
1	B	870	GLN
1	B	879	ASN
1	B	904	HIS
1	B	912	GLN
1	B	927	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	$\#\|Z\| > 2$
3	NAG	A	1002	1,3	14,14,15	0.80	0	15,19,21	2.35	6 (40%)
3	NAG	A	1003	3	14,14,15	0.41	0	15,19,21	1.65	2 (13%)
3	NAG	A	1004	1,3	14,14,15	0.62	0	15,19,21	1.72	2 (13%)
3	NAG	A	1005	3	14,14,15	0.59	0	15,19,21	0.76	0
7	MAN	B	1001	7	11,11,12	0.68	0	14,15,17	1.03	0
7	MAN	B	1002	7	11,11,12	0.58	0	14,15,17	0.69	0
7	NAG	B	1003	1,7	14,14,15	0.37	0	15,19,21	1.58	3 (20%)
7	NAG	B	1004	7	14,14,15	0.54	0	15,19,21	1.11	1 (6%)
3	NAG	B	1007	1,3	14,14,15	0.47	0	15,19,21	0.71	0
3	NAG	B	1008	3	14,14,15	0.53	0	15,19,21	1.16	1 (6%)

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
3	NAG	A	1002	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1003	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1004	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1005	3	-	0/6/23/26	0/1/1/1
7	MAN	B	1001	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1002	7	-	0/2/19/22	0/1/1/1
7	NAG	B	1003	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	1004	7	-	0/6/23/26	0/1/1/1
3	NAG	B	1007	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1008	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1002	NAG	C3-C4-C5	-4.28	102.73	110.20
3	A	1002	NAG	C1-O5-C5	-4.07	107.08	112.25
3	A	1004	NAG	C2-N2-C7	-3.54	118.49	123.04
7	B	1003	NAG	C4-C3-C2	-3.53	105.75	111.23
3	A	1002	NAG	C2-N2-C7	-3.47	118.58	123.04
3	A	1002	NAG	O7-C7-C8	-2.45	117.58	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1003	NAG	C2-N2-C7	-2.16	120.26	123.04
7	B	1003	NAG	C3-C2-N2	2.05	115.47	110.56
3	A	1002	NAG	O4-C4-C3	3.08	117.28	110.34
7	B	1004	NAG	C1-O5-C5	3.34	116.49	112.25
3	A	1002	NAG	O5-C5-C6	3.39	114.68	107.35
3	B	1008	NAG	C1-O5-C5	3.48	116.66	112.25
7	B	1003	NAG	C1-O5-C5	3.61	116.83	112.25
3	A	1004	NAG	C1-O5-C5	4.50	117.96	112.25
3	A	1003	NAG	C1-O5-C5	5.03	118.64	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	NAG	5	0
3	A	1003	NAG	1	0
3	A	1004	NAG	2	0
3	A	1005	NAG	1	0
7	B	1001	MAN	6	0
7	B	1002	MAN	5	0
3	B	1007	NAG	2	0
3	B	1008	NAG	1	0

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LYS	A	1001	6	6,9,9	0.33	0	4,10,10	0.41	0
4	NAG	A	1006	1	14,14,15	0.51	0	15,19,21	1.52	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1007	1	14,14,15	0.58	0	15,19,21	2.26	5 (33%)
4	NAG	A	1008	1	14,14,15	0.47	0	15,19,21	0.85	0
5	MES	A	1009	-	11,12,12	0.64	0	14,16,16	2.90	7 (50%)
2	LYS	B	1005	6	6,9,9	0.35	0	4,10,10	0.34	0
4	NAG	B	1009	1	14,14,15	0.41	0	15,19,21	1.42	3 (20%)
5	MES	B	1010	-	11,12,12	0.67	0	14,16,16	2.75	7 (50%)

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	LYS	A	1001	6	-	0/5/9/9	0/0/0/0
4	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
5	MES	A	1009	-	-	0/6/14/14	0/1/1/1
2	LYS	B	1005	6	-	0/5/9/9	0/0/0/0
4	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
5	MES	B	1010	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1010	MES	C6-C5-N4	-4.43	103.41	110.12
4	A	1007	NAG	C3-C4-C5	-4.33	102.64	110.20
4	A	1007	NAG	C2-N2-C7	-4.12	117.75	123.04
5	A	1009	MES	C6-C5-N4	-3.76	104.42	110.12
5	B	1010	MES	C2-C3-N4	-3.40	104.98	110.12
5	A	1009	MES	C2-C3-N4	-3.35	105.06	110.12
4	A	1006	NAG	C2-N2-C7	-2.56	119.75	123.04
4	B	1009	NAG	C4-C3-C2	-2.38	107.53	111.23
4	B	1009	NAG	C2-N2-C7	-2.07	120.38	123.04
5	B	1010	MES	O2S-S-C8	2.13	108.73	106.91
4	A	1007	NAG	O4-C4-C5	2.16	114.96	109.24
4	A	1007	NAG	O5-C5-C6	2.44	112.64	107.35
5	A	1009	MES	O2S-S-C8	2.88	109.36	106.91
5	A	1009	MES	C7-N4-C5	3.27	119.65	111.27
5	B	1010	MES	C7-N4-C3	3.42	120.03	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1010	MES	C7-N4-C5	3.61	120.51	111.27
5	B	1010	MES	O1S-S-C8	3.70	110.06	106.91
5	A	1009	MES	C7-N4-C3	3.76	120.90	111.27
4	B	1009	NAG	C1-O5-C5	3.79	117.06	112.25
4	A	1006	NAG	C1-O5-C5	4.16	117.53	112.25
4	A	1007	NAG	C1-O5-C5	4.38	117.80	112.25
5	A	1009	MES	C5-N4-C3	4.87	119.44	108.90
5	B	1010	MES	C5-N4-C3	4.87	119.45	108.90
5	A	1009	MES	O1S-S-C8	5.43	111.54	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1007	NAG	2	0
5	A	1009	MES	1	0
2	B	1005	LYS	4	0
5	B	1010	MES	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	869/967 (89%)	-0.04	4 (0%)	91	87	33, 67, 111, 147	2 (0%)
1	B	859/967 (88%)	0.20	59 (6%)	20	12	34, 70, 116, 146	0
All	All	1728/1934 (89%)	0.08	63 (3%)	46	33	33, 68, 114, 147	2 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	615	PRO	5.3
1	B	613	ASP	5.0
1	B	559	LEU	4.9
1	B	561	LEU	4.8
1	B	553	LYS	4.8
1	B	554	GLN	4.7
1	B	153	PRO	4.6
1	B	612	LEU	4.5
1	B	534	VAL	4.4
1	B	550	LEU	4.1
1	B	570	VAL	4.0
1	B	602	ARG	3.9
1	B	105	THR	3.8
1	B	640	TRP	3.7
1	B	532	ALA	3.6
1	B	563	GLN	3.5
1	B	639	GLY	3.4
1	B	623	PHE	3.3
1	B	500	SER	3.3
1	A	924	GLN	3.3
1	B	569	GLY	3.3
1	B	552	VAL	3.2
1	B	603	HIS	3.2
1	B	558	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	598	ASN	3.1
1	B	635	TYR	3.1
1	B	610	ASP	3.1
1	B	556	GLY	3.1
1	B	101	VAL	3.1
1	B	99	VAL	3.0
1	B	555	ASP	2.9
1	B	538	MET	2.9
1	B	162	TYR	2.9
1	B	118	THR	2.8
1	B	591	THR	2.8
1	B	72	VAL	2.7
1	B	102	SER	2.6
1	B	611	THR	2.6
1	B	551	VAL	2.5
1	B	557	CYS	2.5
1	B	107	PHE	2.5
1	B	150	LEU	2.4
1	B	152	VAL	2.4
1	B	169	GLN	2.4
1	B	616	GLU	2.4
1	A	160	LEU	2.4
1	B	638	HIS	2.4
1	B	592	TYR	2.3
1	B	617	LYS	2.3
1	B	465	LEU	2.3
1	A	72	VAL	2.3
1	B	597	SER	2.3
1	A	559	LEU	2.3
1	B	637	GLY	2.2
1	B	167	ASP	2.2
1	B	73	VAL	2.1
1	B	607	SER	2.1
1	B	106	GLN	2.1
1	B	137	LEU	2.1
1	B	634	HIS	2.1
1	B	647	LEU	2.1
1	B	121	THR	2.0
1	B	119	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	1002	14/15	0.85	0.28	0.92	64,79,83,87	0
7	NAG	B	1003	14/15	0.92	0.24	0.25	56,73,85,87	0
3	NAG	B	1007	14/15	0.91	0.26	0.02	68,91,111,112	0
7	NAG	B	1004	14/15	0.90	0.19	-0.17	50,77,92,102	0
3	NAG	A	1003	14/15	0.93	0.14	-0.91	65,82,87,91	0
3	NAG	A	1004	14/15	0.92	0.15	-2.72	46,53,69,70	0
7	MAN	B	1001	11/12	0.80	0.17	-	72,97,108,112	0
7	MAN	B	1002	11/12	0.82	0.31	-	96,113,135,142	0
3	NAG	B	1008	14/15	0.75	0.33	-	84,113,127,133	0
3	NAG	A	1005	14/15	0.86	0.21	-	60,81,88,99	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	MES	A	1009	12/12	0.78	0.43	7.87	57,72,86,95	12
5	MES	B	1010	12/12	0.82	0.40	4.07	57,65,73,84	12
2	LYS	B	1005	10/10	0.92	0.33	3.66	46,59,65,69	0
2	LYS	A	1001	10/10	0.97	0.31	2.01	34,45,52,53	0
6	ZN	B	1006	1/1	0.99	0.20	0.42	46,46,46,46	0
6	ZN	A	1010	1/1	0.99	0.26	-0.67	32,32,32,32	0
4	NAG	A	1006	14/15	0.92	0.19	-1.48	62,85,87,88	0
4	NAG	B	1009	14/15	0.79	0.28	-	76,101,110,112	0
4	NAG	A	1008	14/15	0.87	0.14	-	96,107,114,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	A	1007	14/15	0.86	0.28	-	88,104,121,130	0

6.5 Other polymers (i)

There are no such residues in this entry.