Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:27 am BST

PDB ID	:	3TKN
Title	:	Structure of the Nup82-Nup159-Nup98 heterotrimer
Authors	:	Stuwe, T.T.; Hoelz, A.
Deposited on	:	2011-08-28
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

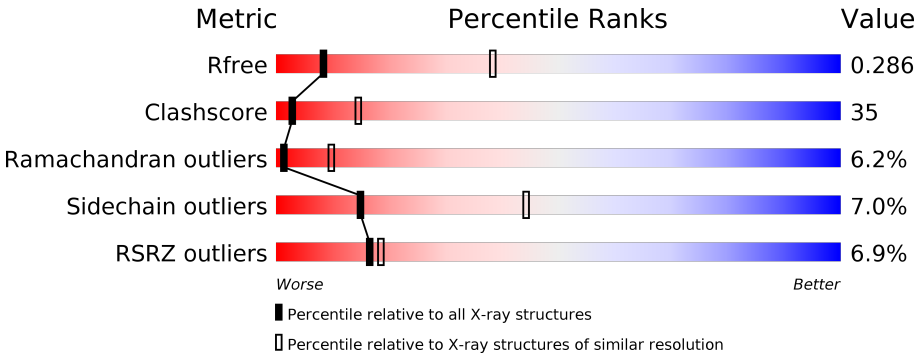
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	452	7% 44% 48% 8%
1	D	452	% 44% 47% 8%
1	G	452	6% 38% 53% 8%
2	B	39	46% 18% 8% 28%
2	E	39	36% 28% 8% 28%
2	H	39	5% 38% 26% 8% 28%

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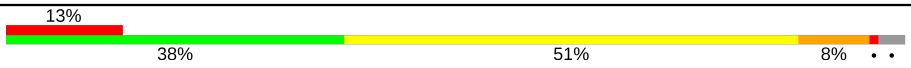
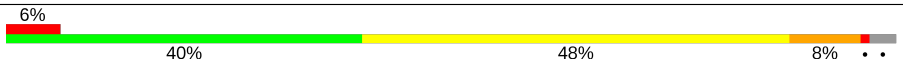
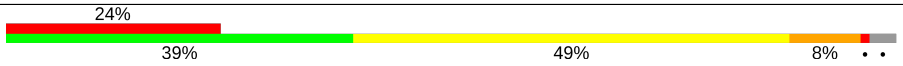
Mol	Chain	Length	Quality of chain
3	C	152	
3	F	152	
3	I	152	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15021 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 Nucleoporin NUP82.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3628	2323	587	707	11			
1	D	447	Total	C	N	O	S	0	0	0
			3601	2309	582	699	11			
1	G	447	Total	C	N	O	S	0	0	0
			3601	2309	582	699	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	SER	CYS	CONFLICT	UNP P40368
D	396	SER	CYS	CONFLICT	UNP P40368
G	396	SER	CYS	CONFLICT	UNP P40368

- Molecule 2 is a protein called Nucleoporin NUP159.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	28	Total	C	N	O	S	0	0	0
			221	144	37	37	3			
2	E	28	Total	C	N	O	S	0	0	0
			221	144	37	37	3			
2	H	28	Total	C	N	O	S	0	0	0
			221	144	37	37	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1422	GLY	-	EXPRESSION TAG	UNP P40477
B	1423	PRO	-	EXPRESSION TAG	UNP P40477
B	1424	HIS	-	EXPRESSION TAG	UNP P40477
E	1422	GLY	-	EXPRESSION TAG	UNP P40477
E	1423	PRO	-	EXPRESSION TAG	UNP P40477

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1424	HIS	-	EXPRESSION TAG	UNP P40477
H	1422	GLY	-	EXPRESSION TAG	UNP P40477
H	1423	PRO	-	EXPRESSION TAG	UNP P40477
H	1424	HIS	-	EXPRESSION TAG	UNP P40477

- Molecule 3 is a protein called Nucleoporin 98.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	147	Total	C	N	O	S	0	0	0
			1176	745	202	226	3			
3	F	147	Total	C	N	O	S	0	0	0
			1176	745	202	226	3			
3	I	147	Total	C	N	O	S	0	0	0
			1176	745	202	226	3			

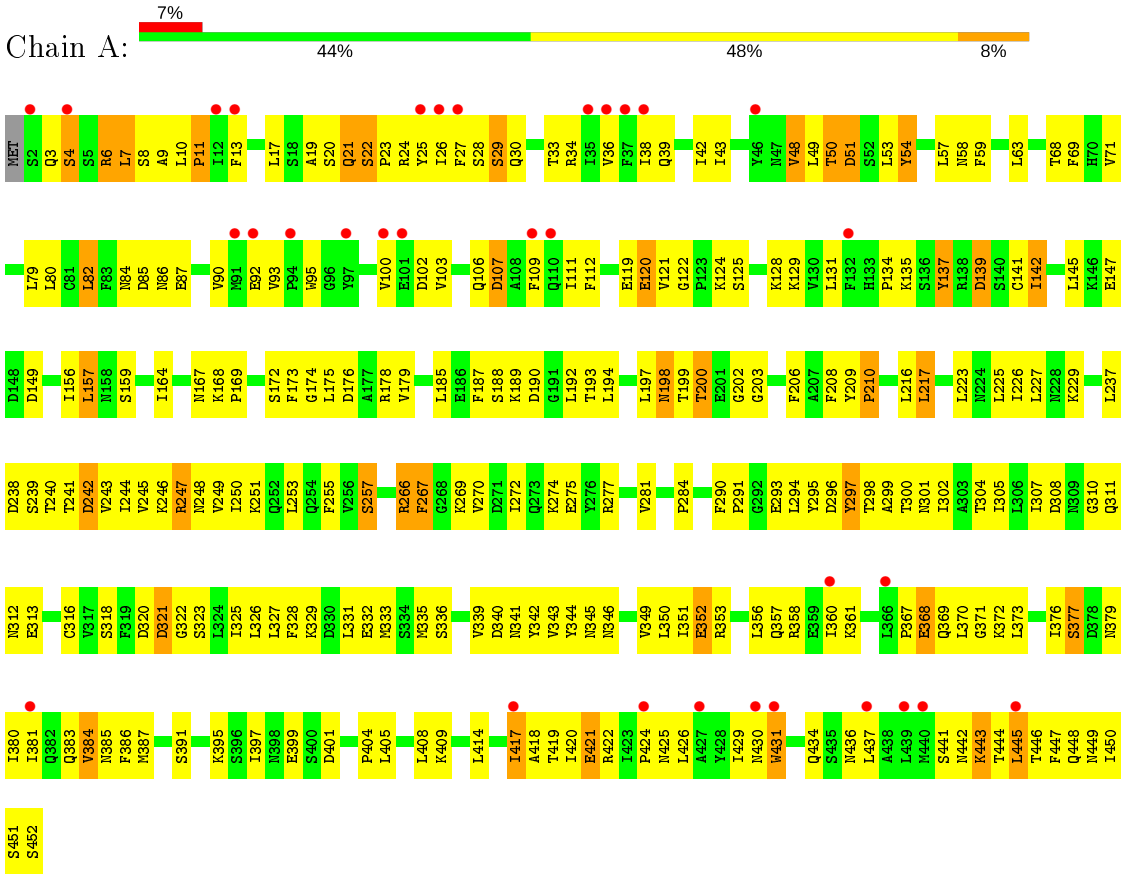
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	729	GLY	-	EXPRESSION TAG	UNP Q6PFD9
C	730	PRO	-	EXPRESSION TAG	UNP Q6PFD9
C	731	HIS	-	EXPRESSION TAG	UNP Q6PFD9
F	729	GLY	-	EXPRESSION TAG	UNP Q6PFD9
F	730	PRO	-	EXPRESSION TAG	UNP Q6PFD9
F	731	HIS	-	EXPRESSION TAG	UNP Q6PFD9
I	729	GLY	-	EXPRESSION TAG	UNP Q6PFD9
I	730	PRO	-	EXPRESSION TAG	UNP Q6PFD9
I	731	HIS	-	EXPRESSION TAG	UNP Q6PFD9

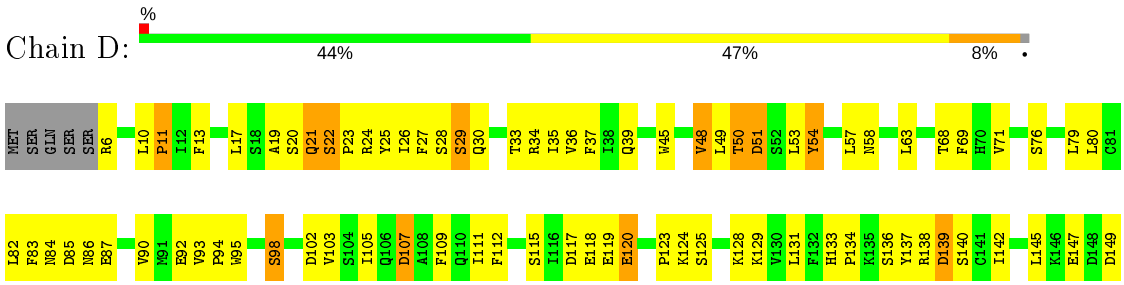
3 Residue-property plots (i)

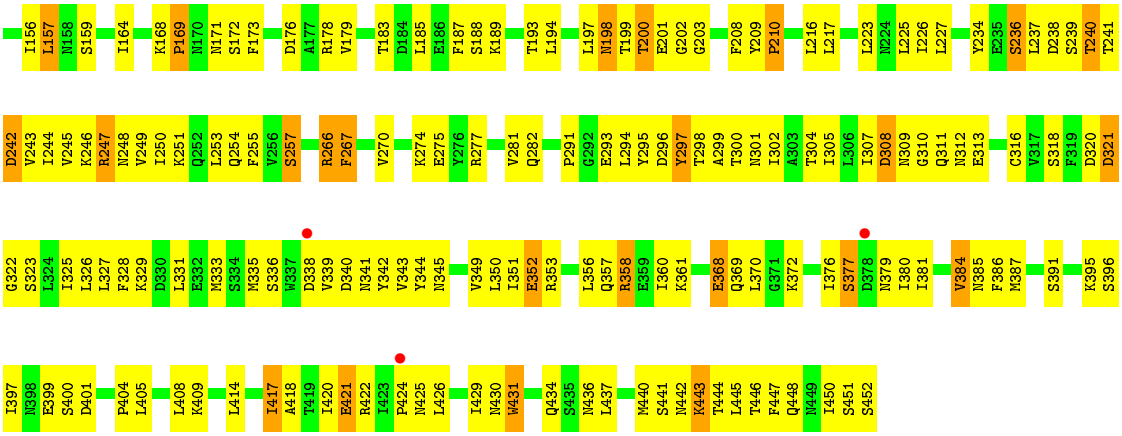
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Nucleoporin NUP82



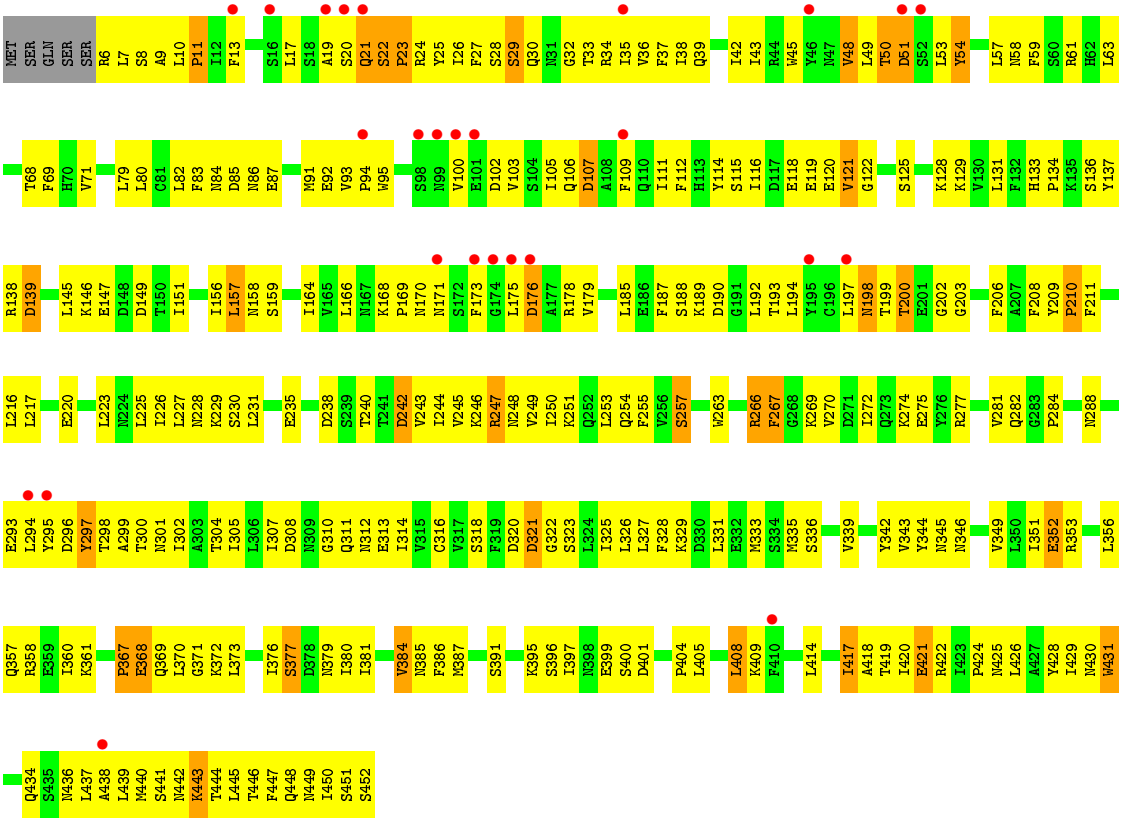
- Molecule 1: Nucleoporin NUP82





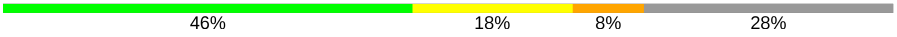
• Molecule 1: Nucleoporin NUP82

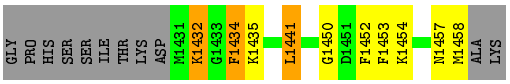
Chain G:



• Molecule 2: Nucleoporin NUP159

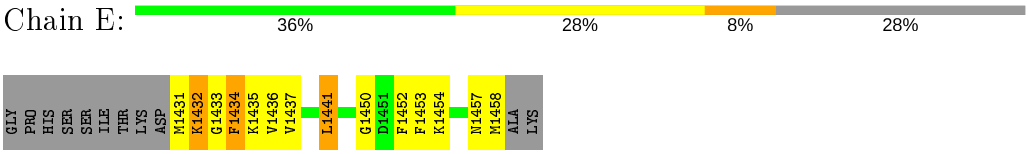
Chain B:





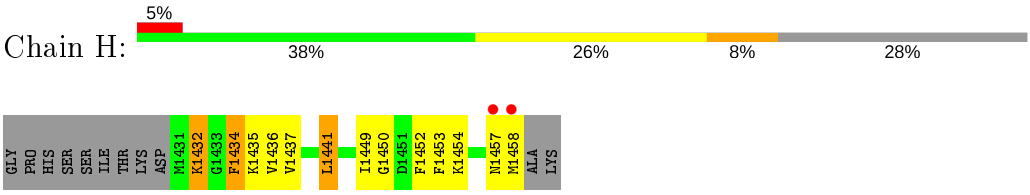
• Molecule 2: Nucleoporin NUP159

Chain E:



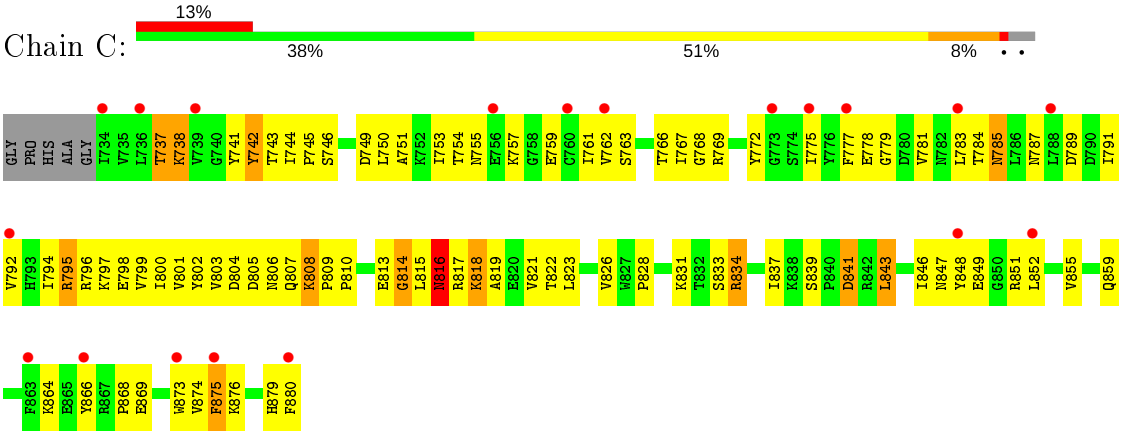
- Molecule 2: Nucleoporin NUP159

Chain H:



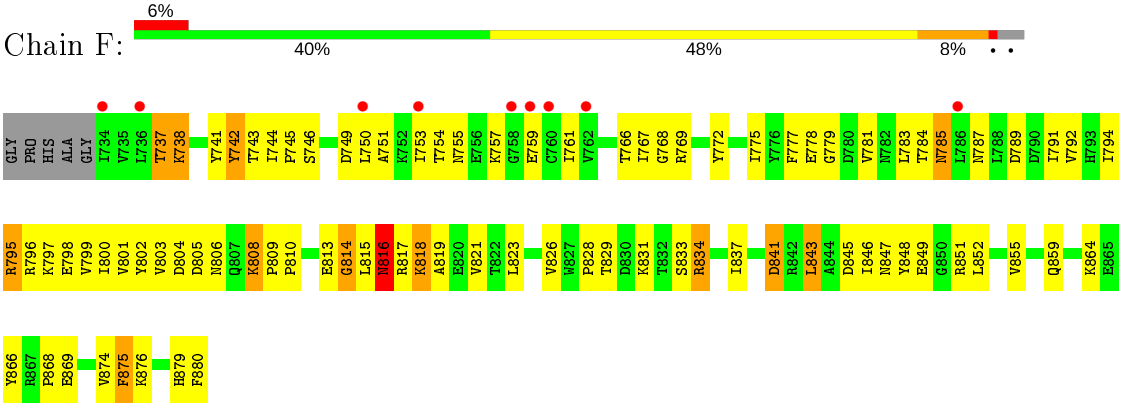
- Molecule 3: Nucleoporin 98

Chain C:



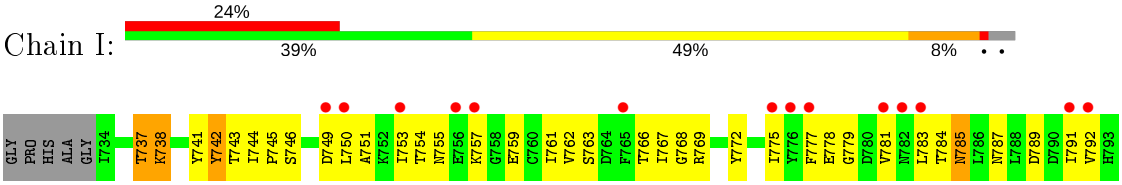
- Molecule 3: Nucleoporin 98

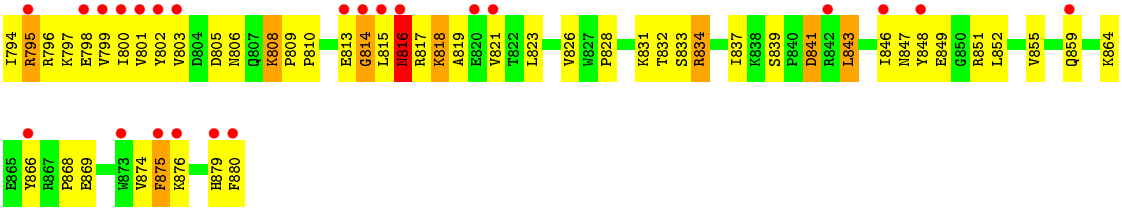
Chain F:



- Molecule 3: Nucleoporin 98

Chain I:




I794
R795
R796
K797
E798
V799
I800
V801
Y802
V803
D804
D805
N806
Q807
K808
P809
P810
E813
G814
L815
N816
R817
K818
A819
E820
V821
T822
L823
V826
W827
P828
K831
T832
S833
R834
I837
K838
S839
P840
D841
R842
L843
I846
N847
Y848
E849
G850
R851
L852
V855
Q859
K864
E865
Y866
R867
P868
E869
W873
V874
F875
K876
H879
F880

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.91Å 115.85Å 118.49Å 90.00° 111.06° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 49.90 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.40) 92.5 (49.90-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.285 0.250 , 0.286	Depositor DCC
R_{free} test set	3659 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	96.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15021	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.48	0/3701	0.70	0/5025
1	D	0.49	0/3674	0.69	0/4989
1	G	0.48	0/3674	0.69	0/4989
2	B	0.60	0/223	0.69	0/293
2	E	0.60	0/223	0.71	0/293
2	H	0.57	0/223	0.66	0/293
3	C	0.35	0/1199	0.59	0/1620
3	F	0.36	0/1199	0.59	0/1620
3	I	0.36	0/1199	0.58	0/1620
All	All	0.46	0/15315	0.67	0/20742

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3628	0	3594	251	0
1	D	3601	0	3571	239	0
1	G	3601	0	3571	272	0
2	B	221	0	235	12	0
2	E	221	0	235	17	0
2	H	221	0	235	17	0
3	C	1176	0	1170	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1176	0	1170	102	0
3	I	1176	0	1170	98	0
All	All	15021	0	14951	1053	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (1053) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:LEU:HD22	1:G:100:VAL:HG11	1.36	1.02
1:A:121:VAL:HG12	1:A:122:GLY:H	1.32	0.95
1:A:6:ARG:HB2	1:A:431:TRP:HH2	1.30	0.93
1:D:142:ILE:HG23	1:D:156:ILE:HD11	1.53	0.89
1:D:381:ILE:HD11	1:D:424:PRO:HG3	1.55	0.89
1:A:381:ILE:HD11	1:A:424:PRO:HG3	1.54	0.88
1:G:381:ILE:HD11	1:G:424:PRO:HG3	1.54	0.87
1:G:112:PHE:HB2	1:G:156:ILE:HG23	1.55	0.87
1:A:384:VAL:HG13	1:A:414:LEU:HD13	1.56	0.86
1:D:169:PRO:HA	1:D:178:ARG:HH11	1.40	0.86
1:D:384:VAL:HG13	1:D:414:LEU:HD13	1.60	0.84
1:A:6:ARG:HB2	1:A:431:TRP:CH2	2.13	0.84
1:G:384:VAL:HG13	1:G:414:LEU:HD13	1.58	0.84
1:G:169:PRO:HA	1:G:178:ARG:HH11	1.42	0.83
1:G:267:PHE:H	1:G:267:PHE:HD1	1.27	0.83
1:G:208:PHE:CZ	1:G:281:VAL:HG22	2.12	0.82
2:B:1434:PHE:HD1	2:B:1435:LYS:H	1.26	0.82
1:D:267:PHE:H	1:D:267:PHE:HD1	1.26	0.82
2:E:1434:PHE:HD1	2:E:1435:LYS:H	1.26	0.82
1:D:203:GLY:O	3:F:831:LYS:HE3	1.80	0.82
1:D:246:LYS:O	1:D:250:ILE:HG12	1.80	0.82
1:A:174:GLY:H	3:C:859:GLN:HE22	1.26	0.81
1:G:247:ARG:HH11	1:G:247:ARG:HG2	1.45	0.81
2:H:1434:PHE:HD1	2:H:1435:LYS:H	1.27	0.81
1:G:368:GLU:H	1:G:368:GLU:CD	1.84	0.81
3:C:864:LYS:HE3	3:C:876:LYS:HE2	1.61	0.81
3:I:864:LYS:HE3	3:I:876:LYS:HE2	1.63	0.80
1:G:37:PHE:HE1	1:G:440:MET:HE1	1.47	0.80
1:G:179:VAL:HG21	1:G:281:VAL:HG11	1.63	0.79
1:D:169:PRO:HA	1:D:178:ARG:NH1	1.98	0.79
1:G:246:LYS:O	1:G:250:ILE:HG12	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:HH	1:A:267:PHE:HD2	1.31	0.79
1:A:129:LYS:HE2	1:A:131:LEU:HD21	1.65	0.78
1:A:267:PHE:H	1:A:267:PHE:HD1	1.27	0.78
1:A:6:ARG:CB	1:A:431:TRP:HH2	1.97	0.78
1:D:247:ARG:HH11	1:D:247:ARG:HG2	1.46	0.78
3:F:864:LYS:HE3	3:F:876:LYS:HE2	1.63	0.78
1:D:179:VAL:HG21	1:D:281:VAL:HG11	1.66	0.78
1:A:30:GLN:HG3	1:A:34:ARG:HD3	1.65	0.78
1:D:142:ILE:CG2	1:D:156:ILE:HD11	2.13	0.78
1:A:208:PHE:CZ	1:A:281:VAL:HG22	2.19	0.77
1:A:247:ARG:HH11	1:A:247:ARG:HG2	1.49	0.77
3:C:805:ASP:HA	3:C:808:LYS:HB2	1.66	0.77
1:G:129:LYS:HE2	1:G:131:LEU:HD21	1.66	0.77
1:A:368:GLU:CD	1:A:368:GLU:H	1.87	0.77
1:A:125:SER:OG	1:A:147:GLU:HB2	1.84	0.77
1:A:301:ASN:H	1:A:318:SER:HB2	1.50	0.77
1:G:30:GLN:HG3	1:G:34:ARG:HD3	1.67	0.77
3:I:805:ASP:HA	3:I:808:LYS:HB2	1.67	0.77
3:F:805:ASP:HA	3:F:808:LYS:HB2	1.67	0.77
1:A:27:PHE:HZ	1:A:71:VAL:HG23	1.50	0.76
3:I:767:ILE:HD13	3:I:792:VAL:HG11	1.67	0.76
1:D:30:GLN:HG3	1:D:34:ARG:HD3	1.67	0.76
3:F:851:ARG:HG3	3:F:851:ARG:HH21	1.51	0.76
1:G:27:PHE:HZ	1:G:71:VAL:HG23	1.49	0.76
1:D:368:GLU:CD	1:D:368:GLU:H	1.89	0.75
3:I:767:ILE:CD1	3:I:792:VAL:HG11	2.17	0.75
3:F:767:ILE:CD1	3:F:792:VAL:HG11	2.17	0.75
3:I:851:ARG:HG3	3:I:851:ARG:HH21	1.51	0.75
1:A:300:THR:HB	1:A:318:SER:HB2	1.69	0.74
1:D:129:LYS:HE2	1:D:131:LEU:HD21	1.69	0.74
1:D:380:ILE:HG22	1:D:381:ILE:N	2.02	0.74
3:C:851:ARG:HH21	3:C:851:ARG:HG3	1.51	0.74
1:A:34:ARG:HB3	1:A:95:TRP:CH2	2.23	0.74
1:A:173:PHE:HA	3:C:859:GLN:OE1	1.86	0.74
1:A:358:ARG:CZ	1:A:380:ILE:HD12	2.17	0.74
1:A:174:GLY:H	3:C:859:GLN:NE2	1.86	0.74
3:F:767:ILE:HD13	3:F:792:VAL:HG11	1.69	0.74
1:G:37:PHE:HE1	1:G:440:MET:CE	2.00	0.74
3:I:828:PRO:HG2	3:I:837:ILE:HB	1.69	0.74
1:G:405:LEU:HB3	2:H:1452:PHE:HE1	1.53	0.73
3:C:767:ILE:CD1	3:C:792:VAL:HG11	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:PHE:HZ	1:D:71:VAL:HG23	1.51	0.73
1:A:349:VAL:HG11	2:B:1453:PHE:HB2	1.71	0.73
1:G:45:TRP:HH2	1:G:100:VAL:HG21	1.55	0.72
1:D:208:PHE:CZ	1:D:281:VAL:HG22	2.24	0.72
1:G:380:ILE:HG22	1:G:381:ILE:N	2.04	0.72
1:A:297:TYR:HB3	1:A:320:ASP:HB2	1.70	0.72
1:A:112:PHE:HB2	1:A:156:ILE:HG23	1.71	0.71
3:F:767:ILE:HG12	3:F:768:GLY:N	2.05	0.71
3:C:767:ILE:HD13	3:C:792:VAL:HG11	1.70	0.71
1:A:380:ILE:HG22	1:A:381:ILE:N	2.05	0.71
1:D:358:ARG:CZ	1:D:380:ILE:HD12	2.20	0.71
1:A:246:LYS:O	1:A:250:ILE:HG12	1.90	0.71
1:D:112:PHE:HB2	1:D:156:ILE:HG23	1.71	0.71
1:A:174:GLY:N	3:C:859:GLN:HE22	1.89	0.71
3:C:828:PRO:HG2	3:C:837:ILE:HB	1.72	0.71
3:C:767:ILE:HG12	3:C:768:GLY:N	2.06	0.70
3:I:809:PRO:HG2	3:I:814:GLY:HA3	1.74	0.70
1:D:300:THR:HB	1:D:318:SER:HB2	1.73	0.70
3:C:818:LYS:HD2	3:C:818:LYS:H	1.57	0.70
1:D:343:VAL:HG11	3:F:834:ARG:CZ	2.21	0.70
1:G:34:ARG:HB3	1:G:95:TRP:CH2	2.26	0.70
1:D:34:ARG:HB3	1:D:95:TRP:CH2	2.27	0.70
3:F:828:PRO:HG2	3:F:837:ILE:HB	1.73	0.70
2:E:1432:LYS:HD3	2:E:1432:LYS:C	2.12	0.70
1:G:169:PRO:HA	1:G:178:ARG:NH1	2.05	0.70
1:D:209:TYR:CE2	1:D:335:MET:HG3	2.27	0.69
1:A:443:LYS:HD2	1:A:443:LYS:H	1.58	0.69
1:G:326:LEU:HD12	1:G:352:GLU:HG2	1.74	0.69
1:G:358:ARG:CZ	1:G:380:ILE:HD12	2.21	0.69
1:G:301:ASN:H	1:G:318:SER:HB2	1.58	0.69
3:I:767:ILE:HG12	3:I:768:GLY:N	2.08	0.69
1:A:425:ASN:C	1:A:426:LEU:HD12	2.13	0.69
1:A:6:ARG:HD3	1:A:431:TRP:CH2	2.28	0.69
3:C:851:ARG:O	3:C:855:VAL:HG23	1.93	0.69
1:D:238:ASP:CG	1:D:239:SER:H	1.96	0.69
1:D:301:ASN:H	1:D:318:SER:HB2	1.57	0.69
1:G:238:ASP:OD2	1:G:240:THR:HG22	1.93	0.69
1:D:443:LYS:H	1:D:443:LYS:HD2	1.58	0.69
3:F:767:ILE:HG12	3:F:768:GLY:H	1.57	0.69
1:G:300:THR:HB	1:G:318:SER:HB2	1.74	0.69
3:I:818:LYS:H	3:I:818:LYS:HD2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:LEU:HD12	3:I:797:LYS:HB3	1.75	0.68
1:G:245:VAL:O	1:G:249:VAL:HG23	1.94	0.68
3:I:761:ILE:HG23	3:I:781:VAL:O	1.93	0.68
1:A:387:MET:HE3	1:A:391:SER:HB3	1.75	0.68
1:D:297:TYR:HB3	1:D:320:ASP:HB2	1.73	0.68
1:D:441:SER:HB3	1:D:444:THR:HB	1.76	0.68
1:G:441:SER:HB3	1:G:444:THR:HB	1.75	0.68
3:C:761:ILE:HG23	3:C:781:VAL:O	1.94	0.68
1:D:326:LEU:HD12	1:D:352:GLU:HG2	1.75	0.68
1:G:157:LEU:N	1:G:157:LEU:HD23	2.09	0.68
1:A:209:TYR:CE2	1:A:335:MET:HG3	2.28	0.67
1:A:441:SER:HB3	1:A:444:THR:HB	1.77	0.67
1:G:247:ARG:HG2	1:G:247:ARG:NH1	2.09	0.67
3:C:809:PRO:HG2	3:C:814:GLY:HA3	1.77	0.67
1:D:245:VAL:O	1:D:249:VAL:HG23	1.95	0.67
1:G:267:PHE:N	1:G:267:PHE:CD1	2.63	0.67
1:G:284:PRO:O	3:I:834:ARG:NH2	2.27	0.67
1:G:297:TYR:HB3	1:G:320:ASP:HB2	1.75	0.67
3:C:817:ARG:HH21	3:C:818:LYS:HD3	1.60	0.66
1:D:349:VAL:HG11	2:E:1453:PHE:HB2	1.76	0.66
3:F:761:ILE:HG23	3:F:781:VAL:O	1.96	0.66
1:D:380:ILE:HG22	1:D:381:ILE:H	1.61	0.66
1:G:170:ASN:HD21	1:G:176:ASP:HB3	1.61	0.66
3:I:767:ILE:HG12	3:I:768:GLY:H	1.60	0.66
3:C:767:ILE:HG12	3:C:768:GLY:H	1.60	0.66
1:G:209:TYR:CE2	1:G:335:MET:HG3	2.31	0.66
1:G:443:LYS:HD2	1:G:443:LYS:H	1.60	0.66
1:A:322:GLY:HA2	1:A:360:ILE:HG13	1.78	0.66
1:A:426:LEU:HD23	1:A:437:LEU:HD11	1.77	0.66
1:A:3:GLN:HG2	1:A:3:GLN:O	1.96	0.66
3:F:851:ARG:O	3:F:855:VAL:HG23	1.95	0.66
1:G:179:VAL:CG2	1:G:281:VAL:HG11	2.26	0.66
1:A:321:ASP:OD2	1:A:323:SER:HB2	1.96	0.65
1:G:380:ILE:HG22	1:G:381:ILE:H	1.60	0.65
1:G:426:LEU:HD23	1:G:437:LEU:HD11	1.77	0.65
1:D:10:LEU:HG	1:D:11:PRO:HD2	1.76	0.65
1:G:10:LEU:HG	1:G:11:PRO:HD2	1.78	0.65
1:D:426:LEU:HD23	1:D:437:LEU:HD11	1.78	0.65
1:D:203:GLY:O	3:F:831:LYS:CE	2.44	0.65
1:D:247:ARG:NH1	1:D:247:ARG:HG2	2.09	0.65
1:D:297:TYR:N	1:D:297:TYR:CD1	2.63	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:THR:O	3:F:851:ARG:HD2	1.95	0.65
1:G:121:VAL:HG12	1:G:122:GLY:H	1.61	0.65
1:G:216:LEU:HB3	1:G:270:VAL:CG1	2.27	0.65
1:G:297:TYR:N	1:G:297:TYR:CD1	2.64	0.65
1:A:10:LEU:HG	1:A:11:PRO:HD2	1.77	0.65
1:A:121:VAL:HG12	1:A:122:GLY:N	2.09	0.65
3:F:809:PRO:HG2	3:F:814:GLY:HA3	1.77	0.65
1:G:25:TYR:HD2	1:G:425:ASN:HD22	1.43	0.65
3:I:817:ARG:HH21	3:I:818:LYS:HD3	1.62	0.65
1:D:425:ASN:C	1:D:426:LEU:HD12	2.17	0.65
1:G:133:HIS:HB3	1:G:136:SER:HB3	1.79	0.65
1:G:349:VAL:HG11	2:H:1453:PHE:HB2	1.79	0.65
1:A:169:PRO:HA	1:A:178:ARG:HH11	1.61	0.64
1:A:326:LEU:HD12	1:A:352:GLU:HG2	1.79	0.64
1:D:267:PHE:N	1:D:267:PHE:CD1	2.63	0.64
1:A:174:GLY:HA2	3:C:873:TRP:CH2	2.33	0.64
1:A:157:LEU:HD23	1:A:157:LEU:N	2.12	0.64
2:E:1434:PHE:HD1	2:E:1435:LYS:N	1.96	0.64
1:A:267:PHE:CD1	1:A:267:PHE:N	2.66	0.64
3:F:817:ARG:HH21	3:F:818:LYS:HD3	1.61	0.64
3:F:818:LYS:H	3:F:818:LYS:HD2	1.60	0.64
3:C:833:SER:C	3:C:834:ARG:HG2	2.17	0.64
3:F:833:SER:C	3:F:834:ARG:HG2	2.18	0.64
1:G:425:ASN:C	1:G:426:LEU:HD12	2.18	0.64
1:A:198:ASN:O	1:A:203:GLY:HA2	1.98	0.64
3:F:746:SER:O	3:F:750:LEU:HG	1.97	0.64
1:A:245:VAL:O	1:A:249:VAL:HG23	1.98	0.64
3:I:851:ARG:O	3:I:855:VAL:HG23	1.96	0.64
1:A:297:TYR:N	1:A:297:TYR:CD1	2.64	0.63
1:D:157:LEU:N	1:D:157:LEU:HD23	2.13	0.63
1:G:208:PHE:CE1	1:G:281:VAL:HG22	2.33	0.63
2:H:1458:MET:HA	2:H:1458:MET:HE2	1.79	0.63
1:A:119:GLU:O	1:A:124:LYS:HE2	1.97	0.63
1:A:179:VAL:HG21	1:A:281:VAL:HG11	1.79	0.63
3:C:746:SER:O	3:C:750:LEU:HG	1.98	0.63
1:A:302:ILE:HA	1:A:316:CYS:O	1.97	0.63
1:A:300:THR:HB	1:A:318:SER:CB	2.29	0.63
1:G:322:GLY:HA2	1:G:360:ILE:HG13	1.81	0.63
1:A:197:LEU:HD21	1:A:299:ALA:HB1	1.81	0.63
2:H:1434:PHE:HD1	2:H:1435:LYS:N	1.96	0.63
1:G:267:PHE:N	1:G:267:PHE:HD1	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:833:SER:C	3:I:834:ARG:HG2	2.18	0.62
1:G:302:ILE:HA	1:G:316:CYS:O	1.98	0.62
1:A:380:ILE:HG22	1:A:381:ILE:H	1.63	0.62
1:G:7:LEU:HD22	1:G:436:ASN:ND2	2.15	0.62
1:A:57:LEU:HD22	1:A:100:VAL:HG11	1.82	0.62
1:A:79:LEU:HD23	1:A:92:GLU:HA	1.81	0.62
1:G:17:LEU:HD13	1:G:17:LEU:O	2.00	0.62
3:I:746:SER:O	3:I:750:LEU:HG	2.00	0.62
1:D:275:GLU:H	1:D:275:GLU:CD	2.03	0.62
1:D:321:ASP:OD2	1:D:323:SER:HB2	2.00	0.61
1:G:79:LEU:HD23	1:G:92:GLU:HA	1.82	0.61
1:D:17:LEU:HD13	1:D:17:LEU:O	1.99	0.61
1:A:405:LEU:HB3	2:B:1452:PHE:HE1	1.66	0.61
2:B:1458:MET:HE2	2:B:1458:MET:HA	1.82	0.61
1:D:322:GLY:HA2	1:D:360:ILE:HG13	1.81	0.61
1:D:239:SER:OG	1:D:240:THR:N	2.34	0.61
1:A:63:LEU:HD11	1:A:69:PHE:CE2	2.36	0.61
1:D:198:ASN:O	1:D:203:GLY:HA2	2.01	0.61
1:G:198:ASN:O	1:G:203:GLY:HA2	2.01	0.61
1:A:331:LEU:HB3	1:A:345:ASN:OD1	2.01	0.61
1:G:275:GLU:CD	1:G:275:GLU:H	2.04	0.61
1:A:253:LEU:O	1:A:257:SER:HB2	2.01	0.61
1:A:275:GLU:H	1:A:275:GLU:CD	2.03	0.61
1:G:210:PRO:HD3	1:G:335:MET:HG2	1.82	0.61
3:F:808:LYS:HE3	3:F:880:PHE:O	2.01	0.61
1:G:331:LEU:HB3	1:G:345:ASN:OD1	2.00	0.61
2:B:1434:PHE:HD1	2:B:1435:LYS:N	1.97	0.60
1:G:297:TYR:CE2	1:G:321:ASP:HB3	2.36	0.60
1:A:17:LEU:HD13	1:A:17:LEU:O	2.01	0.60
1:D:179:VAL:HG23	1:D:281:VAL:HG21	1.81	0.60
1:A:189:LYS:N	1:A:313:GLU:OE1	2.33	0.60
1:D:63:LEU:HD11	1:D:69:PHE:CE2	2.36	0.60
1:G:321:ASP:OD2	1:G:323:SER:HB2	2.01	0.60
1:A:237:LEU:CD2	1:A:241:THR:HG21	2.31	0.60
1:A:28:SER:O	1:A:29:SER:HB2	2.01	0.60
1:D:250:ILE:HG21	2:H:1441:LEU:HG	1.83	0.60
1:D:137:TYR:CE2	1:D:138:ARG:HG3	2.36	0.60
1:G:115:SER:N	1:G:118:GLU:OE2	2.33	0.60
1:A:226:ILE:HG23	1:A:227:LEU:N	2.17	0.60
1:D:179:VAL:CG2	1:D:281:VAL:HG11	2.31	0.60
1:D:302:ILE:HA	1:D:316:CYS:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:808:LYS:HE3	3:I:880:PHE:O	2.02	0.59
1:A:169:PRO:HA	1:A:178:ARG:NH1	2.18	0.59
1:G:253:LEU:O	1:G:257:SER:HB2	2.02	0.59
1:A:79:LEU:HD12	1:A:139:ASP:HB2	1.85	0.59
1:G:231:LEU:O	1:G:235:GLU:HG3	2.01	0.59
1:G:57:LEU:HD13	1:G:100:VAL:HB	1.84	0.59
3:C:808:LYS:HE3	3:C:880:PHE:O	2.02	0.59
1:D:53:LEU:HD13	1:D:54:TYR:N	2.18	0.59
1:G:431:TRP:O	1:G:434:GLN:HB2	2.03	0.59
3:F:837:ILE:HG22	3:F:843:LEU:HD13	1.85	0.58
1:G:179:VAL:HG23	1:G:281:VAL:HG21	1.84	0.58
1:G:430:ASN:HA	1:G:434:GLN:O	2.03	0.58
1:G:63:LEU:HD11	1:G:69:PHE:CE2	2.38	0.58
1:A:208:PHE:CE1	1:A:281:VAL:HG22	2.37	0.58
3:C:769:ARG:NH1	3:C:772:TYR:HE1	2.00	0.58
1:G:28:SER:O	1:G:29:SER:HB2	2.02	0.58
1:A:305:ILE:HD12	1:A:305:ILE:N	2.19	0.58
1:D:79:LEU:HD23	1:D:92:GLU:HA	1.84	0.58
1:G:175:LEU:O	3:I:798:GLU:HB2	2.03	0.58
3:I:837:ILE:HG22	3:I:843:LEU:HD13	1.86	0.58
1:D:387:MET:HE3	1:D:391:SER:HB3	1.86	0.58
3:I:769:ARG:NH1	3:I:772:TYR:HE1	2.02	0.58
2:E:1432:LYS:HG3	2:E:1433:GLY:N	2.19	0.58
1:G:300:THR:HB	1:G:318:SER:CB	2.34	0.58
1:G:329:LYS:HE2	1:G:333:MET:HG3	1.85	0.58
1:D:300:THR:HB	1:D:318:SER:CB	2.33	0.58
1:A:255:PHE:CD2	1:A:335:MET:HE1	2.39	0.58
1:A:321:ASP:CG	1:A:323:SER:HB2	2.25	0.57
1:D:267:PHE:N	1:D:267:PHE:HD1	1.96	0.57
1:D:298:THR:HG22	1:D:299:ALA:N	2.19	0.57
3:F:851:ARG:NH2	3:F:851:ARG:HG3	2.19	0.57
1:G:29:SER:HB3	1:G:34:ARG:HB2	1.85	0.57
2:B:1441:LEU:HG	1:G:250:ILE:HG21	1.85	0.57
1:G:216:LEU:HB2	1:G:272:ILE:CD1	2.34	0.57
1:A:145:LEU:HD22	1:A:185:LEU:HD13	1.85	0.57
1:A:267:PHE:HD1	1:A:267:PHE:N	1.98	0.57
1:A:29:SER:HB3	1:A:34:ARG:HB2	1.87	0.57
1:G:125:SER:OG	1:G:147:GLU:HB2	2.04	0.57
1:G:300:THR:HG22	1:G:301:ASN:OD1	2.05	0.57
1:G:405:LEU:HB3	2:H:1452:PHE:CE1	2.38	0.57
1:A:307:ILE:HG12	1:A:312:ASN:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:837:ILE:HG22	3:C:843:LEU:HD13	1.87	0.57
1:D:451:SER:O	1:D:452:SER:HB3	2.04	0.57
1:G:451:SER:O	1:G:452:SER:HB3	2.05	0.57
1:A:349:VAL:CG1	2:B:1453:PHE:HB2	2.35	0.57
3:C:851:ARG:HG3	3:C:851:ARG:NH2	2.19	0.57
1:A:84:ASN:HD21	1:A:86:ASN:HB3	1.69	0.57
1:D:227:LEU:HD12	1:D:227:LEU:O	2.04	0.57
3:I:851:ARG:HG3	3:I:851:ARG:NH2	2.19	0.57
1:D:305:ILE:HD12	1:D:305:ILE:N	2.20	0.57
1:D:352:GLU:HG3	1:D:353:ARG:N	2.19	0.57
1:D:429:ILE:O	1:D:436:ASN:HB2	2.05	0.57
1:D:441:SER:CB	1:D:444:THR:HB	2.35	0.57
3:F:864:LYS:HE3	3:F:876:LYS:CE	2.34	0.57
1:G:121:VAL:HG12	1:G:122:GLY:N	2.20	0.57
1:A:189:LYS:HG2	1:A:304:THR:HG21	1.87	0.56
3:C:864:LYS:HE3	3:C:876:LYS:CE	2.31	0.56
1:D:48:VAL:HG12	1:D:48:VAL:O	2.04	0.56
2:E:1432:LYS:CG	2:E:1433:GLY:N	2.66	0.56
3:I:775:ILE:HD11	3:I:799:VAL:HG21	1.87	0.56
1:A:451:SER:O	1:A:452:SER:HB3	2.04	0.56
1:D:253:LEU:O	1:D:257:SER:HB2	2.05	0.56
1:D:297:TYR:CE2	1:D:321:ASP:HB3	2.40	0.56
1:D:376:ILE:O	1:D:376:ILE:HG22	2.04	0.56
1:D:6:ARG:O	1:D:6:ARG:HG3	2.05	0.56
1:G:429:ILE:O	1:G:436:ASN:HB2	2.05	0.56
1:D:300:THR:HG22	1:D:301:ASN:OD1	2.05	0.56
1:G:175:LEU:CD1	3:I:797:LYS:HD3	2.36	0.56
1:G:441:SER:CB	1:G:444:THR:HB	2.34	0.56
3:I:864:LYS:HE3	3:I:876:LYS:CE	2.33	0.56
1:A:19:ALA:C	1:A:21:GLN:H	2.09	0.56
3:F:781:VAL:HG22	3:F:817:ARG:HH11	1.70	0.56
1:G:19:ALA:C	1:G:21:GLN:H	2.09	0.56
1:G:339:VAL:HG11	1:G:342:TYR:CD1	2.41	0.56
1:A:431:TRP:O	1:A:434:GLN:HB2	2.05	0.56
1:D:19:ALA:C	1:D:21:GLN:H	2.09	0.56
1:A:356:LEU:O	1:A:358:ARG:HG3	2.05	0.56
1:A:358:ARG:HD3	1:A:377:SER:HB3	1.88	0.56
3:C:781:VAL:HG22	3:C:817:ARG:HH11	1.71	0.56
1:D:226:ILE:HG23	1:D:227:LEU:N	2.20	0.56
1:G:53:LEU:HD13	1:G:54:TYR:N	2.21	0.56
3:I:798:GLU:HG2	3:I:799:VAL:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:781:VAL:HG22	3:I:817:ARG:HH11	1.70	0.56
1:A:107:ASP:C	1:A:109:PHE:H	2.10	0.56
3:F:798:GLU:HG2	3:F:799:VAL:N	2.21	0.56
1:D:321:ASP:CG	1:D:323:SER:HB2	2.26	0.55
1:D:401:ASP:OD1	1:D:404:PRO:HD3	2.06	0.55
1:G:352:GLU:HG3	1:G:353:ARG:N	2.20	0.55
1:G:358:ARG:HD3	1:G:377:SER:HB3	1.87	0.55
1:G:387:MET:CE	1:G:391:SER:HB3	2.36	0.55
1:A:297:TYR:CE2	1:A:321:ASP:HB3	2.41	0.55
1:D:331:LEU:HB3	1:D:345:ASN:OD1	2.06	0.55
3:I:742:TYR:O	3:I:743:THR:HG23	2.06	0.55
3:I:864:LYS:HB3	3:I:874:VAL:HG23	1.88	0.55
1:G:119:GLU:OE1	1:G:146:LYS:NZ	2.40	0.55
1:G:356:LEU:O	1:G:358:ARG:HG3	2.06	0.55
1:A:199:THR:O	1:A:202:GLY:N	2.39	0.55
1:A:48:VAL:HG12	1:A:48:VAL:O	2.07	0.55
3:C:866:TYR:O	3:C:868:PRO:HD3	2.07	0.55
1:D:142:ILE:HG23	1:D:156:ILE:CD1	2.34	0.55
1:D:237:LEU:HD21	1:D:249:VAL:HB	1.88	0.55
2:E:1458:MET:HA	2:E:1458:MET:HE2	1.88	0.55
1:A:90:VAL:HG11	1:A:156:ILE:HD13	1.89	0.55
1:A:247:ARG:HG2	1:A:247:ARG:NH1	2.13	0.55
1:A:387:MET:CE	1:A:391:SER:HB3	2.36	0.55
1:G:156:ILE:HG22	1:G:157:LEU:HD23	1.87	0.55
3:I:866:TYR:O	3:I:868:PRO:HD3	2.07	0.55
1:A:352:GLU:HG3	1:A:353:ARG:N	2.22	0.55
3:C:745:PRO:HB2	3:C:749:ASP:HB3	1.89	0.55
3:C:775:ILE:HD11	3:C:799:VAL:HG21	1.89	0.55
3:F:801:VAL:O	3:F:802:TYR:HB2	2.07	0.55
1:G:344:TYR:CZ	1:G:345:ASN:ND2	2.75	0.55
1:A:227:LEU:O	1:A:227:LEU:HD12	2.07	0.55
1:A:53:LEU:HD13	1:A:54:TYR:N	2.22	0.55
1:A:174:GLY:HA2	3:C:873:TRP:HH2	1.69	0.55
1:G:134:PRO:HD2	1:G:187:PHE:CE1	2.42	0.55
3:C:801:VAL:O	3:C:802:TYR:HB2	2.07	0.55
1:D:343:VAL:HG11	3:F:834:ARG:NH2	2.22	0.55
3:F:866:TYR:O	3:F:868:PRO:HD3	2.06	0.55
1:G:84:ASN:HD21	1:G:86:ASN:HB3	1.71	0.55
3:F:769:ARG:NH1	3:F:772:TYR:HE1	2.05	0.54
1:G:145:LEU:HD22	1:G:185:LEU:HD13	1.89	0.54
1:G:321:ASP:CG	1:G:323:SER:HB2	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:SER:O	1:D:29:SER:HB2	2.07	0.54
1:D:356:LEU:O	1:D:358:ARG:HG3	2.06	0.54
1:G:401:ASP:OD1	1:G:404:PRO:HD3	2.07	0.54
2:H:1450:GLY:O	2:H:1454:LYS:HG3	2.07	0.54
1:A:401:ASP:OD1	1:A:404:PRO:HD3	2.08	0.54
1:G:107:ASP:C	1:G:109:PHE:H	2.11	0.54
1:A:3:GLN:O	1:A:4:SER:C	2.44	0.54
1:A:300:THR:HG22	1:A:301:ASN:OD1	2.08	0.54
1:D:208:PHE:CE1	1:D:281:VAL:HG22	2.42	0.54
1:D:189:LYS:HG2	1:D:304:THR:HG21	1.89	0.54
1:D:84:ASN:HD21	1:D:86:ASN:HB3	1.73	0.54
1:G:79:LEU:HD12	1:G:139:ASP:HB2	1.89	0.54
3:C:798:GLU:HG2	3:C:799:VAL:N	2.22	0.54
1:D:250:ILE:CG2	2:H:1441:LEU:HG	2.37	0.54
1:D:420:ILE:HD12	1:D:420:ILE:O	2.07	0.54
3:I:745:PRO:HB2	3:I:749:ASP:HB3	1.89	0.54
1:A:441:SER:CB	1:A:444:THR:HB	2.37	0.54
1:D:156:ILE:HG22	1:D:157:LEU:HD23	1.90	0.54
1:D:29:SER:HB3	1:D:34:ARG:HB2	1.89	0.54
1:D:408:LEU:HD23	1:D:409:LYS:H	1.71	0.54
1:A:168:LYS:HB3	1:A:169:PRO:CD	2.38	0.54
1:A:429:ILE:O	1:A:436:ASN:HB2	2.08	0.54
3:F:745:PRO:HB2	3:F:749:ASP:HB3	1.90	0.54
1:A:250:ILE:HG21	2:E:1441:LEU:HG	1.89	0.53
1:A:343:VAL:HG12	1:A:343:VAL:O	2.08	0.53
1:D:320:ASP:C	1:D:322:GLY:H	2.10	0.53
1:D:344:TYR:CZ	1:D:345:ASN:ND2	2.76	0.53
1:G:199:THR:O	1:G:202:GLY:N	2.39	0.53
1:A:24:ARG:HG2	1:A:39:GLN:HG3	1.90	0.53
2:B:1432:LYS:O	2:B:1432:LYS:HD2	2.08	0.53
1:D:197:LEU:HD21	1:D:299:ALA:HB1	1.90	0.53
3:F:738:LYS:HB2	3:F:741:TYR:HD2	1.73	0.53
1:D:107:ASP:C	1:D:109:PHE:H	2.11	0.53
1:D:210:PRO:HD3	1:D:335:MET:HG2	1.89	0.53
1:D:405:LEU:HB3	2:E:1452:PHE:HE1	1.72	0.53
1:A:379:ASN:HA	1:A:420:ILE:O	2.08	0.53
1:A:174:GLY:CA	3:C:859:GLN:HE22	2.21	0.53
1:G:376:ILE:HG22	1:G:376:ILE:O	2.07	0.53
1:G:48:VAL:HG12	1:G:48:VAL:O	2.08	0.53
1:A:210:PRO:HD3	1:A:335:MET:HG2	1.88	0.53
3:C:777:PHE:CD1	3:C:819:ALA:HB2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:LYS:HZ1	1:D:304:THR:HB	1.73	0.53
1:A:176:ASP:HB3	3:C:798:GLU:OE2	2.09	0.53
1:G:227:LEU:HD12	1:G:227:LEU:O	2.08	0.53
1:G:298:THR:HG22	1:G:299:ALA:N	2.23	0.53
1:A:430:ASN:HA	1:A:434:GLN:O	2.09	0.53
1:D:169:PRO:CA	1:D:178:ARG:HH11	2.19	0.53
3:F:742:TYR:O	3:F:743:THR:HG23	2.09	0.53
1:G:17:LEU:O	1:G:17:LEU:CD1	2.57	0.53
1:G:305:ILE:N	1:G:305:ILE:HD12	2.24	0.53
1:A:417:ILE:HG23	1:A:448:GLN:OE1	2.09	0.53
1:A:7:LEU:C	1:A:9:ALA:H	2.13	0.53
1:D:92:GLU:HB2	1:D:111:ILE:CD1	2.39	0.53
1:D:307:ILE:HG12	1:D:312:ASN:O	2.09	0.53
1:G:226:ILE:HG23	1:G:227:LEU:N	2.24	0.53
1:A:237:LEU:HD22	1:A:241:THR:HG21	1.89	0.53
1:A:451:SER:O	1:A:452:SER:CB	2.57	0.53
1:D:408:LEU:HD23	1:D:409:LYS:N	2.24	0.53
3:F:828:PRO:HB3	3:F:848:TYR:CE1	2.43	0.53
1:A:446:THR:HG22	1:A:447:PHE:N	2.24	0.52
1:D:17:LEU:O	1:D:17:LEU:CD1	2.57	0.52
1:G:169:PRO:CA	1:G:178:ARG:HH11	2.14	0.52
1:G:379:ASN:HA	1:G:420:ILE:O	2.09	0.52
3:I:777:PHE:CD1	3:I:819:ALA:HB2	2.44	0.52
1:A:121:VAL:CG1	1:A:122:GLY:H	2.14	0.52
3:I:777:PHE:CE2	3:I:815:LEU:HD11	2.44	0.52
1:A:405:LEU:HB3	2:B:1452:PHE:CE1	2.44	0.52
1:G:446:THR:HG22	1:G:447:PHE:N	2.24	0.52
1:A:329:LYS:HE2	1:A:333:MET:HG3	1.90	0.52
1:D:431:TRP:O	1:D:434:GLN:HB2	2.09	0.52
1:A:293:GLU:O	1:A:295:TYR:N	2.43	0.52
1:D:201:GLU:CD	3:F:829:THR:H	2.13	0.52
1:D:387:MET:CE	1:D:391:SER:HB3	2.39	0.52
1:G:238:ASP:OD1	1:G:238:ASP:N	2.43	0.52
1:G:255:PHE:CD2	1:G:335:MET:HE1	2.44	0.52
1:D:199:THR:O	1:D:202:GLY:N	2.43	0.52
3:F:815:LEU:C	3:F:817:ARG:H	2.12	0.52
3:F:775:ILE:HD11	3:F:799:VAL:HG21	1.89	0.52
1:G:21:GLN:O	1:G:22:SER:C	2.48	0.52
1:G:57:LEU:HD11	1:G:106:GLN:HG3	1.91	0.52
1:A:376:ILE:HG22	1:A:376:ILE:O	2.09	0.52
1:D:227:LEU:HD21	2:H:1432:LYS:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ARG:HG3	1:G:431:TRP:HZ3	1.75	0.52
3:I:738:LYS:HB2	3:I:741:TYR:HD2	1.74	0.52
1:A:137:TYR:CE2	1:A:269:LYS:HD3	2.45	0.52
3:C:783:LEU:HD12	3:C:783:LEU:N	2.25	0.52
1:D:358:ARG:HD3	1:D:377:SER:HB3	1.92	0.52
3:F:816:ASN:ND2	3:F:879:HIS:HB2	2.25	0.52
1:G:176:ASP:HB2	1:G:178:ARG:CG	2.40	0.52
1:G:37:PHE:CE1	1:G:440:MET:CE	2.88	0.52
1:A:298:THR:HG22	1:A:299:ALA:N	2.25	0.52
3:C:778:GLU:HG2	3:C:779:GLY:N	2.24	0.52
3:F:777:PHE:CD1	3:F:819:ALA:HB2	2.44	0.52
1:D:21:GLN:O	1:D:22:SER:C	2.48	0.51
1:D:379:ASN:HA	1:D:420:ILE:O	2.10	0.51
3:F:864:LYS:HB3	3:F:874:VAL:HG23	1.91	0.51
1:G:57:LEU:HD13	1:G:100:VAL:CG1	2.39	0.51
1:A:216:LEU:HB3	1:A:270:VAL:CG1	2.40	0.51
1:A:420:ILE:HD12	1:A:420:ILE:O	2.10	0.51
3:C:864:LYS:HB3	3:C:874:VAL:HG23	1.91	0.51
1:G:358:ARG:HH11	1:G:358:ARG:HG2	1.74	0.51
3:I:815:LEU:C	3:I:817:ARG:H	2.14	0.51
1:A:137:TYR:OH	1:A:267:PHE:HD2	1.90	0.51
1:A:344:TYR:CZ	1:A:345:ASN:ND2	2.78	0.51
3:F:783:LEU:N	3:F:783:LEU:HD12	2.25	0.51
1:G:380:ILE:CG2	1:G:381:ILE:N	2.71	0.51
3:I:801:VAL:O	3:I:802:TYR:HB2	2.09	0.51
1:D:380:ILE:CG2	1:D:381:ILE:N	2.70	0.51
1:G:45:TRP:CH2	1:G:100:VAL:HG21	2.40	0.51
1:A:27:PHE:CZ	1:A:71:VAL:HG23	2.39	0.51
1:G:216:LEU:HB3	1:G:270:VAL:HG12	1.93	0.51
1:G:320:ASP:C	1:G:322:GLY:H	2.14	0.51
1:G:380:ILE:CG2	1:G:381:ILE:H	2.23	0.51
3:I:816:ASN:ND2	3:I:879:HIS:HB2	2.25	0.51
1:A:21:GLN:O	1:A:22:SER:C	2.49	0.51
1:A:25:TYR:HD2	1:A:425:ASN:HD22	1.58	0.51
3:C:754:THR:O	3:C:754:THR:HG23	2.10	0.51
1:D:238:ASP:CG	1:D:239:SER:N	2.63	0.51
1:D:266:ARG:HB2	1:D:267:PHE:HD1	1.76	0.51
1:G:166:LEU:HD12	1:G:211:PHE:CE1	2.46	0.51
1:A:444:THR:HG22	1:A:445:LEU:N	2.25	0.51
3:I:843:LEU:HD23	3:I:868:PRO:HB3	1.92	0.51
1:A:274:LYS:HG3	1:A:275:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TYR:HD1	1:A:297:TYR:H	1.59	0.51
1:A:6:ARG:CG	1:A:431:TRP:HH2	2.24	0.51
3:C:738:LYS:HB2	3:C:741:TYR:HD2	1.74	0.51
1:G:274:LYS:O	1:G:277:ARG:HB2	2.10	0.51
2:B:1450:GLY:O	2:B:1454:LYS:HG3	2.11	0.51
3:C:815:LEU:C	3:C:817:ARG:H	2.14	0.51
3:F:742:TYR:C	3:F:742:TYR:CD1	2.85	0.51
1:D:173:PHE:HA	3:F:859:GLN:OE1	2.09	0.51
1:G:26:ILE:HD13	1:G:438:ALA:CB	2.41	0.51
1:G:274:LYS:HG3	1:G:275:GLU:OE2	2.11	0.51
1:G:307:ILE:HG12	1:G:312:ASN:O	2.10	0.51
1:G:451:SER:O	1:G:452:SER:CB	2.58	0.51
1:A:255:PHE:HD2	1:A:335:MET:HE1	1.75	0.51
3:C:737:THR:O	3:C:738:LYS:O	2.29	0.51
1:D:358:ARG:HH11	1:D:358:ARG:HG2	1.75	0.51
3:I:795:ARG:HH21	3:I:800:ILE:HD11	1.75	0.51
1:A:36:VAL:HG11	1:A:80:LEU:HD11	1.92	0.50
3:C:777:PHE:CE2	3:C:815:LEU:HD11	2.46	0.50
3:C:797:LYS:HG2	3:C:826:VAL:HG22	1.93	0.50
1:G:420:ILE:O	1:G:420:ILE:HD12	2.11	0.50
3:I:767:ILE:HD11	3:I:792:VAL:HG11	1.94	0.50
1:A:188:SER:HB2	1:A:193:THR:HB	1.93	0.50
3:C:787:ASN:O	3:C:791:ILE:HG13	2.10	0.50
1:D:145:LEU:HD22	1:D:185:LEU:HD13	1.93	0.50
1:D:380:ILE:CG2	1:D:381:ILE:H	2.24	0.50
3:F:767:ILE:HD11	3:F:792:VAL:HG11	1.93	0.50
3:F:787:ASN:O	3:F:791:ILE:HG13	2.11	0.50
1:G:175:LEU:HD13	3:I:797:LYS:HD3	1.92	0.50
1:A:189:LYS:HG2	1:A:304:THR:CG2	2.40	0.50
1:G:137:TYR:CE2	1:G:269:LYS:HD3	2.46	0.50
1:G:417:ILE:HG23	1:G:448:GLN:OE1	2.11	0.50
3:I:737:THR:O	3:I:738:LYS:O	2.29	0.50
1:A:274:LYS:O	1:A:277:ARG:HB2	2.12	0.50
3:C:767:ILE:HD11	3:C:792:VAL:HG11	1.93	0.50
1:D:125:SER:OG	1:D:147:GLU:HB2	2.12	0.50
1:D:200:THR:O	3:F:851:ARG:HB3	2.11	0.50
3:I:783:LEU:HD12	3:I:783:LEU:N	2.25	0.50
1:A:179:VAL:HG23	1:A:281:VAL:HG21	1.93	0.50
1:A:320:ASP:C	1:A:322:GLY:H	2.14	0.50
1:A:328:PHE:HB2	1:A:351:ILE:HD11	1.94	0.50
3:C:742:TYR:CD1	3:C:742:TYR:C	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:SER:O	1:D:452:SER:CB	2.59	0.50
2:E:1450:GLY:O	2:E:1454:LYS:HG3	2.11	0.50
3:F:821:VAL:HB	3:F:875:PHE:CE1	2.47	0.50
1:G:36:VAL:HG11	1:G:80:LEU:HD11	1.94	0.50
1:G:84:ASN:OD1	1:G:87:GLU:HG2	2.11	0.50
3:C:816:ASN:ND2	3:C:879:HIS:HB2	2.26	0.50
1:D:430:ASN:HA	1:D:434:GLN:O	2.12	0.50
1:D:446:THR:HG22	1:D:447:PHE:N	2.26	0.50
1:D:201:GLU:OE2	3:F:828:PRO:HA	2.12	0.50
1:A:339:VAL:HG11	1:A:342:TYR:CD1	2.46	0.50
1:D:239:SER:O	1:D:241:THR:N	2.45	0.50
1:D:343:VAL:HG12	1:D:343:VAL:O	2.12	0.50
1:G:27:PHE:CZ	1:G:71:VAL:HG23	2.37	0.50
3:I:787:ASN:O	3:I:791:ILE:HG13	2.11	0.50
3:I:797:LYS:HG2	3:I:826:VAL:HG22	1.93	0.50
3:C:828:PRO:HB3	3:C:848:TYR:CE1	2.47	0.50
3:F:777:PHE:CE2	3:F:815:LEU:HD11	2.47	0.50
1:D:343:VAL:CG1	3:F:834:ARG:CZ	2.90	0.50
3:I:772:TYR:CE2	3:I:796:ARG:NH2	2.80	0.50
1:A:142:ILE:HG12	1:A:156:ILE:HG13	1.94	0.49
1:A:175:LEU:HD12	3:C:797:LYS:HD3	1.92	0.49
1:A:229:LYS:HE3	1:A:332:GLU:OE1	2.12	0.49
3:C:810:PRO:HD2	3:C:813:GLU:HG3	1.94	0.49
1:G:6:ARG:HG3	1:G:431:TRP:CZ3	2.47	0.49
3:I:778:GLU:HG2	3:I:779:GLY:N	2.27	0.49
1:G:358:ARG:NH1	1:G:358:ARG:HG2	2.27	0.49
1:G:372:LYS:HG2	1:G:385:ASN:OD1	2.12	0.49
1:A:92:GLU:HB2	1:A:111:ILE:CD1	2.41	0.49
3:F:767:ILE:CG1	3:F:768:GLY:H	2.25	0.49
1:D:149:ASP:HB2	1:D:178:ARG:NH2	2.27	0.49
1:D:444:THR:HG22	1:D:445:LEU:N	2.28	0.49
3:F:795:ARG:HH21	3:F:800:ILE:HD11	1.77	0.49
3:I:802:TYR:CE1	3:I:809:PRO:HD2	2.47	0.49
3:I:828:PRO:HB3	3:I:848:TYR:CE1	2.47	0.49
1:A:50:THR:HG22	1:A:51:ASP:N	2.27	0.49
1:D:297:TYR:H	1:D:297:TYR:HD1	1.58	0.49
3:F:767:ILE:CG1	3:F:768:GLY:N	2.74	0.49
1:G:387:MET:HE3	1:G:391:SER:HB3	1.93	0.49
1:G:444:THR:HG22	1:G:445:LEU:N	2.27	0.49
3:C:742:TYR:O	3:C:743:THR:HG23	2.12	0.49
1:D:421:GLU:OE1	1:D:422:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:742:TYR:HD1	3:F:743:THR:N	2.10	0.49
3:F:754:THR:HG23	3:F:754:THR:O	2.12	0.49
1:G:210:PRO:HG3	1:G:335:MET:CE	2.43	0.49
1:G:255:PHE:HD2	1:G:335:MET:HE1	1.77	0.49
1:G:53:LEU:HD13	1:G:54:TYR:O	2.13	0.49
3:C:742:TYR:HD1	3:C:743:THR:N	2.11	0.49
1:D:216:LEU:HB3	1:D:270:VAL:CG1	2.42	0.49
1:G:297:TYR:H	1:G:297:TYR:HD1	1.58	0.49
1:D:50:THR:HG22	1:D:51:ASP:N	2.28	0.49
3:F:778:GLU:HG2	3:F:779:GLY:N	2.27	0.49
3:F:805:ASP:HA	3:F:808:LYS:CB	2.42	0.49
1:A:156:ILE:HG22	1:A:157:LEU:HD23	1.94	0.49
1:A:17:LEU:CD1	1:A:17:LEU:O	2.60	0.49
1:A:42:ILE:HD11	1:A:58:ASN:HD22	1.78	0.49
1:D:234:TYR:HA	1:D:237:LEU:CD1	2.42	0.49
1:D:53:LEU:HD13	1:D:54:TYR:O	2.13	0.49
1:G:137:TYR:CE2	1:G:138:ARG:HG3	2.48	0.49
3:I:754:THR:HG23	3:I:754:THR:O	2.13	0.49
3:I:821:VAL:HB	3:I:875:PHE:CE1	2.48	0.49
1:A:238:ASP:OD2	1:A:240:THR:N	2.36	0.49
3:C:805:ASP:HA	3:C:808:LYS:CB	2.40	0.49
3:F:772:TYR:CE2	3:F:796:ARG:NH2	2.81	0.49
1:A:216:LEU:HB2	1:A:272:ILE:CD1	2.43	0.48
1:A:408:LEU:HD23	1:A:409:LYS:N	2.28	0.48
3:C:795:ARG:HH21	3:C:800:ILE:HD11	1.78	0.48
1:A:137:TYR:CD1	1:A:269:LYS:HB3	2.48	0.48
1:A:189:LYS:NZ	1:A:304:THR:HB	2.29	0.48
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.77	0.48
3:C:750:LEU:HA	3:C:753:ILE:HD11	1.94	0.48
1:D:199:THR:O	1:D:200:THR:C	2.51	0.48
1:G:24:ARG:NH2	1:G:443:LYS:O	2.46	0.48
1:G:293:GLU:O	1:G:295:TYR:N	2.46	0.48
3:I:742:TYR:HD1	3:I:743:THR:N	2.11	0.48
1:A:92:GLU:HB2	1:A:111:ILE:HD12	1.94	0.48
1:G:199:THR:O	1:G:200:THR:C	2.51	0.48
3:I:742:TYR:CD1	3:I:742:TYR:C	2.86	0.48
1:A:238:ASP:CG	1:A:239:SER:H	2.16	0.48
1:A:384:VAL:HG13	1:A:414:LEU:CD1	2.37	0.48
1:D:164:ILE:HD12	1:D:277:ARG:CZ	2.44	0.48
1:D:343:VAL:CG1	3:F:834:ARG:NH1	2.77	0.48
1:G:210:PRO:HG3	1:G:335:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:O	1:A:124:LYS:CE	2.61	0.48
1:D:349:VAL:CG1	2:E:1453:PHE:HB2	2.41	0.48
1:G:216:LEU:HB2	1:G:272:ILE:HD12	1.94	0.48
3:I:810:PRO:HD2	3:I:813:GLU:HG3	1.94	0.48
1:A:53:LEU:HD13	1:A:54:TYR:O	2.14	0.48
3:C:766:THR:HG22	3:C:767:ILE:N	2.29	0.48
3:C:767:ILE:CG1	3:C:768:GLY:H	2.26	0.48
1:A:175:LEU:O	3:C:798:GLU:HB2	2.14	0.48
3:F:797:LYS:HG2	3:F:826:VAL:HG22	1.96	0.48
1:G:7:LEU:O	1:G:9:ALA:N	2.46	0.48
3:I:767:ILE:CG1	3:I:768:GLY:N	2.77	0.48
1:A:147:GLU:C	1:A:149:ASP:H	2.16	0.48
1:A:358:ARG:HG2	1:A:358:ARG:NH1	2.29	0.48
1:A:358:ARG:NH1	1:A:380:ILE:HD12	2.28	0.48
1:A:380:ILE:CG2	1:A:381:ILE:N	2.72	0.48
3:C:769:ARG:NH1	3:C:772:TYR:CE1	2.81	0.48
1:D:356:LEU:O	1:D:358:ARG:N	2.46	0.48
1:A:168:LYS:O	1:A:178:ARG:HD2	2.14	0.48
3:C:767:ILE:CG1	3:C:768:GLY:N	2.74	0.48
1:D:188:SER:HB2	1:D:193:THR:HB	1.96	0.48
1:G:112:PHE:CB	1:G:156:ILE:HG23	2.36	0.48
1:G:176:ASP:HB2	1:G:178:ARG:HG2	1.96	0.48
1:A:84:ASN:OD1	1:A:87:GLU:HG2	2.13	0.48
1:G:24:ARG:HG2	1:G:39:GLN:HG3	1.96	0.48
1:A:179:VAL:CG2	1:A:281:VAL:HG11	2.44	0.47
1:D:13:PHE:HE1	1:D:26:ILE:HD12	1.79	0.47
1:D:293:GLU:O	1:D:295:TYR:N	2.47	0.47
3:F:828:PRO:HB3	3:F:848:TYR:CD1	2.49	0.47
1:G:248:ASN:HD21	1:G:339:VAL:HG21	1.78	0.47
1:G:33:THR:HG23	1:G:49:LEU:HG	1.96	0.47
1:A:295:TYR:HB3	3:C:846:ILE:HG22	1.95	0.47
3:C:772:TYR:CE2	3:C:796:ARG:NH2	2.82	0.47
1:D:147:GLU:C	1:D:149:ASP:H	2.17	0.47
1:D:189:LYS:HG2	1:D:304:THR:CG2	2.44	0.47
3:F:737:THR:O	3:F:738:LYS:O	2.32	0.47
1:G:50:THR:HG22	1:G:51:ASP:N	2.29	0.47
1:D:384:VAL:HG13	1:D:414:LEU:CD1	2.37	0.47
3:F:791:ILE:HG23	3:F:802:TYR:CE2	2.50	0.47
3:F:869:GLU:H	3:F:869:GLU:CD	2.17	0.47
1:G:168:LYS:O	1:G:178:ARG:HD2	2.14	0.47
1:G:238:ASP:OD2	1:G:240:THR:CG2	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:LEU:C	1:G:9:ALA:N	2.68	0.47
3:I:769:ARG:NH1	3:I:772:TYR:CE1	2.82	0.47
1:A:33:THR:HG23	1:A:49:LEU:HG	1.97	0.47
1:D:329:LYS:HE2	1:D:333:MET:HG3	1.95	0.47
3:F:810:PRO:HD2	3:F:813:GLU:HG3	1.95	0.47
1:G:343:VAL:CG1	3:I:834:ARG:CZ	2.92	0.47
1:A:372:LYS:HG2	1:A:385:ASN:OD1	2.13	0.47
3:C:843:LEU:HD23	3:C:868:PRO:HB3	1.95	0.47
1:D:343:VAL:CG1	3:F:834:ARG:NH2	2.77	0.47
1:G:91:MET:HA	1:G:109:PHE:O	2.14	0.47
1:G:147:GLU:C	1:G:149:ASP:H	2.18	0.47
2:H:1434:PHE:CD1	2:H:1435:LYS:N	2.78	0.47
1:D:82:LEU:N	1:D:82:LEU:HD12	2.29	0.47
1:A:199:THR:O	1:A:200:THR:C	2.53	0.47
1:D:210:PRO:HD3	1:D:335:MET:HE2	1.97	0.47
2:E:1432:LYS:C	2:E:1432:LYS:CD	2.77	0.47
3:F:791:ILE:HG21	3:F:815:LEU:HD23	1.97	0.47
3:F:802:TYR:CE1	3:F:809:PRO:HD2	2.50	0.47
1:A:266:ARG:HB2	1:A:267:PHE:HD1	1.79	0.47
3:C:791:ILE:HG21	3:C:815:LEU:HD23	1.97	0.47
3:C:848:TYR:CE2	3:C:852:LEU:HD22	2.50	0.47
1:D:189:LYS:N	1:D:313:GLU:OE1	2.42	0.47
3:I:828:PRO:HB3	3:I:848:TYR:CD1	2.50	0.47
1:A:290:PHE:CE2	3:C:831:LYS:HD2	2.49	0.47
1:A:421:GLU:OE1	1:A:422:ARG:HG2	2.15	0.47
1:D:417:ILE:HG23	1:D:448:GLN:OE1	2.15	0.47
3:F:818:LYS:HB3	3:F:818:LYS:NZ	2.30	0.47
3:I:767:ILE:CG1	3:I:768:GLY:H	2.27	0.47
3:C:809:PRO:CB	3:C:814:GLY:H	2.28	0.47
1:D:358:ARG:NH1	1:D:358:ARG:HG2	2.29	0.47
1:D:27:PHE:CZ	1:D:71:VAL:HG23	2.41	0.47
1:G:92:GLU:HB2	1:G:111:ILE:CD1	2.45	0.47
1:G:121:VAL:CG1	1:G:122:GLY:H	2.25	0.47
1:G:295:TYR:HE1	3:I:831:LYS:HZ3	1.62	0.47
1:G:328:PHE:HB2	1:G:351:ILE:HD11	1.96	0.47
1:G:38:ILE:HG12	1:G:43:ILE:HG12	1.97	0.47
1:A:310:GLY:O	1:A:312:ASN:N	2.48	0.46
1:A:408:LEU:HD23	1:A:409:LYS:H	1.78	0.46
3:C:749:ASP:O	3:C:753:ILE:HG13	2.15	0.46
3:C:818:LYS:NZ	3:C:818:LYS:HB3	2.30	0.46
1:D:90:VAL:HB	1:D:112:PHE:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:TYR:HA	1:D:237:LEU:HD12	1.96	0.46
1:D:298:THR:HG22	1:D:299:ALA:H	1.80	0.46
1:G:61:ARG:NH2	1:G:103:VAL:HG13	2.30	0.46
1:G:188:SER:HB2	1:G:193:THR:HB	1.97	0.46
1:G:266:ARG:HB2	1:G:267:PHE:HD1	1.80	0.46
1:G:37:PHE:CE1	1:G:440:MET:HE3	2.51	0.46
1:G:384:VAL:HG13	1:G:414:LEU:CD1	2.36	0.46
1:A:380:ILE:CG2	1:A:381:ILE:H	2.25	0.46
3:C:791:ILE:HG23	3:C:802:TYR:CE2	2.50	0.46
1:D:115:SER:O	1:D:118:GLU:HG3	2.16	0.46
1:D:6:ARG:O	1:D:6:ARG:CG	2.63	0.46
3:F:833:SER:O	3:F:834:ARG:HG2	2.15	0.46
3:F:749:ASP:O	3:F:753:ILE:HG13	2.16	0.46
3:F:766:THR:HG22	3:F:767:ILE:N	2.31	0.46
3:F:816:ASN:O	3:F:816:ASN:ND2	2.43	0.46
1:G:26:ILE:HD13	1:G:438:ALA:HB1	1.97	0.46
3:I:750:LEU:HA	3:I:753:ILE:HD11	1.97	0.46
3:I:809:PRO:CB	3:I:814:GLY:H	2.28	0.46
1:A:174:GLY:H	3:C:859:GLN:CD	2.18	0.46
1:A:248:ASN:ND2	1:A:342:TYR:CZ	2.82	0.46
1:A:356:LEU:O	1:A:358:ARG:N	2.47	0.46
3:F:791:ILE:HG23	3:F:802:TYR:CD2	2.51	0.46
1:D:76:SER:OG	1:D:139:ASP:OD2	2.32	0.46
1:D:84:ASN:OD1	1:D:87:GLU:HG2	2.16	0.46
3:F:778:GLU:O	3:F:817:ARG:NH2	2.49	0.46
1:A:189:LYS:HZ1	1:A:304:THR:HB	1.79	0.46
1:G:297:TYR:CD2	1:G:321:ASP:HB3	2.51	0.46
1:G:71:VAL:CG1	1:G:82:LEU:HD23	2.46	0.46
1:A:90:VAL:HB	1:A:112:PHE:HB3	1.96	0.46
1:D:274:LYS:HG3	1:D:275:GLU:OE2	2.16	0.46
1:D:399:GLU:O	1:D:400:SER:HB2	2.15	0.46
1:A:119:GLU:O	1:A:120:GLU:C	2.53	0.46
3:C:802:TYR:CE1	3:C:809:PRO:HD2	2.50	0.46
1:D:134:PRO:HD2	1:D:187:PHE:CE1	2.51	0.46
1:D:255:PHE:CD2	1:D:335:MET:HE1	2.51	0.46
1:G:166:LEU:HD12	1:G:211:PHE:HE1	1.81	0.46
3:I:749:ASP:O	3:I:753:ILE:HG13	2.16	0.46
3:I:778:GLU:O	3:I:817:ARG:NH2	2.49	0.46
1:D:372:LYS:HG2	1:D:385:ASN:OD1	2.15	0.46
2:E:1431:MET:HG3	2:E:1431:MET:O	2.16	0.46
3:F:809:PRO:CB	3:F:814:GLY:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:ASN:OD1	3:I:832:THR:HB	2.16	0.46
1:G:343:VAL:HG12	1:G:343:VAL:O	2.15	0.46
3:I:791:ILE:HG23	3:I:802:TYR:CE2	2.51	0.46
3:I:833:SER:O	3:I:834:ARG:HG2	2.16	0.46
1:A:223:LEU:O	1:A:226:ILE:HG22	2.16	0.45
3:F:750:LEU:HA	3:F:753:ILE:HD11	1.97	0.45
3:F:781:VAL:HG22	3:F:817:ARG:NH1	2.31	0.45
1:G:57:LEU:CD2	1:G:100:VAL:HG11	2.26	0.45
1:G:173:PHE:HA	3:I:859:GLN:OE1	2.16	0.45
1:G:216:LEU:HB2	1:G:272:ILE:HD11	1.98	0.45
1:G:310:GLY:O	1:G:312:ASN:N	2.49	0.45
3:C:841:ASP:OD2	3:C:841:ASP:N	2.49	0.45
1:G:408:LEU:HD23	1:G:409:LYS:N	2.31	0.45
1:G:57:LEU:HD13	1:G:100:VAL:CB	2.47	0.45
1:A:84:ASN:C	1:A:86:ASN:H	2.20	0.45
3:C:821:VAL:HB	3:C:875:PHE:CE1	2.51	0.45
1:G:314:ILE:HG23	1:G:327:LEU:O	2.17	0.45
1:G:370:LEU:O	1:G:372:LYS:HG3	2.17	0.45
1:A:343:VAL:HA	1:A:346:ASN:ND2	2.32	0.45
1:D:296:ASP:HB2	1:D:297:TYR:CD1	2.51	0.45
1:D:325:ILE:HD12	1:D:327:LEU:HD21	1.99	0.45
1:D:37:PHE:HE1	1:D:440:MET:HE1	1.82	0.45
1:A:13:PHE:HE1	1:A:26:ILE:HD12	1.81	0.45
1:A:343:VAL:CG1	1:A:343:VAL:O	2.64	0.45
1:A:444:THR:CG2	1:A:445:LEU:N	2.79	0.45
3:C:791:ILE:HG23	3:C:802:TYR:CD2	2.51	0.45
1:D:250:ILE:O	1:D:254:GLN:HG3	2.16	0.45
1:D:282:GLN:HG2	1:D:342:TYR:HB3	1.99	0.45
1:D:358:ARG:NH1	1:D:380:ILE:HD12	2.31	0.45
3:I:791:ILE:HG21	3:I:815:LEU:HD23	1.99	0.45
1:A:71:VAL:CG1	1:A:82:LEU:HD23	2.47	0.45
2:B:1457:ASN:O	2:B:1458:MET:HE3	2.17	0.45
3:C:828:PRO:HB3	3:C:848:TYR:CD1	2.51	0.45
1:D:189:LYS:NZ	1:D:304:THR:HB	2.31	0.45
1:D:84:ASN:C	1:D:86:ASN:H	2.20	0.45
1:G:53:LEU:HD22	1:G:54:TYR:H	1.82	0.45
1:A:242:ASP:OD1	1:A:244:ILE:N	2.50	0.45
1:A:7:LEU:O	1:A:9:ALA:N	2.47	0.45
1:G:13:PHE:HE1	1:G:26:ILE:HD12	1.82	0.45
1:G:296:ASP:HB2	1:G:297:TYR:CD1	2.52	0.45
3:I:791:ILE:HG23	3:I:802:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:GLU:CD	1:A:368:GLU:N	2.64	0.45
1:A:443:LYS:CD	1:A:443:LYS:H	2.22	0.45
1:G:82:LEU:HD12	1:G:82:LEU:N	2.32	0.45
1:D:248:ASN:HD21	1:D:339:VAL:HG21	1.81	0.44
1:D:320:ASP:O	1:D:322:GLY:N	2.50	0.44
1:G:197:LEU:HD21	1:G:299:ALA:HB1	1.99	0.44
1:G:35:ILE:O	1:G:45:TRP:HA	2.16	0.44
1:D:69:PHE:HA	1:D:83:PHE:O	2.17	0.44
3:F:843:LEU:HD23	3:F:868:PRO:HB3	1.98	0.44
1:G:7:LEU:HD13	1:G:431:TRP:CG	2.52	0.44
1:G:443:LYS:H	1:G:443:LYS:CD	2.25	0.44
1:G:444:THR:CG2	1:G:445:LEU:N	2.80	0.44
1:G:173:PHE:O	3:I:799:VAL:HG12	2.16	0.44
3:I:805:ASP:HA	3:I:808:LYS:CB	2.42	0.44
1:A:370:LEU:O	1:A:372:LYS:HG3	2.18	0.44
3:C:818:LYS:HD2	3:C:818:LYS:N	2.28	0.44
1:G:373:LEU:HB3	1:G:384:VAL:HG23	1.98	0.44
3:C:869:GLU:H	3:C:869:GLU:CD	2.21	0.44
1:D:24:ARG:HG2	1:D:39:GLN:HG3	1.99	0.44
3:F:848:TYR:CE2	3:F:852:LEU:HD22	2.52	0.44
1:G:408:LEU:HD23	1:G:409:LYS:H	1.81	0.44
1:A:376:ILE:HD13	1:A:424:PRO:HD2	1.99	0.44
3:C:781:VAL:HG22	3:C:817:ARG:NH1	2.31	0.44
3:C:822:THR:HG23	3:C:874:VAL:CG1	2.47	0.44
1:G:358:ARG:NH1	1:G:380:ILE:HD12	2.32	0.44
1:G:369:GLN:OE1	1:G:450:ILE:HG21	2.18	0.44
3:I:818:LYS:HB3	3:I:818:LYS:NZ	2.33	0.44
1:D:223:LEU:O	1:D:226:ILE:HG22	2.18	0.44
1:D:295:TYR:O	3:F:846:ILE:HG22	2.17	0.44
3:I:768:GLY:HA2	3:I:794:ILE:CD1	2.48	0.44
1:D:340:ASP:O	1:D:341:ASN:HB2	2.18	0.44
3:F:783:LEU:O	3:F:785:ASN:N	2.51	0.44
3:F:841:ASP:N	3:F:841:ASP:OD2	2.50	0.44
1:G:216:LEU:HB3	1:G:270:VAL:HG13	1.99	0.44
1:D:237:LEU:HD22	1:D:246:LYS:HA	1.99	0.44
1:D:36:VAL:HG11	1:D:80:LEU:HD11	1.98	0.44
1:G:349:VAL:CG1	2:H:1453:PHE:HB2	2.47	0.44
3:I:783:LEU:O	3:I:785:ASN:N	2.51	0.44
3:I:841:ASP:N	3:I:841:ASP:OD2	2.51	0.44
1:A:102:ASP:O	1:A:106:GLN:HB2	2.18	0.44
3:C:742:TYR:C	3:C:742:TYR:HD1	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LYS:O	1:D:277:ARG:HB2	2.17	0.44
1:D:370:LEU:O	1:D:372:LYS:HG3	2.18	0.44
1:G:228:ASN:O	1:G:231:LEU:N	2.51	0.44
1:G:421:GLU:OE1	1:G:422:ARG:HG2	2.18	0.44
1:G:437:LEU:HB2	1:G:450:ILE:HD11	2.00	0.44
2:H:1457:ASN:O	2:H:1458:MET:HE3	2.17	0.44
1:A:82:LEU:HD12	1:A:82:LEU:N	2.32	0.43
1:D:168:LYS:O	1:D:178:ARG:HD2	2.17	0.43
1:A:395:LYS:HD3	1:A:399:GLU:OE2	2.18	0.43
3:C:778:GLU:O	3:C:817:ARG:NH2	2.51	0.43
1:D:138:ARG:O	1:D:140:SER:N	2.51	0.43
1:G:189:LYS:HD3	1:G:189:LYS:HA	1.87	0.43
1:G:93:VAL:HB	1:G:95:TRP:NE1	2.34	0.43
1:A:176:ASP:CB	3:C:798:GLU:OE2	2.66	0.43
1:A:226:ILE:CG2	1:A:227:LEU:N	2.81	0.43
1:D:216:LEU:HB3	1:D:270:VAL:HG12	2.00	0.43
3:F:769:ARG:NH1	3:F:772:TYR:CE1	2.85	0.43
1:G:343:VAL:HA	1:G:346:ASN:ND2	2.33	0.43
3:I:742:TYR:O	3:I:767:ILE:HG13	2.19	0.43
1:A:383:GLN:HG2	1:A:383:GLN:O	2.18	0.43
1:A:373:LEU:HB3	1:A:384:VAL:HG23	2.00	0.43
1:A:38:ILE:HG12	1:A:43:ILE:HG12	2.00	0.43
1:A:93:VAL:HB	1:A:95:TRP:HE1	1.83	0.43
1:D:92:GLU:HB2	1:D:111:ILE:HD12	2.00	0.43
1:D:247:ARG:NH2	1:D:338:ASP:OD2	2.52	0.43
1:G:84:ASN:C	1:G:86:ASN:H	2.20	0.43
1:A:379:ASN:O	1:A:419:THR:HA	2.19	0.43
1:D:10:LEU:HG	1:D:11:PRO:CD	2.47	0.43
1:D:356:LEU:C	1:D:358:ARG:H	2.22	0.43
1:D:395:LYS:O	1:D:397:ILE:N	2.51	0.43
1:D:444:THR:CG2	1:D:445:LEU:N	2.82	0.43
1:D:71:VAL:CG1	1:D:82:LEU:HD23	2.49	0.43
3:F:742:TYR:C	3:F:742:TYR:HD1	2.22	0.43
3:F:851:ARG:NH2	3:F:851:ARG:CG	2.80	0.43
3:C:762:VAL:HG22	3:C:763:SER:N	2.34	0.43
3:C:833:SER:O	3:C:834:ARG:HG2	2.18	0.43
1:G:114:TYR:HA	1:G:118:GLU:OE2	2.18	0.43
1:G:134:PRO:HD2	1:G:187:PHE:CD1	2.53	0.43
1:G:367:PRO:HB2	1:G:368:GLU:OE2	2.18	0.43
1:A:93:VAL:HB	1:A:95:TRP:NE1	2.33	0.43
1:D:321:ASP:OD1	1:D:323:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:TYR:CD1	1:D:54:TYR:C	2.91	0.43
1:G:32:GLY:HA2	1:G:428:TYR:O	2.19	0.43
1:A:200:THR:O	3:C:851:ARG:HD2	2.19	0.43
1:G:190:ASP:OD1	1:G:192:LEU:N	2.47	0.43
1:G:206:PHE:CZ	1:G:284:PRO:HG3	2.54	0.43
1:G:304:THR:HG21	1:G:313:GLU:OE1	2.18	0.43
1:G:387:MET:HE1	1:G:391:SER:HB3	2.01	0.43
1:A:128:LYS:O	1:A:129:LYS:HB2	2.19	0.43
1:A:194:LEU:HB3	1:A:208:PHE:HB2	2.01	0.43
1:A:209:TYR:HA	1:A:210:PRO:HA	1.78	0.43
1:A:275:GLU:N	1:A:275:GLU:CD	2.72	0.43
1:A:336:SER:HB2	1:A:342:TYR:CD2	2.53	0.43
3:C:851:ARG:NH2	3:C:851:ARG:CG	2.81	0.43
1:D:297:TYR:CD2	1:D:321:ASP:HB3	2.54	0.43
1:D:328:PHE:HB2	1:D:351:ILE:HD11	2.01	0.43
1:D:376:ILE:HD13	1:D:424:PRO:HD2	2.01	0.43
3:F:768:GLY:HA2	3:F:794:ILE:CD1	2.49	0.43
3:F:815:LEU:O	3:F:817:ARG:N	2.45	0.43
3:I:766:THR:HG22	3:I:767:ILE:N	2.33	0.43
1:D:209:TYR:HA	1:D:210:PRO:HA	1.84	0.43
1:G:227:LEU:O	1:G:230:SER:HB2	2.18	0.43
1:G:242:ASP:OD1	1:G:244:ILE:N	2.52	0.43
1:G:381:ILE:CD1	1:G:424:PRO:HG3	2.39	0.43
3:I:744:ILE:HB	3:I:766:THR:HB	2.00	0.43
3:I:781:VAL:HG22	3:I:817:ARG:NH1	2.32	0.43
1:A:24:ARG:CD	1:A:39:GLN:HG3	2.49	0.42
1:A:381:ILE:CD1	1:A:424:PRO:HG3	2.39	0.42
1:A:53:LEU:HD22	1:A:54:TYR:H	1.84	0.42
3:C:768:GLY:HA2	3:C:794:ILE:CD1	2.49	0.42
1:D:275:GLU:N	1:D:275:GLU:CD	2.72	0.42
1:G:164:ILE:HD12	1:G:277:ARG:CZ	2.49	0.42
1:A:135:LYS:HD3	1:A:217:LEU:O	2.19	0.42
1:A:417:ILE:HG22	1:A:418:ALA:N	2.34	0.42
1:D:117:ASP:HA	1:D:124:LYS:HD3	2.01	0.42
1:D:128:LYS:O	1:D:129:LYS:HB2	2.18	0.42
1:D:189:LYS:HA	1:D:189:LYS:HD3	1.82	0.42
2:E:1436:VAL:HG13	2:E:1437:VAL:N	2.33	0.42
3:F:847:ASN:O	3:F:847:ASN:CG	2.57	0.42
1:G:145:LEU:HD13	1:G:151:ILE:HG12	2.01	0.42
1:G:28:SER:HB2	1:G:428:TYR:O	2.20	0.42
1:G:298:THR:HG22	1:G:299:ALA:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:343:VAL:HG11	3:I:834:ARG:CZ	2.50	0.42
1:G:395:LYS:O	1:G:397:ILE:N	2.51	0.42
1:G:379:ASN:O	1:G:419:THR:HA	2.19	0.42
3:I:839:SER:O	3:I:843:LEU:HB2	2.19	0.42
1:G:295:TYR:HB3	3:I:846:ILE:HG22	2.01	0.42
3:C:783:LEU:O	3:C:785:ASN:N	2.52	0.42
1:D:171:ASN:O	1:D:171:ASN:ND2	2.51	0.42
1:D:183:THR:HG22	1:D:183:THR:O	2.20	0.42
1:G:25:TYR:HD2	1:G:425:ASN:ND2	2.12	0.42
2:H:1458:MET:CE	2:H:1458:MET:HA	2.48	0.42
3:I:848:TYR:CE2	3:I:852:LEU:HD22	2.53	0.42
1:A:296:ASP:HB2	1:A:297:TYR:CD1	2.54	0.42
1:A:321:ASP:OD1	1:A:323:SER:HB2	2.19	0.42
3:C:744:ILE:HB	3:C:766:THR:HB	2.01	0.42
1:D:119:GLU:O	1:D:120:GLU:C	2.57	0.42
1:D:136:SER:OG	1:D:139:ASP:HA	2.20	0.42
1:D:242:ASP:OD1	1:D:244:ILE:N	2.52	0.42
1:D:343:VAL:O	1:D:343:VAL:CG1	2.67	0.42
1:D:93:VAL:HA	1:D:94:PRO:HD3	1.83	0.42
3:C:751:ALA:O	3:C:754:THR:HG22	2.20	0.42
3:F:745:PRO:HG2	3:F:750:LEU:HD21	2.02	0.42
1:G:275:GLU:N	1:G:275:GLU:CD	2.73	0.42
3:I:745:PRO:HG2	3:I:750:LEU:HD21	2.02	0.42
1:A:340:ASP:O	1:A:341:ASN:HB2	2.19	0.42
3:C:799:VAL:HB	3:C:823:LEU:HD21	2.01	0.42
1:D:25:TYR:HD2	1:D:425:ASN:HD22	1.68	0.42
1:D:440:MET:HB2	1:D:440:MET:HE2	1.88	0.42
1:D:33:THR:HG23	1:D:49:LEU:HG	2.00	0.42
3:F:742:TYR:O	3:F:767:ILE:HG13	2.20	0.42
1:G:57:LEU:HD11	1:G:106:GLN:CG	2.48	0.42
1:G:282:GLN:HG2	1:G:342:TYR:HB3	2.02	0.42
3:I:851:ARG:NH2	3:I:851:ARG:CG	2.82	0.42
1:A:356:LEU:C	1:A:358:ARG:H	2.22	0.42
3:C:742:TYR:O	3:C:767:ILE:HG13	2.20	0.42
1:G:128:LYS:O	1:G:129:LYS:HB2	2.20	0.42
1:G:21:GLN:O	1:G:23:PRO:N	2.53	0.42
1:G:373:LEU:HD23	1:G:384:VAL:HG21	2.02	0.42
1:G:371:GLY:HA3	1:G:387:MET:HG2	2.02	0.42
1:G:69:PHE:HA	1:G:83:PHE:O	2.19	0.42
3:I:799:VAL:HB	3:I:823:LEU:HD21	2.01	0.42
1:A:164:ILE:HD12	1:A:277:ARG:CZ	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASP:OD1	1:A:192:LEU:N	2.48	0.42
1:A:297:TYR:CD2	1:A:321:ASP:HB3	2.55	0.42
1:A:369:GLN:OE1	1:A:450:ILE:HG21	2.20	0.42
3:F:817:ARG:NH2	3:F:818:LYS:HD3	2.33	0.42
1:G:102:ASP:O	1:G:106:GLN:HB2	2.19	0.42
1:G:356:LEU:O	1:G:358:ARG:N	2.52	0.42
1:G:399:GLU:O	1:G:400:SER:HB2	2.20	0.42
1:A:189:LYS:HD3	1:A:189:LYS:HA	1.83	0.42
1:D:53:LEU:HD22	1:D:54:TYR:H	1.84	0.42
1:D:90:VAL:HG11	1:D:156:ILE:HD13	2.02	0.42
1:G:228:ASN:O	1:G:229:LYS:C	2.58	0.42
1:G:220:GLU:HB2	1:G:263:TRP:CH2	2.54	0.42
1:G:42:ILE:HD11	1:G:58:ASN:HD22	1.84	0.42
1:D:291:PRO:HD3	1:D:350:LEU:HD22	2.02	0.42
1:D:395:LYS:HD3	1:D:399:GLU:OE2	2.20	0.42
1:D:57:LEU:HD12	1:D:58:ASN:H	1.85	0.42
1:G:248:ASN:ND2	1:G:342:TYR:CZ	2.84	0.42
1:A:167:ASN:OD1	1:A:178:ARG:HB2	2.19	0.41
1:D:164:ILE:CD1	1:D:277:ARG:CZ	2.98	0.41
1:D:336:SER:HB2	1:D:342:TYR:CD2	2.55	0.41
3:C:847:ASN:ND2	3:C:847:ASN:O	2.53	0.41
1:D:320:ASP:C	1:D:322:GLY:N	2.73	0.41
1:G:250:ILE:O	1:G:254:GLN:HG3	2.20	0.41
1:G:397:ILE:HG12	2:H:1449:ILE:HD12	2.01	0.41
3:I:768:GLY:HA2	3:I:794:ILE:HD12	2.02	0.41
1:A:291:PRO:HD3	1:A:350:LEU:HD22	2.01	0.41
1:A:437:LEU:HB2	1:A:450:ILE:HD11	2.03	0.41
1:A:43:ILE:HG13	1:A:59:PHE:CE2	2.56	0.41
2:B:1434:PHE:CD1	2:B:1435:LYS:N	2.79	0.41
3:C:816:ASN:ND2	3:C:816:ASN:O	2.46	0.41
3:F:738:LYS:HB2	3:F:741:TYR:CD2	2.52	0.41
1:G:325:ILE:HD12	1:G:327:LEU:HD21	2.01	0.41
1:A:134:PRO:HD2	1:A:187:PHE:CE1	2.55	0.41
1:A:137:TYR:HA	1:A:217:LEU:HG	2.02	0.41
1:D:226:ILE:CG2	1:D:227:LEU:N	2.83	0.41
1:D:210:PRO:HG3	1:D:335:MET:CE	2.50	0.41
2:E:1457:ASN:O	2:E:1458:MET:HE3	2.20	0.41
3:C:839:SER:O	3:C:843:LEU:HB2	2.20	0.41
1:D:103:VAL:O	1:D:103:VAL:HG12	2.19	0.41
3:F:802:TYR:O	3:F:804:ASP:N	2.52	0.41
2:H:1441:LEU:HD23	2:H:1441:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ASN:O	1:A:450:ILE:HD13	2.20	0.41
1:D:308:ASP:OD1	1:D:309:ASN:N	2.54	0.41
1:D:417:ILE:HG22	1:D:418:ALA:N	2.35	0.41
1:G:116:ILE:C	1:G:118:GLU:H	2.24	0.41
1:G:223:LEU:O	1:G:226:ILE:HG22	2.21	0.41
1:G:417:ILE:HG22	1:G:418:ALA:N	2.35	0.41
3:I:742:TYR:C	3:I:742:TYR:HD1	2.24	0.41
3:I:818:LYS:N	3:I:818:LYS:HD2	2.30	0.41
1:A:103:VAL:O	1:A:103:VAL:HG12	2.21	0.41
1:A:325:ILE:HD12	1:A:327:LEU:HD21	2.03	0.41
3:C:753:ILE:HD12	3:C:753:ILE:C	2.41	0.41
1:D:93:VAL:HB	1:D:95:TRP:NE1	2.35	0.41
1:G:356:LEU:HD21	1:G:414:LEU:HD21	2.03	0.41
1:G:425:ASN:HB3	1:G:440:MET:HB3	2.02	0.41
1:G:93:VAL:HB	1:G:95:TRP:HE1	1.85	0.41
3:I:755:ASN:HB2	3:I:759:GLU:O	2.21	0.41
1:A:248:ASN:HD21	1:A:339:VAL:HG21	1.85	0.41
1:A:395:LYS:O	1:A:397:ILE:N	2.54	0.41
1:D:369:GLN:OE1	1:D:450:ILE:HG21	2.20	0.41
2:H:1436:VAL:HG13	2:H:1437:VAL:N	2.36	0.41
3:I:751:ALA:O	3:I:754:THR:HG22	2.20	0.41
3:I:847:ASN:O	3:I:847:ASN:CG	2.59	0.41
1:A:119:GLU:O	1:A:124:LYS:NZ	2.53	0.41
1:A:149:ASP:HB2	1:A:178:ARG:NH2	2.36	0.41
3:F:742:TYR:CD1	3:F:743:THR:N	2.89	0.41
1:G:449:ASN:O	1:G:450:ILE:HD13	2.21	0.41
1:A:395:LYS:C	1:A:397:ILE:N	2.74	0.41
3:C:755:ASN:HB2	3:C:759:GLU:O	2.20	0.41
3:C:802:TYR:O	3:C:804:ASP:N	2.54	0.41
3:F:818:LYS:N	3:F:818:LYS:HD2	2.31	0.41
1:G:102:ASP:HB3	1:G:105:ILE:HB	2.02	0.41
3:C:768:GLY:HA2	3:C:794:ILE:HD12	2.03	0.41
3:C:837:ILE:N	3:C:837:ILE:HD12	2.36	0.41
1:D:102:ASP:HB3	1:D:105:ILE:HB	2.02	0.41
1:D:296:ASP:OD1	3:F:845:ASP:HB3	2.21	0.41
1:D:37:PHE:HE1	1:D:440:MET:CE	2.33	0.41
1:D:35:ILE:O	1:D:45:TRP:HA	2.21	0.41
1:D:79:LEU:HD12	1:D:139:ASP:HB2	2.03	0.41
3:F:847:ASN:ND2	3:F:847:ASN:O	2.54	0.41
1:G:194:LEU:HB3	1:G:208:PHE:HB2	2.02	0.41
1:G:336:SER:HB2	1:G:342:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:356:LEU:C	1:G:358:ARG:H	2.24	0.41
1:G:43:ILE:HG13	1:G:59:PHE:CE2	2.56	0.41
3:I:738:LYS:HB2	3:I:741:TYR:CD2	2.53	0.41
3:I:843:LEU:HD12	3:I:843:LEU:HA	1.88	0.41
1:A:142:ILE:HD11	1:A:156:ILE:HG12	2.03	0.40
1:A:371:GLY:HA3	1:A:387:MET:HG2	2.03	0.40
1:D:234:TYR:C	1:D:236:SER:H	2.23	0.40
1:D:339:VAL:HG11	1:D:342:TYR:CD1	2.56	0.40
1:G:395:LYS:HD3	1:G:399:GLU:OE2	2.20	0.40
1:A:216:LEU:HB2	1:A:272:ILE:HD11	2.03	0.40
3:C:815:LEU:O	3:C:817:ARG:N	2.48	0.40
1:A:250:ILE:CG2	2:E:1441:LEU:HG	2.51	0.40
3:F:744:ILE:HB	3:F:766:THR:HB	2.02	0.40
3:F:834:ARG:HB3	3:F:834:ARG:HE	1.61	0.40
1:G:93:VAL:HA	1:G:94:PRO:HD3	1.83	0.40
3:C:807:GLN:O	3:C:809:PRO:CD	2.70	0.40
3:F:755:ASN:HB2	3:F:759:GLU:O	2.21	0.40
1:G:103:VAL:HG12	1:G:103:VAL:O	2.21	0.40
1:G:297:TYR:HD2	1:G:320:ASP:HB2	1.87	0.40
1:G:321:ASP:OD1	1:G:323:SER:HB2	2.21	0.40
3:I:742:TYR:CD1	3:I:743:THR:N	2.89	0.40
3:I:762:VAL:HG22	3:I:763:SER:N	2.36	0.40
1:A:10:LEU:HG	1:A:11:PRO:CD	2.49	0.40
1:A:206:PHE:CZ	1:A:284:PRO:HG3	2.56	0.40
1:A:422:ARG:HG2	1:A:422:ARG:H	1.72	0.40
1:A:174:GLY:HA2	3:C:859:GLN:HE22	1.86	0.40
1:D:133:HIS:HB3	1:D:136:SER:HB3	2.03	0.40
1:D:194:LEU:HB3	1:D:208:PHE:HB2	2.03	0.40
3:F:751:ALA:O	3:F:754:THR:HG22	2.22	0.40
1:G:121:VAL:CG1	1:G:122:GLY:N	2.83	0.40
1:A:216:LEU:HB2	1:A:272:ILE:HD12	2.04	0.40
1:D:237:LEU:CD2	1:D:246:LYS:HA	2.52	0.40
1:D:310:GLY:O	1:D:312:ASN:N	2.55	0.40
2:E:1432:LYS:HG3	2:E:1433:GLY:H	1.84	0.40
3:F:799:VAL:HB	3:F:823:LEU:HD21	2.03	0.40
1:G:137:TYR:CZ	1:G:269:LYS:HD3	2.56	0.40
1:G:418:ALA:HB3	1:G:439:LEU:CD1	2.51	0.40
3:I:869:GLU:H	3:I:869:GLU:CD	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	449/452 (99%)	358 (80%)	64 (14%)	27 (6%)	1 10
1	D	445/452 (98%)	351 (79%)	65 (15%)	29 (6%)	1 8
1	G	445/452 (98%)	358 (80%)	62 (14%)	25 (6%)	2 12
2	B	26/39 (67%)	21 (81%)	5 (19%)	0	100 100
2	E	26/39 (67%)	21 (81%)	4 (15%)	1 (4%)	3 19
2	H	26/39 (67%)	20 (77%)	6 (23%)	0	100 100
3	C	145/152 (95%)	110 (76%)	24 (17%)	11 (8%)	1 6
3	F	145/152 (95%)	110 (76%)	24 (17%)	11 (8%)	1 6
3	I	145/152 (95%)	110 (76%)	24 (17%)	11 (8%)	1 6
All	All	1852/1929 (96%)	1459 (79%)	278 (15%)	115 (6%)	1 10

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	GLU
1	A	266	ARG
1	A	311	GLN
1	A	377	SER
3	C	738	LYS
3	C	784	THR
3	C	803	VAL
1	D	51	ASP
1	D	98	SER
1	D	123	PRO
1	D	139	ASP
1	D	311	GLN
1	D	377	SER
2	E	1432	LYS
3	F	738	LYS
3	F	784	THR

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Mol	Chain	Res	Type
3	F	803	VAL
1	G	311	GLN
1	G	377	SER
3	I	738	LYS
3	I	784	THR
3	I	803	VAL
1	A	4	SER
1	A	48	VAL
1	A	51	ASP
1	A	200	THR
1	A	294	LEU
1	A	308	ASP
3	C	757	LYS
3	C	816	ASN
3	C	849	GLU
1	D	48	VAL
1	D	176	ASP
1	D	200	THR
1	D	240	THR
1	D	266	ARG
1	D	294	LEU
1	D	308	ASP
1	D	321	ASP
3	F	757	LYS
3	F	816	ASN
3	F	849	GLU
1	G	8	SER
1	G	48	VAL
1	G	51	ASP
1	G	120	GLU
1	G	200	THR
1	G	266	ARG
1	G	294	LEU
1	G	308	ASP
1	G	321	ASP
3	I	757	LYS
3	I	816	ASN
3	I	849	GLU
1	A	20	SER
1	A	85	ASP
1	A	137	TYR
1	A	321	ASP

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Mol	Chain	Res	Type
1	A	357	GLN
3	C	814	GLY
1	D	20	SER
1	D	172	SER
1	D	357	GLN
1	D	396	SER
3	F	814	GLY
1	G	20	SER
1	G	85	ASP
1	G	357	GLN
1	G	396	SER
3	I	814	GLY
1	A	8	SER
1	A	22	SER
1	A	29	SER
1	D	22	SER
1	D	29	SER
1	D	85	ASP
1	G	22	SER
1	G	29	SER
1	G	442	ASN
3	I	737	THR
1	A	50	THR
1	A	172	SER
1	A	368	GLU
1	A	442	ASN
1	A	445	LEU
3	C	737	THR
3	C	785	ASN
3	C	806	ASN
1	D	50	THR
1	D	120	GLU
1	D	169	PRO
1	D	368	GLU
1	D	417	ILE
1	D	442	ASN
3	F	737	THR
3	F	785	ASN
3	F	806	ASN
1	G	50	THR
1	G	121	VAL
1	G	368	GLU

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Mol	Chain	Res	Type
1	G	417	ILE
3	I	785	ASN
3	I	806	ASN
1	A	417	ILE
1	G	23	PRO
1	A	11	PRO
3	C	808	LYS
1	D	11	PRO
1	D	23	PRO
1	A	23	PRO
3	F	808	LYS
1	G	11	PRO
1	G	367	PRO
1	A	367	PRO
3	I	808	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/423 (100%)	392 (93%)	30 (7%)	14	44
1	D	418/423 (99%)	391 (94%)	27 (6%)	17	46
1	G	418/423 (99%)	389 (93%)	29 (7%)	15	45
2	B	24/33 (73%)	21 (88%)	3 (12%)	4	17
2	E	24/33 (73%)	22 (92%)	2 (8%)	11	36
2	H	24/33 (73%)	21 (88%)	3 (12%)	4	17
3	C	130/132 (98%)	121 (93%)	9 (7%)	15	45
3	F	130/132 (98%)	121 (93%)	9 (7%)	15	45
3	I	130/132 (98%)	121 (93%)	9 (7%)	15	45
All	All	1720/1764 (98%)	1599 (93%)	121 (7%)	15	44

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	7	LEU
1	A	21	GLN
1	A	54	TYR
1	A	68	THR
1	A	82	LEU
1	A	107	ASP
1	A	139	ASP
1	A	141	CYS
1	A	142	ILE
1	A	157	LEU
1	A	159	SER
1	A	198	ASN
1	A	210	PRO
1	A	217	LEU
1	A	225	LEU
1	A	242	ASP
1	A	243	VAL
1	A	247	ARG
1	A	251	LYS
1	A	257	SER
1	A	267	PHE
1	A	297	TYR
1	A	352	GLU
1	A	361	LYS
1	A	384	VAL
1	A	386	PHE
1	A	421	GLU
1	A	431	TRP
1	A	443	LYS
2	B	1432	LYS
2	B	1434	PHE
2	B	1441	LEU
3	C	742	TYR
3	C	789	ASP
3	C	795	ARG
3	C	816	ASN
3	C	818	LYS
3	C	834	ARG
3	C	841	ASP
3	C	843	LEU
3	C	875	PHE
1	D	21	GLN

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Mol	Chain	Res	Type
1	D	54	TYR
1	D	68	THR
1	D	98	SER
1	D	107	ASP
1	D	157	LEU
1	D	159	SER
1	D	198	ASN
1	D	210	PRO
1	D	217	LEU
1	D	225	LEU
1	D	236	SER
1	D	242	ASP
1	D	243	VAL
1	D	247	ARG
1	D	251	LYS
1	D	257	SER
1	D	267	PHE
1	D	297	TYR
1	D	352	GLU
1	D	358	ARG
1	D	361	LYS
1	D	384	VAL
1	D	386	PHE
1	D	421	GLU
1	D	431	TRP
1	D	443	LYS
2	E	1434	PHE
2	E	1441	LEU
3	F	742	TYR
3	F	789	ASP
3	F	795	ARG
3	F	816	ASN
3	F	818	LYS
3	F	834	ARG
3	F	841	ASP
3	F	843	LEU
3	F	875	PHE
1	G	21	GLN
1	G	54	TYR
1	G	68	THR
1	G	107	ASP
1	G	139	ASP

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Mol	Chain	Res	Type
1	G	157	LEU
1	G	158	ASN
1	G	159	SER
1	G	171	ASN
1	G	176	ASP
1	G	198	ASN
1	G	210	PRO
1	G	217	LEU
1	G	225	LEU
1	G	242	ASP
1	G	243	VAL
1	G	247	ARG
1	G	251	LYS
1	G	257	SER
1	G	267	PHE
1	G	297	TYR
1	G	352	GLU
1	G	361	LYS
1	G	384	VAL
1	G	386	PHE
1	G	408	LEU
1	G	421	GLU
1	G	431	TRP
1	G	443	LYS
2	H	1432	LYS
2	H	1434	PHE
2	H	1441	LEU
3	I	742	TYR
3	I	789	ASP
3	I	795	ARG
3	I	816	ASN
3	I	818	LYS
3	I	834	ARG
3	I	841	ASP
3	I	843	LEU
3	I	875	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	436	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	451/452 (99%)	0.28	33 (7%) 15 17	60, 104, 150, 170	0
1	D	447/452 (98%)	0.32	3 (0%) 87 87	61, 99, 145, 170	0
1	G	447/452 (98%)	0.30	26 (5%) 23 24	63, 104, 148, 170	0
2	B	28/39 (71%)	-0.04	0 100 100	68, 90, 136, 136	0
2	E	28/39 (71%)	0.02	0 100 100	65, 87, 127, 136	0
2	H	28/39 (71%)	0.45	2 (7%) 16 18	69, 88, 126, 137	0
3	C	147/152 (96%)	0.70	19 (12%) 3 4	95, 141, 190, 199	0
3	F	147/152 (96%)	0.40	9 (6%) 21 22	93, 140, 190, 198	0
3	I	147/152 (96%)	1.15	37 (25%) 0 0	96, 141, 190, 199	0
All	All	1870/1929 (96%)	0.40	129 (6%) 16 18	60, 111, 169, 199	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	880	PHE	10.5
1	G	101	GLU	6.4
2	H	1458	MET	5.8
2	H	1457	ASN	5.3
1	G	171	ASN	5.3
3	I	801	VAL	5.1
3	I	815	LEU	5.0
3	I	775	ILE	4.8
3	C	760	CYS	4.7
1	A	26	ILE	4.6
1	G	174	GLY	4.6
1	G	173	PHE	4.4
3	C	873	TRP	4.4
3	I	816	ASN	4.3
1	A	13	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
3	F	750	LEU	4.1
1	G	175	LEU	4.1
1	G	99	ASN	4.1
1	G	100	VAL	4.0
1	G	46	TYR	4.0
3	I	777	PHE	3.9
3	I	866	TYR	3.9
1	A	94	PRO	3.9
1	A	2	SER	3.7
3	I	846	ILE	3.7
3	C	866	TYR	3.6
1	G	109	PHE	3.6
3	F	758	GLY	3.6
3	C	792	VAL	3.5
3	I	783	LEU	3.5
3	I	781	VAL	3.4
3	I	756	GLU	3.4
1	A	37	PHE	3.4
3	I	749	ASP	3.3
3	C	783	LEU	3.3
3	I	803	VAL	3.2
3	I	814	GLY	3.2
3	C	762	VAL	3.2
1	G	98	SER	3.2
1	A	110	GLN	3.1
1	A	417	ILE	3.0
1	G	35	ILE	3.0
1	A	100	VAL	3.0
1	G	176	ASP	3.0
3	F	762	VAL	3.0
3	I	750	LEU	2.9
3	C	880	PHE	2.9
1	A	440	MET	2.9
3	I	757	LYS	2.9
3	C	756	GLU	2.8
3	C	775	ILE	2.8
3	I	821	VAL	2.8
1	G	410	PHE	2.8
1	A	424	PRO	2.8
1	A	109	PHE	2.8
3	C	863	PHE	2.8
1	A	38	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	760	CYS	2.7
1	A	97	TYR	2.7
3	F	753	ILE	2.7
1	A	12	ILE	2.7
1	A	25	TYR	2.7
1	G	52	SER	2.6
3	I	795	ARG	2.6
1	G	197	LEU	2.6
1	A	36	VAL	2.6
3	C	875	PHE	2.6
1	G	294	LEU	2.6
3	I	765	PHE	2.6
1	G	295	TYR	2.6
1	G	51	ASP	2.5
3	F	734	ILE	2.5
3	I	799	VAL	2.5
1	D	378	ASP	2.5
3	I	800	ILE	2.5
1	A	439	LEU	2.5
3	I	875	PHE	2.5
1	G	20	SER	2.5
1	G	438	ALA	2.4
1	G	94	PRO	2.4
3	I	876	LYS	2.4
3	I	873	TRP	2.4
3	C	848	TYR	2.4
1	A	381	ILE	2.4
3	I	879	HIS	2.4
1	A	132	PHE	2.4
3	C	739	VAL	2.4
1	A	431	TRP	2.4
1	A	427	ALA	2.3
1	G	19	ALA	2.3
3	I	798	GLU	2.3
3	I	813	GLU	2.3
1	A	360	ILE	2.3
1	A	437	LEU	2.3
3	C	852	LEU	2.3
3	C	777	PHE	2.3
3	I	782	ASN	2.3
1	A	35	ILE	2.2
3	I	842	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	753	ILE	2.2
3	I	848	TYR	2.2
3	C	736	LEU	2.2
3	I	776	TYR	2.2
1	A	27	PHE	2.2
1	A	92	GLU	2.2
1	G	195	TYR	2.1
3	I	820	GLU	2.1
1	A	366	LEU	2.1
1	A	445	LEU	2.1
3	I	802	TYR	2.1
3	C	788	LEU	2.1
1	A	46	TYR	2.1
3	C	734	ILE	2.1
1	D	424	PRO	2.1
1	A	101	GLU	2.1
1	G	16	SER	2.1
3	F	786	LEU	2.1
1	G	13	PHE	2.1
1	A	430	ASN	2.1
1	D	338	ASP	2.1
1	G	21	GLN	2.0
3	F	759	GLU	2.0
3	I	792	VAL	2.0
3	I	791	ILE	2.0
3	C	773	GLY	2.0
3	I	859	GLN	2.0
3	F	736	LEU	2.0
1	A	91	MET	2.0
1	A	4	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.