Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 05:21 PM EST

PDB ID	:	3TDR
Title	:	Crystal structure of HSC at pH 7.5
Authors	:	Czyzewski, B.K.; Wang, D.-N.
Deposited on	:	2011-08-11
Resolution	:	3.20 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

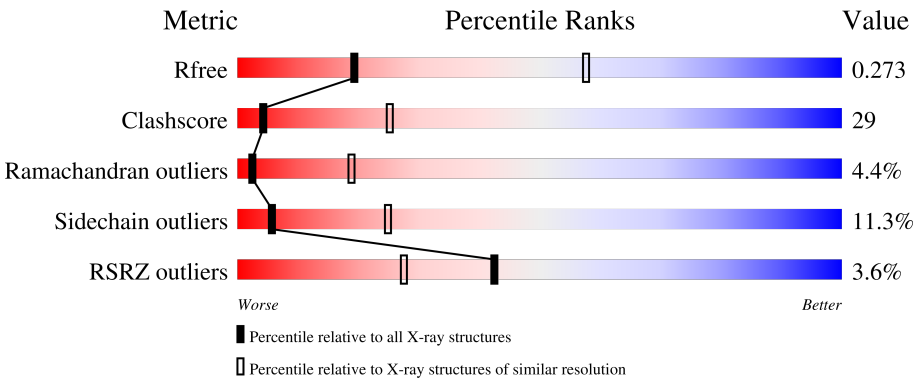
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of 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	268	7% 46% 40% 10% •
1	B	268	8% 37% 51% 7% • •
1	C	268	4% 51% 38% 6% •
1	D	268	6% 41% 47% 7% • •
1	E	268	3% 38% 50% 7% • •

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Mol	Chain	Length	Quality of chain
1	F	268	45% 43% 6%
1	G	268	% 47% 40% 8%
1	H	268	% 39% 46% 9%
1	I	268	% 54% 37%
1	J	268	3% 40% 45% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18927 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 formate/nitrite transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	1886	1238	295	339	14	0	0	0
1	B	256	1890	1241	296	339	14	0	0	0
1	C	257	1898	1247	297	340	14	0	0	0
1	D	256	1890	1241	296	339	14	0	0	0
1	E	256	1890	1241	296	339	14	0	0	0
1	F	256	1886	1238	295	339	14	0	0	0
1	G	256	1890	1241	296	339	14	0	0	0
1	H	256	1890	1241	296	339	14	0	0	0
1	I	256	1890	1241	296	339	14	0	0	0
1	J	256	1890	1241	296	339	14	0	0	0

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q186B7
A	-1	GLY	-	expression tag	UNP Q186B7
A	0	ARG	-	expression tag	UNP Q186B7
A	1	ALA	-	expression tag	UNP Q186B7
A	259	ALA	-	expression tag	UNP Q186B7
A	260	ALA	-	expression tag	UNP Q186B7
A	261	ALA	-	expression tag	UNP Q186B7
A	262	GLU	-	expression tag	UNP Q186B7
A	263	ASN	-	expression tag	UNP Q186B7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	264	LEU	-	expression tag	UNP Q186B7
A	265	TYR	-	expression tag	UNP Q186B7
B	-2	MET	-	expression tag	UNP Q186B7
B	-1	GLY	-	expression tag	UNP Q186B7
B	0	ARG	-	expression tag	UNP Q186B7
B	1	ALA	-	expression tag	UNP Q186B7
B	259	ALA	-	expression tag	UNP Q186B7
B	260	ALA	-	expression tag	UNP Q186B7
B	261	ALA	-	expression tag	UNP Q186B7
B	262	GLU	-	expression tag	UNP Q186B7
B	263	ASN	-	expression tag	UNP Q186B7
B	264	LEU	-	expression tag	UNP Q186B7
B	265	TYR	-	expression tag	UNP Q186B7
C	-2	MET	-	expression tag	UNP Q186B7
C	-1	GLY	-	expression tag	UNP Q186B7
C	0	ARG	-	expression tag	UNP Q186B7
C	1	ALA	-	expression tag	UNP Q186B7
C	259	ALA	-	expression tag	UNP Q186B7
C	260	ALA	-	expression tag	UNP Q186B7
C	261	ALA	-	expression tag	UNP Q186B7
C	262	GLU	-	expression tag	UNP Q186B7
C	263	ASN	-	expression tag	UNP Q186B7
C	264	LEU	-	expression tag	UNP Q186B7
C	265	TYR	-	expression tag	UNP Q186B7
D	-2	MET	-	expression tag	UNP Q186B7
D	-1	GLY	-	expression tag	UNP Q186B7
D	0	ARG	-	expression tag	UNP Q186B7
D	1	ALA	-	expression tag	UNP Q186B7
D	259	ALA	-	expression tag	UNP Q186B7
D	260	ALA	-	expression tag	UNP Q186B7
D	261	ALA	-	expression tag	UNP Q186B7
D	262	GLU	-	expression tag	UNP Q186B7
D	263	ASN	-	expression tag	UNP Q186B7
D	264	LEU	-	expression tag	UNP Q186B7
D	265	TYR	-	expression tag	UNP Q186B7
E	-2	MET	-	expression tag	UNP Q186B7
E	-1	GLY	-	expression tag	UNP Q186B7
E	0	ARG	-	expression tag	UNP Q186B7
E	1	ALA	-	expression tag	UNP Q186B7
E	259	ALA	-	expression tag	UNP Q186B7
E	260	ALA	-	expression tag	UNP Q186B7
E	261	ALA	-	expression tag	UNP Q186B7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	262	GLU	-	expression tag	UNP Q186B7
E	263	ASN	-	expression tag	UNP Q186B7
E	264	LEU	-	expression tag	UNP Q186B7
E	265	TYR	-	expression tag	UNP Q186B7
F	-2	MET	-	expression tag	UNP Q186B7
F	-1	GLY	-	expression tag	UNP Q186B7
F	0	ARG	-	expression tag	UNP Q186B7
F	1	ALA	-	expression tag	UNP Q186B7
F	259	ALA	-	expression tag	UNP Q186B7
F	260	ALA	-	expression tag	UNP Q186B7
F	261	ALA	-	expression tag	UNP Q186B7
F	262	GLU	-	expression tag	UNP Q186B7
F	263	ASN	-	expression tag	UNP Q186B7
F	264	LEU	-	expression tag	UNP Q186B7
F	265	TYR	-	expression tag	UNP Q186B7
G	-2	MET	-	expression tag	UNP Q186B7
G	-1	GLY	-	expression tag	UNP Q186B7
G	0	ARG	-	expression tag	UNP Q186B7
G	1	ALA	-	expression tag	UNP Q186B7
G	259	ALA	-	expression tag	UNP Q186B7
G	260	ALA	-	expression tag	UNP Q186B7
G	261	ALA	-	expression tag	UNP Q186B7
G	262	GLU	-	expression tag	UNP Q186B7
G	263	ASN	-	expression tag	UNP Q186B7
G	264	LEU	-	expression tag	UNP Q186B7
G	265	TYR	-	expression tag	UNP Q186B7
H	-2	MET	-	expression tag	UNP Q186B7
H	-1	GLY	-	expression tag	UNP Q186B7
H	0	ARG	-	expression tag	UNP Q186B7
H	1	ALA	-	expression tag	UNP Q186B7
H	259	ALA	-	expression tag	UNP Q186B7
H	260	ALA	-	expression tag	UNP Q186B7
H	261	ALA	-	expression tag	UNP Q186B7
H	262	GLU	-	expression tag	UNP Q186B7
H	263	ASN	-	expression tag	UNP Q186B7
H	264	LEU	-	expression tag	UNP Q186B7
H	265	TYR	-	expression tag	UNP Q186B7
I	-2	MET	-	expression tag	UNP Q186B7
I	-1	GLY	-	expression tag	UNP Q186B7
I	0	ARG	-	expression tag	UNP Q186B7
I	1	ALA	-	expression tag	UNP Q186B7
I	259	ALA	-	expression tag	UNP Q186B7

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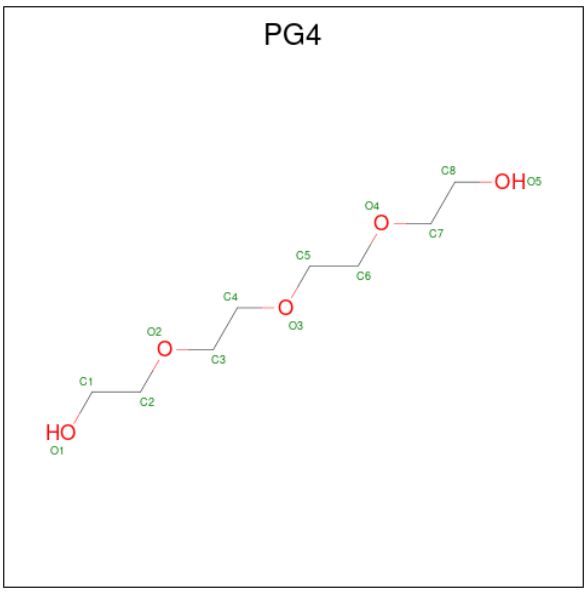
Chain	Residue	Modelled	Actual	Comment	Reference
I	260	ALA	-	expression tag	UNP Q186B7
I	261	ALA	-	expression tag	UNP Q186B7
I	262	GLU	-	expression tag	UNP Q186B7
I	263	ASN	-	expression tag	UNP Q186B7
I	264	LEU	-	expression tag	UNP Q186B7
I	265	TYR	-	expression tag	UNP Q186B7
J	-2	MET	-	expression tag	UNP Q186B7
J	-1	GLY	-	expression tag	UNP Q186B7
J	0	ARG	-	expression tag	UNP Q186B7
J	1	ALA	-	expression tag	UNP Q186B7
J	259	ALA	-	expression tag	UNP Q186B7
J	260	ALA	-	expression tag	UNP Q186B7
J	261	ALA	-	expression tag	UNP Q186B7
J	262	GLU	-	expression tag	UNP Q186B7
J	263	ASN	-	expression tag	UNP Q186B7
J	264	LEU	-	expression tag	UNP Q186B7
J	265	TYR	-	expression tag	UNP Q186B7

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	I	1	13	8	5	0	0

- Molecule 3 is water.

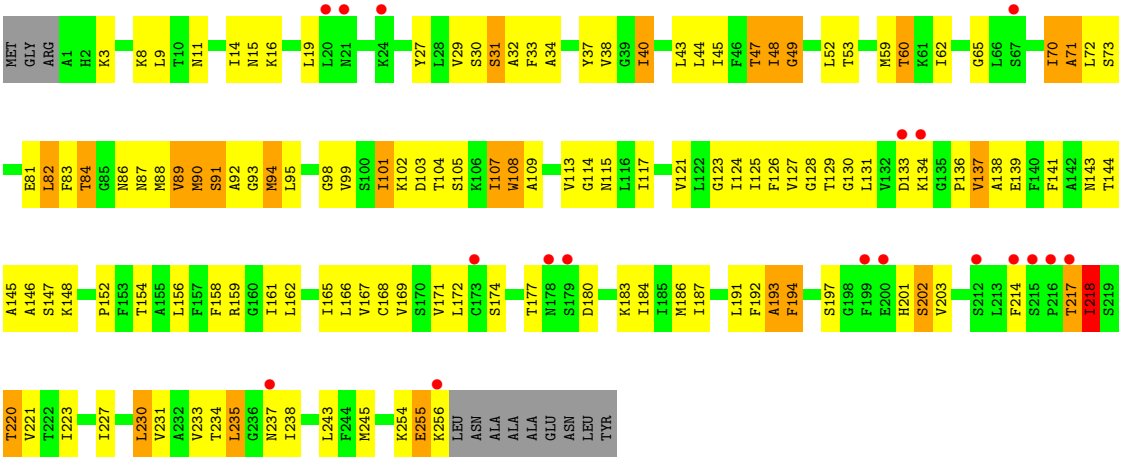
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	2	2	2	0	0
			Total	O		
3	E	1	1	1	0	0
			Total	O		
3	F	3	3	3	0	0
			Total	O		
3	H	1	1	1	0	0
			Total	O		
3	I	6	6	6	0	0
			Total	O		
3	J	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

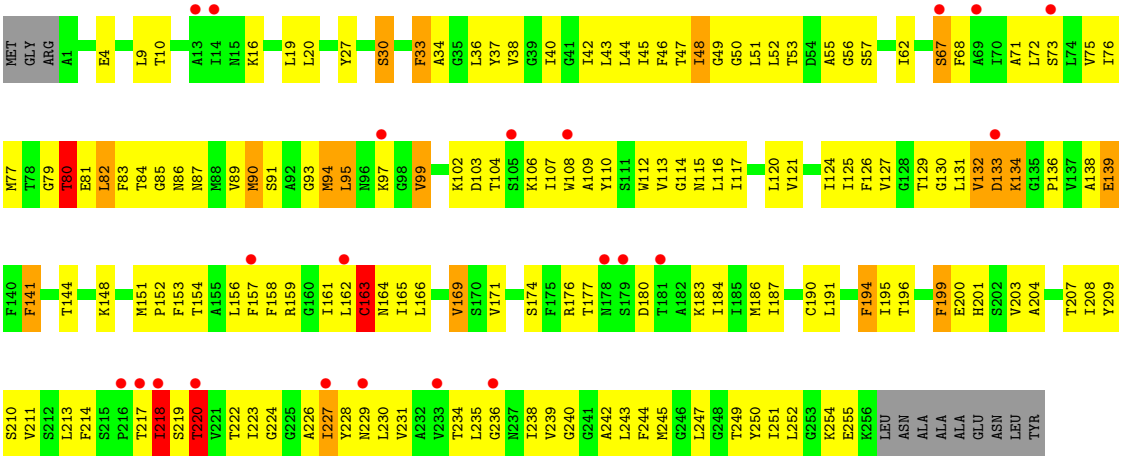
- Molecule 1: formate/nitrite transporter

Chain A:



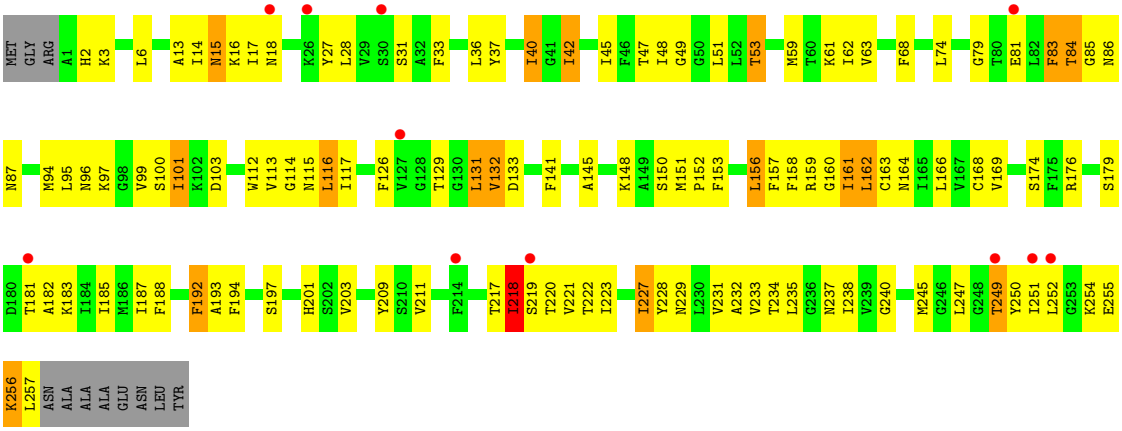
- Molecule 1: formate/nitrite transporter

Chain B:



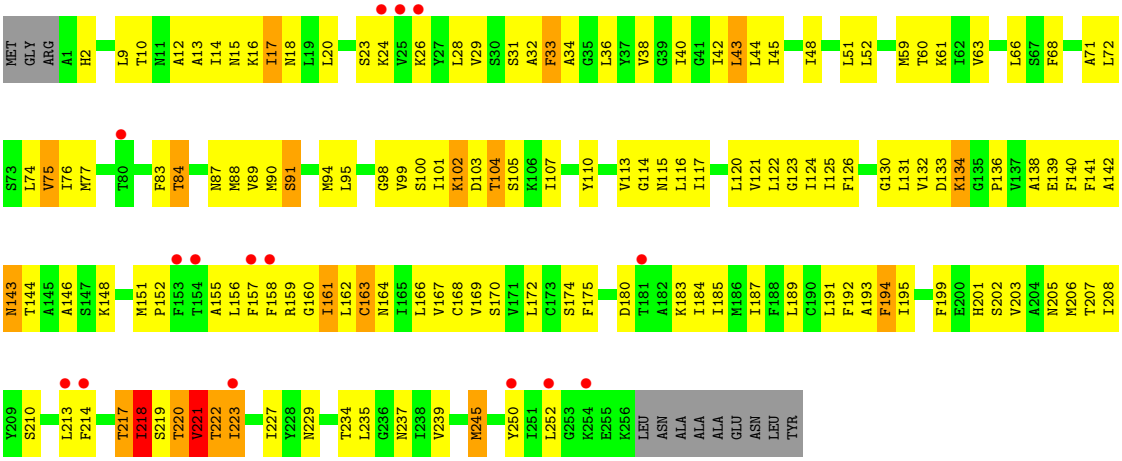
- Molecule 1: formate/nitrite transporter

Chain C:



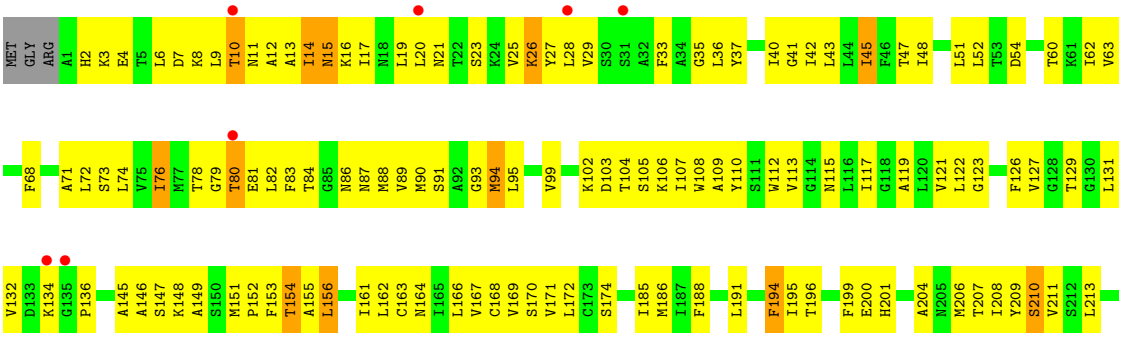
• Molecule 1: formate/nitrite transporter

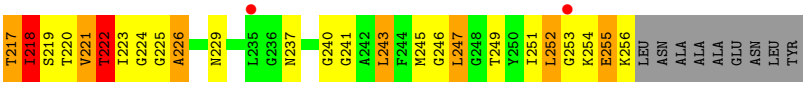
Chain D:



• Molecule 1: formate/nitrite transporter

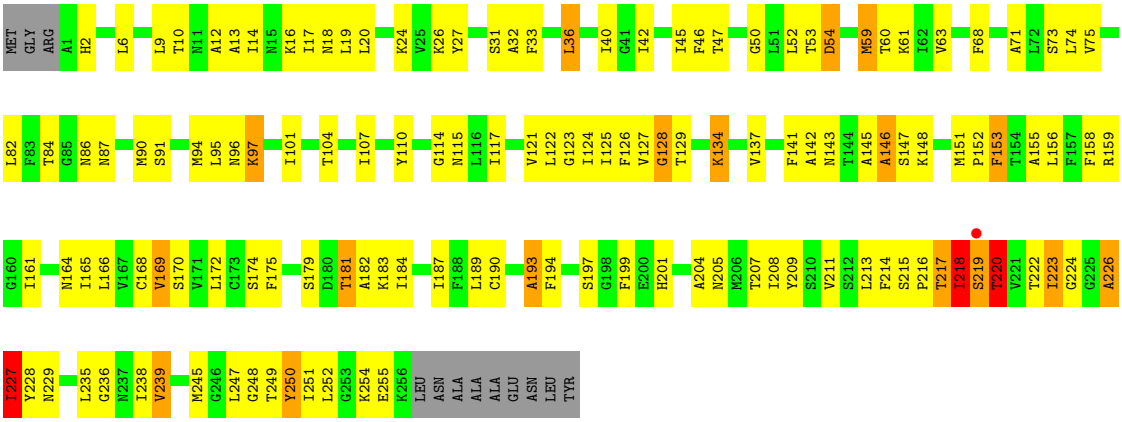
Chain E:





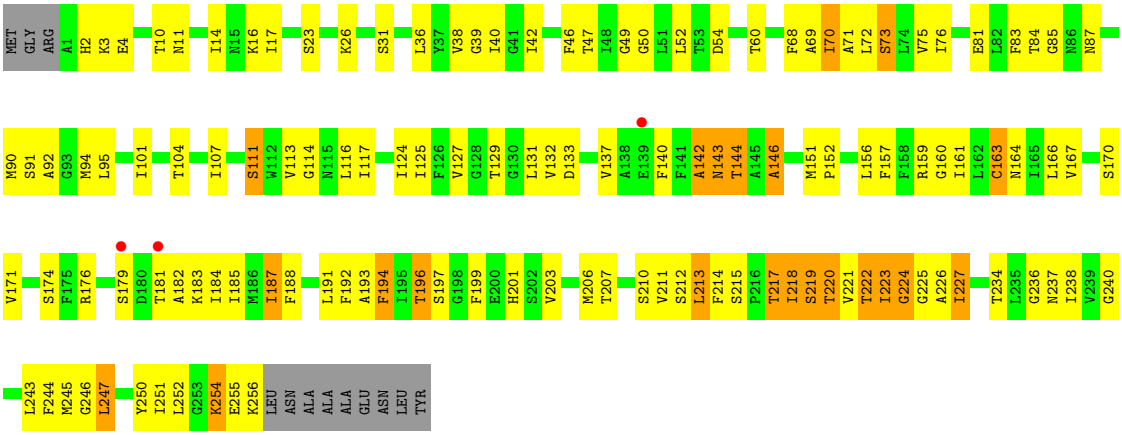
• Molecule 1: formate/nitrite transporter

Chain F:



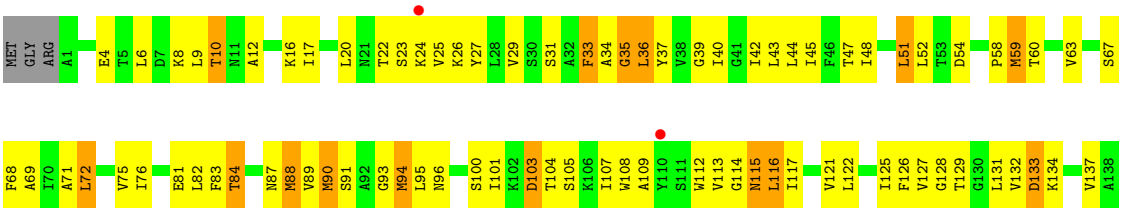
• Molecule 1: formate/nitrite transporter

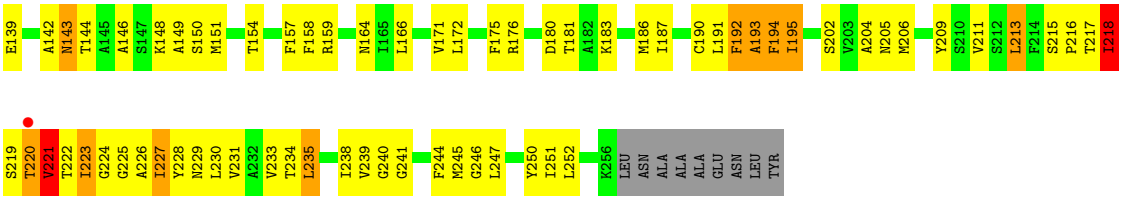
Chain G:



• Molecule 1: formate/nitrite transporter

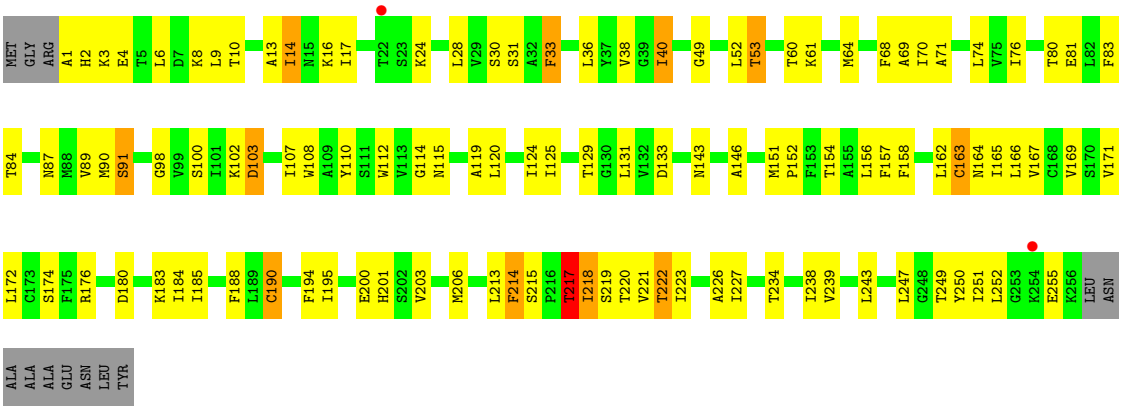
Chain H:





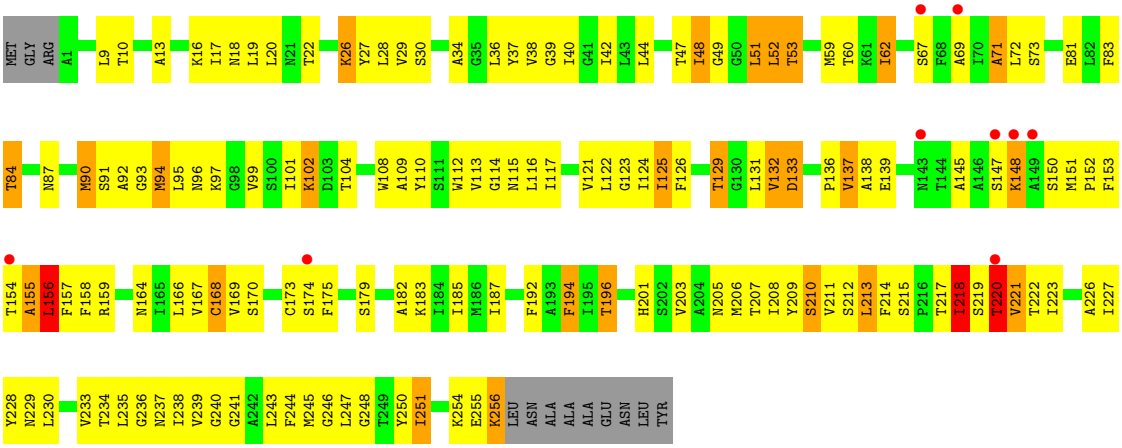
• Molecule 1: formate/nitrite transporter

Chain I:



• Molecule 1: formate/nitrite transporter

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.89Å 101.61Å 168.36Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	48.38 – 3.20 49.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.38-3.20) 93.5 (49.12-3.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.187 , 0.279 0.188 , 0.273	Depositor DCC
R_{free} test set	2686 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	79.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 93.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18927	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4

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	0.30	0/1918	0.51	0/2601
1	B	0.33	0/1922	0.55	2/2605 (0.1%)
1	C	0.36	0/1930	0.56	0/2616
1	D	0.36	0/1922	0.55	0/2605
1	E	0.38	0/1922	0.56	0/2605
1	F	0.47	0/1918	0.65	0/2601
1	G	0.43	0/1922	0.63	1/2605 (0.0%)
1	H	0.42	0/1922	0.60	0/2605
1	I	0.50	0/1922	0.69	1/2605 (0.0%)
1	J	0.41	0/1922	0.59	0/2605
All	All	0.40	0/19220	0.59	4/26053 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	I	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	222	THR	N-CA-CB	-6.64	97.68	110.30
1	G	222	THR	N-CA-CB	5.47	120.69	110.30
1	B	222	THR	N-CA-C	5.06	124.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	190	CYS	CB-CA-C	5.01	120.43	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	ILE	Peptide
1	B	220	THR	Peptide
1	I	217	THR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1886	0	1983	116	0
1	B	1890	0	1994	139	0
1	C	1898	0	2005	107	0
1	D	1890	0	1994	120	0
1	E	1890	0	1994	129	0
1	F	1886	0	1983	114	0
1	G	1890	0	1994	123	0
1	H	1890	0	1994	140	0
1	I	1890	0	1994	94	0
1	J	1890	0	1994	149	0
2	I	13	0	17	5	0
3	C	2	0	0	1	0
3	E	1	0	0	0	0
3	F	3	0	0	0	0
3	H	1	0	0	0	0
3	I	6	0	0	0	0
3	J	1	0	0	0	0
All	All	18927	0	19946	1139	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 29.

All (1139) 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:H:223:ILE:CG2	1:H:227:ILE:HD11	1.76	1.13
1:B:223:ILE:O	1:B:227:ILE:HG22	1.49	1.12
1:H:223:ILE:HG22	1:H:227:ILE:HD11	1.27	1.07
1:J:126:PHE:O	1:J:129:THR:OG1	1.72	1.06
1:B:90:MET:HE2	1:B:104:THR:HA	1.38	1.05
1:I:221:VAL:HG23	1:I:222:THR:H	1.22	1.01
1:E:223:ILE:HD12	1:E:223:ILE:H	1.28	0.98
1:C:151:MET:SD	1:C:159:ARG:NH1	2.38	0.96
1:E:42:ILE:HD11	1:E:204:ALA:HB1	1.46	0.95
1:F:126:PHE:O	1:F:129:THR:OG1	1.87	0.91
1:F:217:THR:O	1:F:218:ILE:HG23	1.69	0.91
1:D:160:GLY:O	1:D:237:ASN:ND2	2.03	0.91
1:H:223:ILE:HG22	1:H:227:ILE:CD1	2.00	0.91
1:F:24:LYS:HE2	1:F:110:TYR:HE2	1.37	0.90
1:G:223:ILE:HD12	1:G:223:ILE:H	1.34	0.90
1:I:219:SER:HB3	1:I:221:VAL:HG22	1.54	0.90
1:A:40:ILE:HG21	1:D:166:LEU:HD21	1.52	0.89
1:E:10:THR:HG23	1:E:93:GLY:HA2	1.57	0.87
1:B:38:VAL:HA	1:B:71:ALA:HB1	1.56	0.87
1:J:151:MET:HG2	1:J:152:PRO:HD2	1.54	0.87
1:C:100:SER:OG	1:C:103:ASP:OD1	1.91	0.86
1:G:193:ALA:HA	1:J:44:LEU:HD13	1.55	0.86
1:H:126:PHE:O	1:H:129:THR:OG1	1.91	0.86
1:J:226:ALA:O	1:J:230:LEU:HG	1.75	0.86
1:J:222:THR:C	1:J:223:ILE:HD12	1.96	0.85
1:E:41:GLY:O	1:E:45:ILE:HG23	1.77	0.85
1:F:24:LYS:HE2	1:F:110:TYR:CE2	2.12	0.84
1:A:159:ARG:HG2	1:B:129:THR:HB	1.57	0.84
1:J:164:ASN:O	1:J:168:CYS:HB2	1.78	0.84
1:C:159:ARG:HH21	1:D:131:LEU:HD23	1.41	0.84
1:G:94:MET:HG2	1:G:95:LEU:HD23	1.58	0.84
1:A:193:ALA:HA	1:B:44:LEU:HD13	1.58	0.84
1:A:167:VAL:O	1:A:171:VAL:HG23	1.77	0.83
1:E:90:MET:HE2	1:E:104:THR:HA	1.59	0.82
1:H:223:ILE:O	1:H:225:GLY:N	2.12	0.82
1:C:129:THR:HB	1:C:131:LEU:HD12	1.62	0.81
1:B:223:ILE:O	1:B:227:ILE:CG2	2.28	0.81
1:B:157:PHE:CZ	1:B:161:ILE:HD11	2.16	0.81
1:H:23:SER:HB2	1:J:256:LYS:NZ	1.94	0.81
1:A:9:LEU:HD23	1:A:89:VAL:HG22	1.62	0.81
1:G:201:HIS:HE1	1:G:203:VAL:HB	1.46	0.81
1:B:109:ALA:O	1:B:113:VAL:HG23	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:VAL:HG23	1:E:245:MET:HE2	1.64	0.80
1:B:42:ILE:HD11	1:B:204:ALA:HB1	1.64	0.80
1:A:30:SER:HB2	1:D:252:LEU:HD21	1.62	0.80
1:D:72:LEU:HD23	1:D:187:ILE:HG23	1.61	0.80
1:D:146:ALA:HA	1:D:221:VAL:CG1	2.12	0.80
1:D:121:VAL:O	1:D:125:ILE:HG13	1.82	0.79
1:I:61:LYS:HD3	2:I:266:PG4:H31	1.63	0.79
1:I:124:ILE:HG13	1:I:214:PHE:CE2	2.16	0.79
1:C:218:ILE:HG22	3:C:266:HOH:O	1.81	0.79
1:G:201:HIS:CE1	1:G:203:VAL:HB	2.17	0.79
1:C:84:THR:HB	1:C:164:ASN:OD1	1.82	0.79
1:I:219:SER:HB3	1:I:221:VAL:CG2	2.12	0.79
1:G:159:ARG:HG2	1:J:129:THR:HG22	1.65	0.79
1:H:10:THR:HG23	1:H:93:GLY:HA2	1.64	0.78
1:G:140:PHE:O	1:G:144:THR:OG1	2.01	0.78
1:G:223:ILE:O	1:G:226:ALA:N	2.14	0.78
1:G:68:PHE:CD2	1:G:191:LEU:HD23	2.18	0.78
1:G:234:THR:O	1:G:238:ILE:HG13	1.84	0.77
1:I:221:VAL:HG23	1:I:222:THR:N	2.00	0.77
1:E:149:ALA:HB1	1:E:225:GLY:HA3	1.66	0.77
1:G:254:LYS:HE2	1:G:255:GLU:H	1.50	0.77
1:A:171:VAL:O	1:A:174:SER:OG	2.04	0.76
1:C:48:ILE:HG23	1:E:62:ILE:HD11	1.67	0.76
1:F:205:ASN:HA	1:F:208:ILE:HD12	1.68	0.76
1:C:94:MET:SD	1:C:101:ILE:HG13	2.26	0.75
1:A:223:ILE:HG22	1:A:227:ILE:HD11	1.68	0.74
1:F:84:THR:HG21	1:F:201:HIS:CD2	2.21	0.74
1:G:217:THR:O	1:G:217:THR:OG1	2.04	0.74
1:H:133:ASP:O	1:H:217:THR:OG1	2.05	0.74
1:D:130:GLY:O	1:D:133:ASP:HB2	1.87	0.74
1:I:87:ASN:O	1:I:91:SER:HB2	1.86	0.74
1:C:45:ILE:HD13	1:C:68:PHE:CD1	2.23	0.74
1:F:218:ILE:O	1:F:219:SER:HB2	1.86	0.74
1:A:166:LEU:HD12	1:A:194:PHE:HB3	1.70	0.73
1:B:184:ILE:HA	1:B:187:ILE:HD12	1.70	0.73
1:E:42:ILE:HG21	1:E:208:ILE:HG12	1.69	0.73
1:D:91:SER:O	1:D:95:LEU:HG	1.89	0.73
1:B:166:LEU:HD21	1:E:40:ILE:HG21	1.70	0.73
1:D:146:ALA:HA	1:D:221:VAL:HG11	1.68	0.73
1:A:31:SER:HB2	1:A:114:GLY:HA3	1.69	0.73
1:H:23:SER:HB2	1:J:256:LYS:HZ1	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:223:ILE:H	1:H:223:ILE:HD12	1.52	0.73
1:J:201:HIS:CE1	1:J:203:VAL:HB	2.24	0.73
1:G:167:VAL:O	1:G:171:VAL:HG23	1.86	0.73
1:C:183:LYS:O	1:C:187:ILE:HG13	1.88	0.73
1:E:219:SER:OG	1:E:221:VAL:HG23	1.88	0.72
1:F:101:ILE:H	1:F:101:ILE:HD12	1.53	0.72
1:F:159:ARG:HG2	1:G:129:THR:HB	1.70	0.72
1:G:250:TYR:OH	1:G:254:LYS:HD3	1.89	0.72
1:H:35:GLY:H	1:H:115:ASN:ND2	1.87	0.72
1:H:109:ALA:O	1:H:113:VAL:HG23	1.90	0.72
1:H:217:THR:O	1:H:218:ILE:HB	1.87	0.72
1:G:114:GLY:HA2	1:G:117:ILE:HD12	1.70	0.72
1:E:166:LEU:O	1:E:169:VAL:HG12	1.90	0.72
1:F:46:PHE:CE2	1:F:208:ILE:HG12	2.25	0.72
1:B:43:LEU:O	1:B:47:THR:OG1	2.06	0.72
1:D:42:ILE:HD13	1:D:45:ILE:HD11	1.72	0.71
1:E:28:LEU:HD21	1:E:110:TYR:HD1	1.54	0.71
1:H:125:ILE:HG23	1:J:158:PHE:HD2	1.53	0.71
1:C:151:MET:HG3	1:C:152:PRO:HD2	1.72	0.71
1:D:223:ILE:O	1:D:227:ILE:HG12	1.90	0.71
1:H:95:LEU:HB3	1:H:250:TYR:CD2	2.25	0.71
1:E:84:THR:HA	1:E:87:ASN:ND2	2.05	0.71
1:G:187:ILE:O	1:G:191:LEU:HD13	1.91	0.71
1:C:234:THR:O	1:C:238:ILE:HG13	1.90	0.71
1:B:36:LEU:O	1:B:40:ILE:HG13	1.90	0.71
1:D:76:ILE:HD12	1:D:187:ILE:HD11	1.72	0.71
1:H:226:ALA:O	1:H:230:LEU:HG	1.91	0.71
1:J:223:ILE:O	1:J:227:ILE:HG12	1.91	0.70
1:C:159:ARG:HE	1:D:131:LEU:HD21	1.57	0.70
1:J:72:LEU:HD23	1:J:187:ILE:HG23	1.72	0.70
1:J:207:THR:O	1:J:211:VAL:HG23	1.92	0.70
1:A:217:THR:O	1:A:218:ILE:HG23	1.91	0.70
1:E:76:ILE:HD11	1:E:171:VAL:HG22	1.73	0.70
1:D:31:SER:HB2	1:D:114:GLY:HA3	1.73	0.70
1:I:24:LYS:HE3	1:I:110:TYR:OH	1.91	0.70
1:C:115:ASN:HB3	1:C:203:VAL:HG13	1.72	0.70
1:G:250:TYR:CZ	1:G:254:LYS:HD3	2.26	0.70
1:E:52:LEU:HB3	1:E:60:THR:OG1	1.90	0.70
1:C:17:ILE:HG12	1:C:103:ASP:HB3	1.74	0.69
1:G:222:THR:HB	1:G:223:ILE:HD12	1.74	0.69
1:A:223:ILE:CG2	1:A:227:ILE:HD11	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:O	1:A:109:ALA:N	2.26	0.69
1:J:10:THR:O	1:J:13:ALA:HB3	1.92	0.69
1:J:132:VAL:HA	1:J:138:ALA:HB2	1.72	0.69
1:H:87:ASN:OD1	1:H:238:ILE:HA	1.92	0.69
1:H:117:ILE:O	1:H:121:VAL:HG23	1.93	0.69
1:H:48:ILE:HG12	1:J:62:ILE:HD13	1.73	0.69
1:B:217:THR:O	1:B:218:ILE:HB	1.91	0.69
1:J:83:PHE:CE2	1:J:112:TRP:HD1	2.10	0.69
1:C:218:ILE:HG13	1:C:220:THR:HG23	1.74	0.69
1:G:16:LYS:NZ	1:G:81:GLU:OE2	2.26	0.69
1:H:75:VAL:HG11	1:H:82:LEU:HB2	1.74	0.69
1:H:211:VAL:O	1:H:215:SER:HB2	1.93	0.68
1:B:108:TRP:O	1:B:112:TRP:HB2	1.94	0.68
1:F:143:ASN:O	1:F:146:ALA:HB3	1.94	0.68
1:C:94:MET:O	1:C:97:LYS:N	2.25	0.68
1:F:151:MET:HG3	1:F:152:PRO:HD2	1.75	0.68
1:A:89:VAL:O	1:A:91:SER:N	2.27	0.68
1:B:129:THR:OG1	1:B:131:LEU:HG	1.93	0.68
1:A:177:THR:OG1	1:B:180:ASP:OD2	2.06	0.68
1:F:42:ILE:HD11	1:F:204:ALA:HB1	1.74	0.68
1:J:240:GLY:O	1:J:244:PHE:HB2	1.94	0.68
1:D:140:PHE:O	1:D:144:THR:OG1	2.11	0.68
1:G:223:ILE:H	1:G:223:ILE:CD1	2.06	0.68
1:J:124:ILE:HG12	1:J:214:PHE:CE2	2.29	0.68
1:A:166:LEU:O	1:A:169:VAL:HG12	1.95	0.67
1:D:34:ALA:O	1:D:38:VAL:HG23	1.94	0.67
1:E:218:ILE:HG21	1:G:218:ILE:O	1.94	0.67
1:H:159:ARG:HG2	1:I:129:THR:HB	1.75	0.67
1:B:226:ALA:O	1:B:230:LEU:HG	1.94	0.67
1:A:166:LEU:HA	1:A:169:VAL:HG12	1.76	0.67
1:E:218:ILE:HD13	1:G:218:ILE:HA	1.77	0.67
1:J:69:ALA:O	1:J:73:SER:HB2	1.94	0.67
1:B:34:ALA:HB2	1:B:80:THR:OG1	1.94	0.67
1:D:217:THR:O	1:D:217:THR:OG1	2.09	0.67
1:J:72:LEU:HD13	1:J:167:VAL:HG13	1.76	0.67
1:F:145:ALA:HB1	1:F:209:TYR:CE1	2.30	0.67
1:B:112:TRP:HE1	1:B:234:THR:CG2	2.08	0.67
1:G:72:LEU:HD23	1:G:187:ILE:HG23	1.76	0.67
1:I:234:THR:O	1:I:238:ILE:HG13	1.95	0.67
1:B:36:LEU:HD21	1:B:40:ILE:HD11	1.75	0.66
1:B:243:LEU:O	1:B:247:LEU:HB3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:LEU:O	1:D:120:LEU:HG	1.95	0.66
1:J:51:LEU:HD12	1:J:51:LEU:H	1.60	0.66
1:B:112:TRP:HE1	1:B:234:THR:HG21	1.60	0.66
1:C:112:TRP:HE1	1:C:234:THR:HG1	1.42	0.66
1:E:6:LEU:HD23	1:E:253:GLY:O	1.96	0.66
1:J:18:ASN:O	1:J:22:THR:OG1	2.05	0.66
1:D:10:THR:O	1:D:14:ILE:HD12	1.96	0.66
1:D:114:GLY:HA2	1:D:117:ILE:HD12	1.76	0.66
1:H:44:LEU:HD12	1:H:44:LEU:O	1.96	0.66
1:B:20:LEU:HD21	1:B:110:TYR:CD2	2.31	0.65
1:D:124:ILE:HG13	1:D:214:PHE:CE2	2.32	0.65
1:A:94:MET:HA	1:A:99:VAL:O	1.96	0.65
1:C:223:ILE:H	1:C:223:ILE:HD12	1.61	0.65
1:J:151:MET:SD	1:J:156:LEU:HD23	2.36	0.65
1:F:226:ALA:O	1:F:228:TYR:N	2.30	0.65
1:B:48:ILE:O	1:B:51:LEU:N	2.29	0.65
1:F:75:VAL:HG11	1:F:82:LEU:HB2	1.78	0.65
1:H:12:ALA:O	1:H:16:LYS:HG3	1.96	0.65
1:J:47:THR:HA	1:J:137:VAL:CG1	2.26	0.65
1:A:83:PHE:O	1:A:87:ASN:ND2	2.30	0.65
1:H:129:THR:HB	1:J:159:ARG:HD3	1.77	0.65
1:H:240:GLY:O	1:H:244:PHE:HB2	1.96	0.65
1:I:215:SER:OG	1:I:217:THR:HG23	1.97	0.65
1:F:40:ILE:HG21	1:I:166:LEU:HD21	1.78	0.64
1:G:151:MET:HG2	1:G:152:PRO:HD2	1.78	0.64
1:C:245:MET:O	1:C:249:THR:OG1	2.15	0.64
1:D:68:PHE:CD2	1:D:191:LEU:HD23	2.33	0.64
1:I:31:SER:HB2	1:I:114:GLY:HA3	1.79	0.64
1:B:190:CYS:SG	1:E:74:LEU:HD21	2.38	0.64
1:F:217:THR:O	1:F:217:THR:OG1	2.14	0.64
1:J:122:LEU:HA	1:J:125:ILE:HG13	1.78	0.64
1:G:192:PHE:O	1:G:196:THR:OG1	2.12	0.64
1:D:12:ALA:O	1:D:16:LYS:HG3	1.98	0.64
1:B:83:PHE:CE2	1:B:112:TRP:HD1	2.16	0.63
1:F:84:THR:HA	1:F:87:ASN:ND2	2.13	0.63
1:J:239:VAL:O	1:J:243:LEU:HB3	1.97	0.63
1:D:187:ILE:O	1:D:191:LEU:HD13	1.99	0.63
1:A:169:VAL:HG21	1:B:37:TYR:CE1	2.33	0.63
1:C:84:THR:HG21	1:C:201:HIS:CD2	2.33	0.63
1:C:129:THR:CB	1:C:131:LEU:HD12	2.28	0.63
1:B:55:ALA:O	1:B:57:SER:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:THR:O	1:C:185:ILE:HG13	1.99	0.63
1:E:33:PHE:HB3	1:E:80:THR:HG21	1.79	0.63
1:B:162:LEU:O	1:B:165:ILE:HB	1.97	0.63
1:C:161:ILE:O	1:C:164:ASN:N	2.32	0.63
1:E:223:ILE:H	1:E:223:ILE:CD1	2.04	0.63
1:B:127:VAL:O	1:B:130:GLY:N	2.31	0.63
1:I:14:ILE:HD11	1:I:98:GLY:HA3	1.81	0.62
1:A:62:ILE:HD11	1:B:48:ILE:HG23	1.80	0.62
1:I:61:LYS:CE	2:I:266:PG4:H22	2.29	0.62
1:J:91:SER:OG	1:J:246:GLY:HA3	1.98	0.62
1:G:23:SER:HB3	1:G:26:LYS:HB2	1.81	0.62
1:J:145:ALA:HB1	1:J:209:TYR:CE1	2.34	0.62
1:C:159:ARG:HH21	1:D:131:LEU:CD2	2.10	0.62
1:B:161:ILE:HA	1:B:236:GLY:O	1.99	0.62
1:G:254:LYS:HE2	1:G:255:GLU:N	2.14	0.62
1:B:157:PHE:CE2	1:B:161:ILE:HD11	2.34	0.62
1:E:117:ILE:O	1:E:121:VAL:HG23	1.99	0.62
1:G:171:VAL:O	1:G:174:SER:HB3	1.99	0.62
1:A:136:PRO:HA	1:A:139:GLU:HB2	1.82	0.61
1:B:245:MET:O	1:B:249:THR:HG23	2.00	0.61
1:G:223:ILE:O	1:G:225:GLY:N	2.33	0.61
1:I:61:LYS:CD	2:I:266:PG4:H31	2.29	0.61
1:J:235:LEU:O	1:J:239:VAL:HG23	1.98	0.61
1:G:220:THR:O	1:G:221:VAL:HG13	2.00	0.61
1:A:27:TYR:O	1:A:31:SER:OG	2.19	0.61
1:H:42:ILE:HD11	1:H:204:ALA:HB1	1.82	0.61
1:I:84:THR:HB	1:I:164:ASN:OD1	2.00	0.61
1:C:160:GLY:O	1:C:237:ASN:ND2	2.31	0.61
1:C:223:ILE:HD12	1:C:223:ILE:N	2.15	0.61
1:I:87:ASN:H	1:I:87:ASN:HD22	1.49	0.61
1:B:171:VAL:O	1:B:174:SER:HB3	2.01	0.61
1:J:113:VAL:O	1:J:117:ILE:HG13	2.01	0.61
1:F:247:LEU:O	1:F:250:TYR:HB3	2.01	0.61
1:G:157:PHE:CE2	1:G:161:ILE:HD11	2.35	0.61
1:I:28:LEU:HD21	1:I:110:TYR:HD2	1.66	0.61
1:A:158:PHE:CD1	1:A:161:ILE:HD12	2.36	0.61
1:B:36:LEU:HD23	1:B:37:TYR:N	2.15	0.61
1:B:234:THR:O	1:B:238:ILE:HG13	2.00	0.61
1:H:223:ILE:HG22	1:H:227:ILE:CG1	2.30	0.61
1:A:183:LYS:O	1:A:187:ILE:HG13	2.01	0.61
1:F:16:LYS:NZ	1:F:86:ASN:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:93:GLY:O	1:J:97:LYS:N	2.33	0.61
1:C:2:HIS:CD2	1:C:252:LEU:HD22	2.35	0.60
1:C:45:ILE:HA	1:C:48:ILE:HD12	1.83	0.60
1:H:88:MET:HG3	1:H:245:MET:HB3	1.82	0.60
1:C:81:GLU:OE1	1:C:86:ASN:ND2	2.34	0.60
1:H:116:LEU:O	1:H:116:LEU:HD12	2.01	0.60
1:H:59:MET:O	1:H:63:VAL:HG23	2.01	0.60
1:A:202:SER:OG	1:A:237:ASN:ND2	2.34	0.60
1:F:87:ASN:HD22	1:F:164:ASN:HD21	1.50	0.60
1:G:184:ILE:HA	1:G:187:ILE:HG13	1.84	0.60
1:G:191:LEU:HD12	1:G:191:LEU:N	2.16	0.60
1:H:40:ILE:HG21	1:J:166:LEU:HD21	1.84	0.60
1:J:205:ASN:HA	1:J:208:ILE:HG13	1.83	0.60
1:G:185:ILE:O	1:G:188:PHE:HB3	2.02	0.60
1:H:39:GLY:HA3	1:H:122:LEU:HD23	1.84	0.60
1:A:143:ASN:O	1:A:147:SER:N	2.28	0.60
1:B:159:ARG:HG2	1:E:129:THR:HB	1.84	0.60
1:F:10:THR:O	1:F:14:ILE:HD12	2.00	0.60
1:G:151:MET:HB3	1:G:156:LEU:HD21	1.84	0.60
1:D:183:LYS:O	1:D:187:ILE:HG13	2.01	0.60
1:F:153:PHE:CD1	1:F:153:PHE:C	2.75	0.60
1:J:221:VAL:O	1:J:222:THR:OG1	2.18	0.60
1:J:211:VAL:O	1:J:215:SER:HB2	2.02	0.60
1:J:109:ALA:O	1:J:113:VAL:HG23	2.02	0.59
1:J:250:TYR:CZ	1:J:254:LYS:HG2	2.37	0.59
1:J:256:LYS:HD3	1:J:256:LYS:N	2.16	0.59
1:B:38:VAL:HA	1:B:71:ALA:CB	2.30	0.59
1:E:129:THR:OG1	1:E:131:LEU:HG	2.03	0.59
1:H:166:LEU:HD21	1:I:40:ILE:HG21	1.83	0.59
1:J:234:THR:O	1:J:238:ILE:HG13	2.02	0.59
1:E:43:LEU:HD11	1:E:122:LEU:HD21	1.84	0.59
1:F:183:LYS:O	1:F:187:ILE:HG13	2.03	0.59
1:J:34:ALA:O	1:J:38:VAL:HG23	2.02	0.59
1:D:83:PHE:CE2	1:D:234:THR:HG23	2.38	0.59
1:G:2:HIS:ND1	1:G:252:LEU:HB3	2.18	0.59
1:H:172:LEU:O	1:H:176:ARG:HG3	2.03	0.59
1:J:209:TYR:O	1:J:212:SER:N	2.36	0.59
1:J:248:GLY:HA2	1:J:251:ILE:HG13	1.83	0.59
1:J:9:LEU:HD23	1:J:175:PHE:HE2	1.66	0.59
1:A:223:ILE:O	1:A:227:ILE:HG12	2.03	0.59
1:D:113:VAL:O	1:D:117:ILE:HG13	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:LEU:O	1:E:40:ILE:HG12	2.03	0.59
1:E:145:ALA:HB1	1:E:209:TYR:CD1	2.38	0.59
1:H:47:THR:HA	1:H:137:VAL:HG22	1.83	0.59
1:J:87:ASN:OD1	1:J:238:ILE:HA	2.03	0.59
1:B:34:ALA:O	1:B:38:VAL:HG23	2.03	0.58
1:B:209:TYR:OH	1:B:229:ASN:ND2	2.23	0.58
1:E:3:LYS:NZ	1:E:7:ASP:OD2	2.32	0.58
1:E:23:SER:CB	1:E:26:LYS:HB2	2.33	0.58
1:E:54:ASP:OD2	1:E:136:PRO:HG3	2.04	0.58
1:E:164:ASN:HD22	1:E:241:GLY:H	1.51	0.58
1:H:223:ILE:C	1:H:225:GLY:H	2.06	0.58
1:J:136:PRO:HA	1:J:139:GLU:HB2	1.84	0.58
1:B:247:LEU:O	1:B:251:ILE:HG13	2.04	0.58
1:D:194:PHE:HA	1:D:199:PHE:CD2	2.38	0.58
1:F:161:ILE:HG12	1:F:239:VAL:HG12	1.85	0.58
1:B:10:THR:HG22	1:B:93:GLY:HA2	1.86	0.58
1:I:61:LYS:HE2	2:I:266:PG4:H22	1.85	0.58
1:A:192:PHE:CE2	1:B:67:SER:HB3	2.38	0.58
1:C:3:LYS:HE2	1:C:255:GLU:OE2	2.04	0.58
1:G:46:PHE:O	1:G:49:GLY:N	2.37	0.58
1:H:194:PHE:CD1	1:H:194:PHE:C	2.77	0.58
1:G:212:SER:O	1:G:213:LEU:HD23	2.04	0.57
1:H:223:ILE:O	1:H:226:ALA:N	2.36	0.57
1:A:86:ASN:O	1:A:90:MET:HB2	2.05	0.57
1:F:197:SER:HB3	1:F:199:PHE:CZ	2.39	0.57
1:C:166:LEU:HA	1:C:169:VAL:HG12	1.86	0.57
1:J:168:CYS:HB3	1:J:245:MET:HG3	1.87	0.57
1:F:74:LEU:HD21	1:I:190:CYS:SG	2.45	0.57
1:F:226:ALA:O	1:F:227:ILE:C	2.42	0.57
1:G:166:LEU:HD21	1:J:40:ILE:HG21	1.86	0.57
1:J:145:ALA:HB1	1:J:209:TYR:HE1	1.69	0.57
1:A:99:VAL:HB	1:A:103:ASP:HB2	1.86	0.57
1:F:90:MET:HE2	1:F:104:THR:HA	1.85	0.57
1:I:49:GLY:O	1:I:53:THR:HB	2.04	0.57
1:D:59:MET:O	1:D:61:LYS:N	2.38	0.57
1:E:151:MET:HG3	1:E:152:PRO:HD2	1.87	0.57
1:F:6:LEU:HG	1:F:96:ASN:ND2	2.20	0.57
1:J:205:ASN:HA	1:J:208:ILE:CD1	2.34	0.57
1:A:121:VAL:O	1:A:125:ILE:HG13	2.05	0.57
1:B:34:ALA:HA	1:B:75:VAL:HG22	1.87	0.57
1:E:23:SER:OG	1:E:26:LYS:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:9:LEU:HD23	1:J:175:PHE:CE2	2.39	0.57
1:J:129:THR:HB	1:J:131:LEU:HG	1.87	0.57
1:J:153:PHE:N	1:J:228:TYR:OH	2.38	0.57
1:D:16:LYS:CE	1:D:89:VAL:HG11	2.35	0.57
1:B:151:MET:HG2	1:B:152:PRO:HD2	1.87	0.57
1:E:27:TYR:OH	1:E:107:ILE:HG23	2.04	0.57
1:F:117:ILE:O	1:F:121:VAL:HG23	2.05	0.57
1:G:206:MET:O	1:G:210:SER:HB2	2.05	0.57
1:A:3:LYS:HE3	1:A:255:GLU:OE2	2.05	0.56
1:C:166:LEU:HD21	1:D:40:ILE:HG21	1.87	0.56
1:A:43:LEU:HD22	1:A:126:PHE:CE2	2.40	0.56
1:E:23:SER:HB3	1:E:26:LYS:HB2	1.86	0.56
1:G:164:ASN:HB2	1:G:237:ASN:ND2	2.20	0.56
1:H:35:GLY:H	1:H:115:ASN:HD22	1.53	0.56
1:I:76:ILE:HD11	1:I:171:VAL:HG22	1.87	0.56
1:J:123:GLY:HA3	1:J:210:SER:OG	2.05	0.56
1:J:213:LEU:HD22	1:J:222:THR:O	2.05	0.56
1:B:83:PHE:HE2	1:B:234:THR:HG23	1.70	0.56
1:C:61:LYS:HD3	1:D:51:LEU:HD11	1.86	0.56
1:C:185:ILE:O	1:C:188:PHE:HB3	2.05	0.56
1:H:76:ILE:HD11	1:H:171:VAL:HG22	1.86	0.56
1:J:201:HIS:HE1	1:J:203:VAL:HB	1.68	0.56
1:E:13:ALA:HA	1:E:16:LYS:HG3	1.86	0.56
1:I:220:THR:H	1:I:221:VAL:HG22	1.70	0.56
1:J:90:MET:HB2	1:J:108:TRP:HE1	1.71	0.56
1:J:112:TRP:HZ3	1:J:116:LEU:HD22	1.71	0.56
1:A:82:LEU:HD23	1:A:82:LEU:O	2.06	0.56
1:A:166:LEU:HD21	1:B:40:ILE:HG21	1.87	0.56
1:B:90:MET:O	1:B:93:GLY:N	2.28	0.56
1:H:219:SER:O	1:H:220:THR:HG23	2.06	0.56
1:F:134:LYS:HG2	1:F:134:LYS:O	2.05	0.56
1:G:52:LEU:HB3	1:G:60:THR:HG23	1.87	0.56
1:D:202:SER:O	1:D:206:MET:HG3	2.05	0.56
1:H:34:ALA:HB3	1:H:115:ASN:HD21	1.71	0.56
1:H:132:VAL:HG11	1:H:211:VAL:CG1	2.36	0.56
1:G:11:ASN:HA	1:G:14:ILE:HD12	1.87	0.56
1:B:95:LEU:HB3	1:B:250:TYR:CD2	2.40	0.56
1:D:104:THR:HG22	1:D:105:SER:N	2.19	0.56
1:H:68:PHE:O	1:H:191:LEU:HD23	2.06	0.56
1:J:222:THR:O	1:J:223:ILE:HD12	2.06	0.56
1:A:94:MET:SD	1:A:101:ILE:HG23	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:HD23	1:C:40:ILE:HG13	1.88	0.56
1:D:151:MET:HG2	1:D:152:PRO:HD2	1.88	0.56
1:A:230:LEU:O	1:A:233:VAL:N	2.39	0.55
1:B:124:ILE:HG12	1:B:214:PHE:CD2	2.41	0.55
1:H:6:LEU:HD12	1:H:6:LEU:O	2.06	0.55
1:A:47:THR:HA	1:A:137:VAL:HG13	1.87	0.55
1:B:136:PRO:HA	1:B:139:GLU:HB2	1.88	0.55
1:I:157:PHE:HZ	1:I:239:VAL:HG21	1.72	0.55
1:F:45:ILE:HD13	1:F:68:PHE:CD1	2.41	0.55
1:A:43:LEU:HD13	1:A:126:PHE:CD1	2.42	0.55
1:H:72:LEU:HB3	1:H:187:ILE:HG23	1.88	0.55
1:C:74:LEU:HD23	1:E:186:MET:HE1	1.89	0.55
1:H:127:VAL:C	1:H:129:THR:H	2.09	0.55
1:J:94:MET:HE1	1:J:95:LEU:HA	1.89	0.55
1:E:78:THR:O	1:E:80:THR:N	2.39	0.55
1:G:84:THR:O	1:G:87:ASN:HB2	2.06	0.55
1:G:161:ILE:HG12	1:G:236:GLY:O	2.06	0.55
1:I:157:PHE:CZ	1:I:239:VAL:HG21	2.42	0.55
1:E:164:ASN:ND2	1:E:237:ASN:O	2.34	0.55
1:E:247:LEU:O	1:E:251:ILE:HG13	2.07	0.55
1:A:16:LYS:HG2	1:A:81:GLU:OE2	2.06	0.55
1:B:82:LEU:HD23	1:B:85:GLY:H	1.71	0.55
1:E:241:GLY:O	1:E:246:GLY:N	2.37	0.55
1:G:159:ARG:HG2	1:J:129:THR:CG2	2.36	0.55
1:H:125:ILE:O	1:H:129:THR:HG23	2.07	0.55
1:H:223:ILE:HD12	1:H:223:ILE:N	2.20	0.55
1:B:36:LEU:CD2	1:B:40:ILE:HD11	2.37	0.55
1:E:151:MET:CE	1:E:156:LEU:HD21	2.37	0.55
1:I:3:LYS:HE3	1:I:255:GLU:OE2	2.06	0.55
1:B:121:VAL:O	1:B:125:ILE:HG13	2.06	0.55
1:B:240:GLY:O	1:B:244:PHE:HB2	2.07	0.55
1:D:115:ASN:HB3	1:D:203:VAL:HG13	1.88	0.55
1:E:94:MET:CE	1:E:95:LEU:HD23	2.36	0.55
1:G:159:ARG:NE	1:J:131:LEU:HD21	2.21	0.55
1:F:10:THR:O	1:F:13:ALA:HB3	2.07	0.54
1:I:166:LEU:HA	1:I:169:VAL:HG12	1.89	0.54
1:B:186:MET:CE	1:E:74:LEU:HD23	2.37	0.54
1:C:218:ILE:HG13	1:C:220:THR:CG2	2.37	0.54
1:H:17:ILE:HD12	1:H:20:LEU:HD23	1.89	0.54
1:H:180:ASP:HA	1:H:183:LYS:HD2	1.88	0.54
1:I:129:THR:OG1	1:I:131:LEU:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:PHE:CE2	1:B:112:TRP:CD1	2.94	0.54
1:D:45:ILE:HD13	1:D:68:PHE:CD1	2.42	0.54
1:J:241:GLY:O	1:J:245:MET:HB2	2.07	0.54
1:B:72:LEU:HD12	1:B:72:LEU:O	2.06	0.54
1:B:94:MET:O	1:B:94:MET:HG2	2.06	0.54
1:B:95:LEU:HB3	1:B:250:TYR:CE2	2.42	0.54
1:A:128:GLY:HA3	1:D:158:PHE:HD2	1.71	0.54
1:I:213:LEU:HD23	1:I:221:VAL:HG21	1.90	0.54
1:C:87:ASN:OD1	1:C:238:ILE:HG12	2.08	0.54
1:E:145:ALA:O	1:E:209:TYR:HE1	1.90	0.54
1:H:48:ILE:HG12	1:J:62:ILE:CD1	2.38	0.54
1:B:151:MET:CE	1:B:156:LEU:HD21	2.38	0.54
1:A:9:LEU:CD2	1:A:89:VAL:HG22	2.37	0.54
1:B:9:LEU:HD22	1:B:89:VAL:HA	1.89	0.54
1:J:102:LYS:HB2	1:J:102:LYS:NZ	2.23	0.54
1:J:112:TRP:CZ3	1:J:116:LEU:HD22	2.43	0.54
1:J:117:ILE:O	1:J:121:VAL:HG23	2.08	0.54
1:G:142:ALA:O	1:G:144:THR:N	2.41	0.54
1:I:38:VAL:HA	1:I:71:ALA:HB1	1.90	0.54
1:F:84:THR:HG21	1:F:201:HIS:NE2	2.23	0.54
1:H:126:PHE:CE2	1:H:132:VAL:HG13	2.43	0.54
1:H:127:VAL:CG1	1:H:216:PRO:HD3	2.37	0.54
1:A:34:ALA:O	1:A:38:VAL:HG23	2.08	0.53
1:C:231:VAL:HG12	1:C:232:ALA:N	2.23	0.53
1:F:46:PHE:HE2	1:F:208:ILE:HG12	1.72	0.53
1:G:220:THR:C	1:G:221:VAL:HG13	2.28	0.53
1:H:221:VAL:O	1:H:222:THR:OG1	2.21	0.53
1:J:83:PHE:CD1	1:J:83:PHE:C	2.81	0.53
1:C:161:ILE:O	1:C:162:LEU:C	2.46	0.53
1:F:142:ALA:HB2	1:F:218:ILE:HG21	1.91	0.53
1:I:2:HIS:HD2	1:I:176:ARG:HH12	1.55	0.53
1:C:148:LYS:HB3	1:C:229:ASN:ND2	2.23	0.53
1:H:72:LEU:HB3	1:H:187:ILE:CG2	2.38	0.53
1:A:44:LEU:O	1:A:48:ILE:HG13	2.08	0.53
1:D:36:LEU:HG	1:D:122:LEU:HB2	1.90	0.53
1:H:132:VAL:HG11	1:H:211:VAL:HG13	1.91	0.53
1:I:17:ILE:CG1	1:I:103:ASP:HB3	2.38	0.53
1:B:113:VAL:O	1:B:117:ILE:HG13	2.08	0.53
1:C:6:LEU:HD11	1:C:96:ASN:HB2	1.89	0.53
1:E:84:THR:HG21	1:E:201:HIS:CD2	2.43	0.53
1:H:116:LEU:HA	1:H:206:MET:SD	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:240:GLY:HA2	1:J:244:PHE:HD2	1.73	0.53
1:B:43:LEU:HD13	1:B:126:PHE:CD1	2.44	0.53
1:H:88:MET:HE1	1:H:171:VAL:HG12	1.90	0.53
1:C:145:ALA:O	1:C:209:TYR:OH	2.18	0.53
1:H:144:THR:O	1:H:148:LYS:HG3	2.08	0.53
1:E:148:LYS:O	1:E:229:ASN:ND2	2.38	0.53
1:H:108:TRP:O	1:H:112:TRP:HB2	2.09	0.53
1:I:154:THR:O	1:I:157:PHE:HB3	2.09	0.53
1:A:161:ILE:O	1:A:165:ILE:HG13	2.09	0.53
1:B:116:LEU:O	1:B:120:LEU:HG	2.08	0.53
1:B:224:GLY:HA2	1:B:227:ILE:CG2	2.39	0.53
1:E:94:MET:HE2	1:E:95:LEU:HD23	1.90	0.53
1:J:121:VAL:O	1:J:125:ILE:HG12	2.09	0.53
1:E:2:HIS:CE1	1:E:252:LEU:HD13	2.44	0.53
1:H:247:LEU:O	1:H:251:ILE:HG13	2.08	0.53
1:J:96:ASN:O	1:J:97:LYS:HB2	2.08	0.53
1:J:183:LYS:O	1:J:187:ILE:HG13	2.07	0.53
1:B:120:LEU:HA	1:B:210:SER:OG	2.09	0.52
1:I:213:LEU:HD13	1:I:223:ILE:HG13	1.90	0.52
1:D:126:PHE:HE2	1:D:141:PHE:CZ	2.27	0.52
1:J:115:ASN:HB3	1:J:203:VAL:HG13	1.90	0.52
1:I:17:ILE:HD13	1:I:103:ASP:HB3	1.91	0.52
1:J:17:ILE:O	1:J:20:LEU:N	2.41	0.52
1:D:221:VAL:HG23	1:D:222:THR:H	1.74	0.52
1:H:31:SER:HB2	1:H:114:GLY:HA3	1.91	0.52
1:D:17:ILE:HD13	1:D:103:ASP:OD1	2.09	0.52
1:J:174:SER:HB2	1:J:183:LYS:HD3	1.90	0.52
1:C:161:ILE:O	1:C:163:CYS:N	2.43	0.52
1:D:87:ASN:O	1:D:91:SER:HB3	2.10	0.52
1:F:2:HIS:NE2	1:F:252:LEU:HD13	2.25	0.52
1:F:169:VAL:HG23	1:F:245:MET:HE1	1.92	0.52
1:J:205:ASN:HA	1:J:208:ILE:CG1	2.40	0.52
1:B:87:ASN:H	1:B:87:ASN:HD22	1.58	0.52
1:C:15:ASN:HA	1:C:18:ASN:HB2	1.91	0.52
1:C:87:ASN:OD1	1:C:238:ILE:HA	2.10	0.52
1:E:74:LEU:O	1:E:78:THR:OG1	2.18	0.52
1:G:159:ARG:CG	1:J:129:THR:HG22	2.38	0.52
1:G:223:ILE:HD12	1:G:223:ILE:N	2.16	0.52
1:B:199:PHE:N	1:B:199:PHE:CD1	2.77	0.52
1:D:133:ASP:O	1:D:134:LYS:HB3	2.10	0.52
1:G:90:MET:HG3	1:G:107:ILE:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:20:LEU:HD11	1:J:110:TYR:CD2	2.45	0.52
1:J:52:LEU:HB3	1:J:60:THR:OG1	2.10	0.52
1:E:90:MET:HB2	1:E:108:TRP:HE1	1.75	0.51
1:F:59:MET:O	1:F:63:VAL:HG23	2.10	0.51
1:J:166:LEU:HD12	1:J:194:PHE:HB3	1.91	0.51
1:A:180:ASP:O	1:A:184:ILE:HG13	2.10	0.51
1:G:166:LEU:HD21	1:J:40:ILE:HD12	1.91	0.51
1:H:36:LEU:O	1:H:40:ILE:HG12	2.10	0.51
1:B:42:ILE:CD1	1:B:204:ALA:HB1	2.36	0.51
1:D:84:THR:HB	1:D:164:ASN:OD1	2.11	0.51
1:B:112:TRP:NE1	1:B:234:THR:HG21	2.24	0.51
1:C:159:ARG:NH2	1:D:131:LEU:HD23	2.20	0.51
1:E:42:ILE:CD1	1:E:204:ALA:HB1	2.32	0.51
1:F:91:SER:O	1:F:95:LEU:HG	2.11	0.51
1:D:17:ILE:HG23	1:D:18:ASN:N	2.25	0.51
1:D:94:MET:SD	1:D:101:ILE:HG23	2.51	0.51
1:H:39:GLY:O	1:H:43:LEU:HG	2.10	0.51
1:A:184:ILE:HG21	1:D:185:ILE:HG21	1.93	0.51
1:E:68:PHE:HE2	1:E:194:PHE:CZ	2.29	0.51
1:G:83:PHE:HA	1:G:111:SER:OG	2.10	0.51
1:G:125:ILE:O	1:G:129:THR:HG23	2.11	0.51
1:G:160:GLY:O	1:G:237:ASN:ND2	2.44	0.51
1:H:209:TYR:CD2	1:H:226:ALA:HB1	2.46	0.51
1:J:13:ALA:O	1:J:16:LYS:HB2	2.10	0.51
1:A:115:ASN:HB3	1:A:203:VAL:HG13	1.92	0.51
1:E:209:TYR:CE1	1:E:221:VAL:HG11	2.46	0.51
1:E:204:ALA:O	1:E:208:ILE:HG13	2.11	0.51
1:F:110:TYR:HD1	1:F:110:TYR:H	1.58	0.51
1:G:68:PHE:CE2	1:G:191:LEU:HD23	2.45	0.51
1:H:10:THR:HG21	1:H:96:ASN:HB3	1.93	0.51
1:H:45:ILE:HD13	1:H:68:PHE:HB2	1.92	0.51
1:E:156:LEU:HD11	1:E:229:ASN:ND2	2.26	0.51
1:F:159:ARG:NH1	1:G:131:LEU:HD21	2.26	0.51
1:G:52:LEU:CB	1:G:60:THR:HG23	2.41	0.51
1:G:254:LYS:HG3	1:G:256:LYS:HG2	1.92	0.51
1:H:68:PHE:O	1:H:68:PHE:CG	2.62	0.51
1:H:87:ASN:HD22	1:H:87:ASN:H	1.59	0.51
1:H:127:VAL:O	1:H:129:THR:N	2.44	0.51
1:I:61:LYS:HD3	2:I:266:PG4:C3	2.38	0.51
1:J:239:VAL:O	1:J:243:LEU:CB	2.58	0.51
1:B:19:LEU:HD23	1:B:27:TYR:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASN:OD1	1:B:238:ILE:HA	2.11	0.51
1:D:189:LEU:O	1:D:192:PHE:N	2.44	0.51
1:E:86:ASN:HB3	1:E:90:MET:HG2	1.92	0.51
1:H:143:ASN:O	1:H:146:ALA:N	2.44	0.51
1:C:148:LYS:O	1:C:229:ASN:HB2	2.10	0.50
1:E:245:MET:O	1:E:249:THR:HG23	2.10	0.50
1:G:251:ILE:O	1:J:26:LYS:HE2	2.11	0.50
1:H:35:GLY:N	1:H:115:ASN:ND2	2.58	0.50
1:J:92:ALA:O	1:J:96:ASN:HB2	2.11	0.50
1:A:146:ALA:HA	1:A:221:VAL:CG1	2.42	0.50
1:B:36:LEU:HD23	1:B:36:LEU:C	2.32	0.50
1:D:132:VAL:O	1:D:138:ALA:HB2	2.10	0.50
1:H:218:ILE:HG23	1:H:220:THR:HG23	1.93	0.50
1:A:89:VAL:HG12	1:A:90:MET:N	2.26	0.50
1:G:179:SER:HB3	1:G:182:ALA:HB3	1.93	0.50
1:G:183:LYS:O	1:G:187:ILE:CG1	2.59	0.50
1:G:38:VAL:HA	1:G:71:ALA:HB1	1.93	0.50
1:I:247:LEU:O	1:I:250:TYR:HB3	2.12	0.50
1:C:168:CYS:HB2	1:C:245:MET:HG3	1.92	0.50
1:E:4:GLU:O	1:E:8:LYS:HG3	2.11	0.50
1:H:72:LEU:HD12	1:H:75:VAL:HB	1.93	0.50
1:J:83:PHE:CD2	1:J:112:TRP:HD1	2.29	0.50
1:A:90:MET:CE	1:A:99:VAL:HG21	2.42	0.50
1:B:90:MET:SD	1:B:107:ILE:HG13	2.52	0.50
1:E:145:ALA:HB1	1:E:209:TYR:HD1	1.77	0.50
1:F:31:SER:HB3	1:F:114:GLY:HA3	1.93	0.50
1:H:127:VAL:HG13	1:H:132:VAL:HG21	1.94	0.50
1:H:202:SER:HB3	1:H:233:VAL:HG12	1.93	0.50
1:I:172:LEU:HD13	1:I:249:THR:HG21	1.92	0.50
1:I:223:ILE:O	1:I:227:ILE:HG12	2.10	0.50
1:B:207:THR:O	1:B:211:VAL:HG23	2.11	0.50
1:D:24:LYS:O	1:D:28:LEU:HG	2.12	0.50
1:E:162:LEU:HD13	1:E:199:PHE:CZ	2.47	0.50
1:D:14:ILE:HD11	1:D:98:GLY:HA3	1.94	0.50
1:G:69:ALA:O	1:G:73:SER:HB2	2.12	0.50
1:H:34:ALA:O	1:H:37:TYR:N	2.45	0.50
1:F:52:LEU:HB3	1:F:60:THR:OG1	2.12	0.50
1:A:90:MET:HE3	1:A:99:VAL:HG21	1.94	0.49
1:B:180:ASP:HA	1:B:183:LYS:HD2	1.94	0.49
1:B:250:TYR:CE1	1:B:254:LYS:HD3	2.47	0.49
1:E:185:ILE:O	1:E:188:PHE:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLY:O	1:A:53:THR:HB	2.12	0.49
1:I:133:ASP:HA	1:I:217:THR:HG21	1.93	0.49
1:J:83:PHE:HD1	1:J:84:THR:N	2.10	0.49
1:B:231:VAL:O	1:B:235:LEU:HG	2.12	0.49
1:D:148:LYS:HB3	1:D:229:ASN:ND2	2.26	0.49
1:D:168:CYS:HB2	1:D:245:MET:HG2	1.95	0.49
1:D:219:SER:O	1:D:220:THR:OG1	2.28	0.49
1:E:194:PHE:CE1	1:E:195:ILE:HD13	2.47	0.49
1:F:179:SER:O	1:F:183:LYS:HG3	2.12	0.49
1:I:31:SER:O	1:I:115:ASN:HA	2.12	0.49
1:A:217:THR:C	1:A:218:ILE:HG13	2.32	0.49
1:B:196:THR:O	1:E:47:THR:HG21	2.12	0.49
1:H:17:ILE:O	1:H:20:LEU:HB3	2.11	0.49
1:D:17:ILE:HG23	1:D:18:ASN:H	1.77	0.49
1:F:110:TYR:N	1:F:110:TYR:CD1	2.81	0.49
1:G:94:MET:HG2	1:G:95:LEU:N	2.28	0.49
1:H:90:MET:HB3	1:H:104:THR:HG23	1.94	0.49
1:H:223:ILE:C	1:H:225:GLY:N	2.65	0.49
1:A:254:LYS:O	1:A:256:LYS:N	2.45	0.49
1:D:9:LEU:HD21	1:D:88:MET:CE	2.43	0.49
1:F:172:LEU:HD13	1:F:249:THR:HG21	1.94	0.49
1:I:219:SER:C	1:I:220:THR:HG23	2.32	0.49
1:J:39:GLY:O	1:J:42:ILE:N	2.45	0.49
1:J:194:PHE:C	1:J:194:PHE:CD1	2.85	0.49
1:A:126:PHE:O	1:A:129:THR:OG1	2.23	0.49
1:C:33:PHE:HE1	1:E:245:MET:SD	2.36	0.49
1:A:52:LEU:HB2	1:A:60:THR:HG23	1.95	0.49
1:A:138:ALA:HA	1:A:141:PHE:HB2	1.95	0.49
1:C:133:ASP:O	1:C:217:THR:HG21	2.13	0.49
1:H:26:LYS:NZ	1:J:254:LYS:O	2.33	0.49
1:C:218:ILE:HD12	1:C:219:SER:N	2.27	0.49
1:D:168:CYS:O	1:D:172:LEU:N	2.31	0.49
1:F:190:CYS:O	1:F:193:ALA:HB3	2.13	0.49
1:F:214:PHE:O	1:F:216:PRO:HD3	2.13	0.49
1:I:2:HIS:CD2	1:I:176:ARG:HH12	2.30	0.49
1:B:194:PHE:CZ	1:B:195:ILE:HD11	2.48	0.48
1:C:251:ILE:O	1:D:26:LYS:HG2	2.12	0.48
1:F:47:THR:HA	1:F:137:VAL:CG2	2.43	0.48
1:I:83:PHE:O	1:I:87:ASN:ND2	2.46	0.48
1:E:72:LEU:HD13	1:E:82:LEU:HD22	1.95	0.48
1:F:84:THR:HA	1:F:87:ASN:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:ALA:O	1:G:197:SER:HB2	2.13	0.48
1:J:17:ILE:HD12	1:J:20:LEU:HB3	1.95	0.48
1:A:89:VAL:C	1:A:91:SER:H	2.17	0.48
1:A:159:ARG:CG	1:B:129:THR:HB	2.36	0.48
1:E:153:PHE:O	1:E:154:THR:C	2.52	0.48
1:H:68:PHE:CD2	1:H:195:ILE:HG13	2.48	0.48
1:J:52:LEU:HD12	1:J:60:THR:HA	1.95	0.48
1:C:218:ILE:HD12	1:C:219:SER:H	1.78	0.48
1:D:151:MET:SD	1:D:159:ARG:NH1	2.86	0.48
1:H:94:MET:SD	1:H:101:ILE:HG13	2.53	0.48
1:A:131:LEU:HG	1:D:159:ARG:HE	1.78	0.48
1:C:156:LEU:HD13	1:C:233:VAL:HG23	1.95	0.48
1:D:94:MET:HA	1:D:99:VAL:O	2.14	0.48
1:D:123:GLY:HA3	1:D:210:SER:OG	2.14	0.48
1:G:151:MET:SD	1:G:159:ARG:NH1	2.87	0.48
1:H:76:ILE:HG13	1:H:187:ILE:HD11	1.94	0.48
1:H:90:MET:HE2	1:H:104:THR:HA	1.95	0.48
1:I:1:ALA:HB1	1:I:176:ARG:HH22	1.77	0.48
1:F:179:SER:HB3	1:F:182:ALA:HB3	1.96	0.48
1:C:96:ASN:OD1	1:C:254:LYS:HD3	2.14	0.48
1:D:95:LEU:HB3	1:D:250:TYR:CD2	2.48	0.48
1:E:17:ILE:O	1:E:21:ASN:N	2.39	0.48
1:A:234:THR:O	1:A:238:ILE:HG13	2.13	0.48
1:B:91:SER:O	1:B:95:LEU:HG	2.14	0.48
1:B:201:HIS:CE1	1:B:203:VAL:HB	2.49	0.48
1:C:235:LEU:O	1:C:238:ILE:N	2.47	0.48
1:E:119:ALA:HB1	1:E:207:THR:HA	1.96	0.48
1:F:158:PHE:HB3	1:G:129:THR:HG22	1.96	0.48
1:G:159:ARG:HH21	1:J:131:LEU:HD23	1.78	0.48
1:E:108:TRP:O	1:E:112:TRP:HB2	2.14	0.48
1:H:23:SER:HB2	1:J:256:LYS:HZ3	1.77	0.48
1:J:230:LEU:N	1:J:230:LEU:HD23	2.29	0.48
1:B:90:MET:HE2	1:B:104:THR:CA	2.27	0.48
1:E:123:GLY:O	1:E:127:VAL:HG23	2.13	0.48
1:J:205:ASN:HA	1:J:208:ILE:HD12	1.96	0.48
1:C:141:PHE:CD2	1:C:211:VAL:HG11	2.49	0.47
1:D:245:MET:HE3	1:D:245:MET:HA	1.95	0.47
1:H:67:SER:C	1:H:69:ALA:H	2.17	0.47
1:A:162:LEU:O	1:A:165:ILE:HB	2.14	0.47
1:C:129:THR:HG21	1:E:162:LEU:HD12	1.94	0.47
1:C:141:PHE:CE2	1:C:211:VAL:HG11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:LEU:HD23	1:E:51:LEU:N	2.29	0.47
1:E:87:ASN:HB2	1:E:241:GLY:HA3	1.95	0.47
1:E:195:ILE:HG22	1:E:196:THR:N	2.29	0.47
1:G:47:THR:HA	1:G:137:VAL:HG13	1.96	0.47
1:J:219:SER:O	1:J:220:THR:HG23	2.14	0.47
1:G:223:ILE:O	1:G:224:GLY:C	2.53	0.47
1:J:87:ASN:HD22	1:J:87:ASN:H	1.61	0.47
1:C:255:GLU:C	1:C:257:LEU:N	2.65	0.47
1:D:23:SER:HB3	1:D:26:LYS:HB2	1.97	0.47
1:E:87:ASN:CB	1:E:241:GLY:HA3	2.44	0.47
1:J:250:TYR:OH	1:J:254:LYS:HE3	2.15	0.47
1:A:124:ILE:HG13	1:A:214:PHE:CE2	2.50	0.47
1:B:218:ILE:CG2	1:B:220:THR:HG23	2.44	0.47
1:F:20:LEU:HD11	1:F:110:TYR:CD2	2.50	0.47
1:H:10:THR:HG23	1:H:93:GLY:CA	2.41	0.47
1:H:133:ASP:O	1:H:217:THR:HG21	2.14	0.47
1:J:26:LYS:O	1:J:29:VAL:N	2.47	0.47
1:G:36:LEU:O	1:G:40:ILE:HG13	2.14	0.47
1:H:9:LEU:HD23	1:H:175:PHE:CE2	2.49	0.47
1:A:89:VAL:C	1:A:91:SER:N	2.68	0.47
1:A:192:PHE:HE2	1:B:67:SER:HB3	1.80	0.47
1:C:49:GLY:O	1:C:53:THR:HB	2.15	0.47
1:C:227:ILE:HD13	1:C:227:ILE:N	2.30	0.47
1:D:43:LEU:HD13	1:D:126:PHE:CD1	2.50	0.47
1:E:151:MET:HE2	1:E:156:LEU:HD21	1.97	0.47
1:E:206:MET:O	1:E:210:SER:HB3	2.15	0.47
1:J:133:ASP:O	1:J:217:THR:OG1	2.14	0.47
1:J:155:ALA:O	1:J:159:ARG:HG2	2.15	0.47
1:E:25:VAL:O	1:E:29:VAL:HG23	2.14	0.47
1:E:169:VAL:O	1:E:172:LEU:HB3	2.15	0.47
1:H:125:ILE:HG23	1:J:158:PHE:CD2	2.43	0.47
1:I:167:VAL:HG21	1:I:201:HIS:CD2	2.50	0.47
1:C:27:TYR:CE1	1:C:81:GLU:HG3	2.50	0.47
1:D:142:ALA:O	1:D:144:THR:N	2.48	0.47
1:F:122:LEU:HD23	1:F:207:THR:HG21	1.97	0.47
1:F:141:PHE:CE1	1:F:211:VAL:HG11	2.50	0.47
1:C:126:PHE:O	1:C:129:THR:OG1	2.27	0.47
1:F:24:LYS:CE	1:F:110:TYR:CE2	2.90	0.47
1:F:254:LYS:HD2	1:F:255:GLU:H	1.79	0.47
1:G:224:GLY:HA2	1:G:227:ILE:HG13	1.97	0.47
1:H:29:VAL:O	1:H:33:PHE:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HA	1:A:169:VAL:CG1	2.44	0.46
1:B:127:VAL:HG22	1:B:132:VAL:HG21	1.97	0.46
1:D:136:PRO:HA	1:D:139:GLU:HB2	1.97	0.46
1:F:12:ALA:O	1:F:16:LYS:HG3	2.14	0.46
1:F:71:ALA:O	1:F:75:VAL:HG23	2.15	0.46
1:I:151:MET:HG2	1:I:156:LEU:HG	1.98	0.46
1:A:194:PHE:CD1	1:A:194:PHE:C	2.88	0.46
1:F:146:ALA:O	1:F:147:SER:C	2.52	0.46
1:G:211:VAL:O	1:G:215:SER:HB2	2.15	0.46
1:H:234:THR:HG22	1:H:238:ILE:CD1	2.46	0.46
1:I:17:ILE:HG12	1:I:103:ASP:HB3	1.97	0.46
1:A:37:TYR:O	1:A:40:ILE:HB	2.16	0.46
1:A:47:THR:HA	1:A:137:VAL:CG1	2.45	0.46
1:A:217:THR:O	1:A:217:THR:OG1	2.32	0.46
1:B:157:PHE:O	1:B:161:ILE:HG13	2.15	0.46
1:E:156:LEU:CD1	1:E:229:ASN:ND2	2.79	0.46
1:A:94:MET:CE	1:A:95:LEU:HD23	2.45	0.46
1:B:16:LYS:HD3	1:B:81:GLU:OE1	2.15	0.46
1:E:6:LEU:O	1:E:9:LEU:HB2	2.16	0.46
1:G:194:PHE:CD1	1:G:194:PHE:C	2.89	0.46
1:H:17:ILE:CD1	1:H:20:LEU:HD23	2.45	0.46
1:I:165:ILE:O	1:I:169:VAL:HG12	2.15	0.46
1:J:38:VAL:HA	1:J:71:ALA:HB1	1.97	0.46
1:E:28:LEU:HD21	1:E:110:TYR:CD1	2.43	0.46
1:E:222:THR:C	1:E:224:GLY:H	2.18	0.46
1:F:53:THR:O	1:F:54:ASP:C	2.54	0.46
1:F:184:ILE:HG21	1:I:185:ILE:HG21	1.96	0.46
1:F:226:ALA:O	1:F:229:ASN:N	2.48	0.46
1:E:12:ALA:O	1:E:16:LYS:HG3	2.16	0.46
1:H:31:SER:O	1:H:115:ASN:ND2	2.48	0.46
1:H:83:PHE:CE2	1:H:234:THR:HG23	2.50	0.46
1:J:37:TYR:O	1:J:40:ILE:N	2.49	0.46
1:A:104:THR:HG22	1:A:105:SER:N	2.30	0.46
1:B:154:THR:HG22	1:B:158:PHE:CE2	2.50	0.46
1:F:26:LYS:HE2	1:I:251:ILE:O	2.15	0.46
1:G:133:ASP:O	1:G:217:THR:HG21	2.16	0.46
1:H:40:ILE:CG2	1:J:166:LEU:HD21	2.46	0.46
1:H:44:LEU:O	1:H:48:ILE:HG13	2.15	0.46
1:G:46:PHE:O	1:G:47:THR:C	2.55	0.46
1:G:183:LYS:O	1:G:187:ILE:HG12	2.16	0.46
1:H:186:MET:SD	1:I:184:ILE:HD13	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ILE:O	1:B:50:GLY:N	2.49	0.46
1:B:83:PHE:O	1:B:86:ASN:N	2.48	0.46
1:B:141:PHE:CE2	1:B:211:VAL:HG11	2.50	0.46
1:B:148:LYS:O	1:B:156:LEU:HD11	2.16	0.46
1:B:239:VAL:O	1:B:243:LEU:HB3	2.15	0.46
1:E:43:LEU:HD22	1:E:126:PHE:CE2	2.51	0.46
1:E:218:ILE:HG12	1:G:218:ILE:O	2.15	0.46
1:G:237:ASN:HD22	1:G:237:ASN:HA	1.63	0.46
1:B:68:PHE:O	1:B:191:LEU:HD23	2.15	0.45
1:C:42:ILE:HD13	1:C:42:ILE:HA	1.64	0.45
1:E:48:ILE:HD13	1:E:63:VAL:HG12	1.98	0.45
1:G:91:SER:OG	1:G:246:GLY:HA3	2.15	0.45
1:H:84:THR:HB	1:H:164:ASN:OD1	2.16	0.45
1:I:17:ILE:CD1	1:I:103:ASP:HB3	2.47	0.45
1:C:113:VAL:O	1:C:117:ILE:HG13	2.16	0.45
1:F:19:LEU:HD23	1:F:27:TYR:HD1	1.81	0.45
1:I:151:MET:HG3	1:I:152:PRO:HD2	1.96	0.45
1:J:34:ALA:CB	1:J:81:GLU:O	2.64	0.45
1:A:148:LYS:O	1:A:156:LEU:HD11	2.16	0.45
1:D:75:VAL:HG12	1:D:76:ILE:N	2.31	0.45
1:F:181:THR:HG22	1:G:181:THR:OG1	2.16	0.45
1:H:103:ASP:O	1:H:107:ILE:HG12	2.15	0.45
1:J:10:THR:HG23	1:J:93:GLY:HA2	1.98	0.45
1:A:128:GLY:HA3	1:D:158:PHE:CD2	2.49	0.45
1:C:161:ILE:HG23	1:C:240:GLY:HA3	1.99	0.45
1:D:13:ALA:O	1:D:16:LYS:HB2	2.16	0.45
1:A:40:ILE:HD12	1:D:166:LEU:HD21	1.97	0.45
1:A:93:GLY:O	1:A:98:GLY:N	2.49	0.45
1:B:19:LEU:HD23	1:B:27:TYR:CD2	2.52	0.45
1:C:17:ILE:HG12	1:C:103:ASP:OD2	2.16	0.45
1:C:84:THR:O	1:C:87:ASN:HB2	2.17	0.45
1:D:100:SER:OG	1:D:103:ASP:N	2.45	0.45
1:G:91:SER:OG	1:G:92:ALA:N	2.50	0.45
1:A:144:THR:HA	1:A:147:SER:OG	2.16	0.45
1:B:130:GLY:O	1:B:133:ASP:HB2	2.17	0.45
1:B:224:GLY:HA2	1:B:227:ILE:HG23	1.97	0.45
1:C:157:PHE:HD2	1:C:158:PHE:CD1	2.34	0.45
1:D:180:ASP:O	1:D:184:ILE:HG13	2.17	0.45
1:E:11:ASN:HA	1:E:14:ILE:HD12	1.99	0.45
1:E:109:ALA:O	1:E:113:VAL:HG23	2.16	0.45
1:A:130:GLY:O	1:A:133:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HD22	1:B:200:GLU:HG3	1.99	0.45
1:F:47:THR:HA	1:F:137:VAL:HG22	1.98	0.45
1:I:143:ASN:O	1:I:146:ALA:HB3	2.16	0.45
1:J:151:MET:SD	1:J:156:LEU:CD2	3.05	0.45
1:J:179:SER:HB3	1:J:182:ALA:HB3	1.98	0.45
1:A:90:MET:HG3	1:A:107:ILE:HG21	1.99	0.45
1:A:144:THR:HA	1:A:147:SER:HB2	1.99	0.45
1:B:201:HIS:HE1	1:B:203:VAL:HB	1.82	0.45
1:D:139:GLU:O	1:D:142:ALA:N	2.50	0.45
1:D:213:LEU:HD21	1:D:222:THR:HA	1.99	0.45
1:E:207:THR:O	1:E:211:VAL:HG23	2.17	0.45
1:F:238:ILE:O	1:F:239:VAL:C	2.55	0.45
1:H:27:TYR:O	1:H:27:TYR:CD1	2.69	0.45
1:H:47:THR:O	1:H:51:LEU:HB2	2.16	0.45
1:H:52:LEU:HD23	1:H:52:LEU:HA	1.51	0.45
1:J:49:GLY:O	1:J:53:THR:HB	2.16	0.45
1:A:71:ALA:O	1:A:73:SER:N	2.50	0.45
1:B:132:VAL:HA	1:B:138:ALA:HB2	1.98	0.45
1:B:153:PHE:N	1:B:228:TYR:OH	2.49	0.45
1:B:249:THR:HA	1:B:252:LEU:HD12	1.97	0.45
1:F:121:VAL:O	1:F:125:ILE:HG13	2.17	0.45
1:F:209:TYR:O	1:F:213:LEU:HG	2.17	0.45
1:G:107:ILE:HD13	1:G:107:ILE:HA	1.89	0.45
1:H:127:VAL:HA	1:H:132:VAL:CG2	2.46	0.45
1:J:114:GLY:HA2	1:J:117:ILE:HD12	1.98	0.45
1:A:144:THR:HA	1:A:147:SER:CB	2.47	0.45
1:A:231:VAL:O	1:A:235:LEU:HB2	2.17	0.45
1:B:30:SER:O	1:B:33:PHE:HB2	2.17	0.45
1:B:110:TYR:O	1:B:114:GLY:N	2.34	0.45
1:C:112:TRP:CE3	1:C:112:TRP:O	2.69	0.45
1:D:102:LYS:O	1:D:102:LYS:HG3	2.13	0.45
1:E:163:CYS:O	1:E:167:VAL:HG23	2.16	0.45
1:E:164:ASN:HB3	1:E:240:GLY:HA3	1.99	0.45
1:F:161:ILE:HD11	1:F:239:VAL:HG11	1.98	0.45
1:F:219:SER:O	1:F:220:THR:HG23	2.17	0.45
1:H:100:SER:N	1:H:103:ASP:OD2	2.50	0.45
1:J:218:ILE:HD12	1:J:218:ILE:HA	1.73	0.45
1:C:48:ILE:HG21	1:C:63:VAL:HG12	1.99	0.44
1:F:151:MET:SD	1:F:156:LEU:HD23	2.56	0.44
1:G:90:MET:CG	1:G:107:ILE:HG21	2.47	0.44
1:G:163:CYS:HB2	1:G:199:PHE:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:MET:O	1:H:228:TYR:OH	2.21	0.44
1:J:87:ASN:HD22	1:J:87:ASN:N	2.16	0.44
1:J:90:MET:HB3	1:J:104:THR:HG23	1.99	0.44
1:J:153:PHE:O	1:J:157:PHE:N	2.48	0.44
1:J:236:GLY:O	1:J:237:ASN:C	2.56	0.44
1:A:166:LEU:CA	1:A:169:VAL:HG12	2.45	0.44
1:F:101:ILE:H	1:F:101:ILE:CD1	2.28	0.44
1:G:129:THR:OG1	1:G:131:LEU:HG	2.17	0.44
1:G:143:ASN:O	1:G:146:ALA:HB3	2.18	0.44
1:J:47:THR:O	1:J:51:LEU:HD11	2.17	0.44
1:J:207:THR:HA	1:J:210:SER:HB3	1.99	0.44
1:A:94:MET:O	1:A:94:MET:HE3	2.16	0.44
1:C:223:ILE:H	1:C:223:ILE:CD1	2.27	0.44
1:D:17:ILE:HD13	1:D:103:ASP:CG	2.37	0.44
1:F:40:ILE:CG2	1:I:166:LEU:HD21	2.45	0.44
1:F:217:THR:C	1:F:218:ILE:HG12	2.37	0.44
1:H:164:ASN:HD22	1:H:241:GLY:HA3	1.83	0.44
1:H:205:ASN:ND2	1:H:229:ASN:OD1	2.44	0.44
1:B:213:LEU:O	1:B:214:PHE:HD1	2.01	0.44
1:C:37:TYR:CE1	1:E:169:VAL:HG21	2.53	0.44
1:E:83:PHE:O	1:E:87:ASN:ND2	2.50	0.44
1:G:183:LYS:O	1:G:187:ILE:HG13	2.18	0.44
1:B:86:ASN:O	1:B:87:ASN:C	2.55	0.44
1:B:115:ASN:HB3	1:B:203:VAL:HG13	1.99	0.44
1:B:132:VAL:HG12	1:B:138:ALA:HA	2.00	0.44
1:B:209:TYR:HD2	1:B:230:LEU:HD21	1.83	0.44
1:D:95:LEU:HB3	1:D:250:TYR:CE2	2.52	0.44
1:D:161:ILE:HG22	1:D:162:LEU:N	2.31	0.44
1:D:161:ILE:HG22	1:D:162:LEU:HD23	2.00	0.44
1:E:16:LYS:HD3	1:E:81:GLU:OE2	2.18	0.44
1:E:20:LEU:HB2	1:E:27:TYR:CD2	2.53	0.44
1:E:88:MET:HG3	1:E:245:MET:C	2.37	0.44
1:F:87:ASN:HD22	1:F:164:ASN:ND2	2.12	0.44
1:I:162:LEU:HD23	1:I:162:LEU:HA	1.77	0.44
1:J:125:ILE:HG12	1:J:125:ILE:H	1.42	0.44
1:A:9:LEU:HD11	1:A:172:LEU:CD1	2.48	0.44
1:B:115:ASN:N	1:B:115:ASN:HD22	2.16	0.44
1:D:90:MET:CE	1:D:107:ILE:HG13	2.48	0.44
1:E:43:LEU:CD1	1:E:122:LEU:HD21	2.47	0.44
1:H:27:TYR:CD1	1:H:27:TYR:C	2.90	0.44
1:I:30:SER:OG	1:I:81:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:LEU:HD23	1:I:36:LEU:O	2.17	0.44
1:B:27:TYR:CE2	1:B:81:GLU:HG3	2.52	0.44
1:B:73:SER:HA	1:B:187:ILE:HD13	2.00	0.44
1:C:114:GLY:HA2	1:C:117:ILE:HD12	2.00	0.44
1:G:179:SER:O	1:G:183:LYS:HG3	2.17	0.44
1:H:127:VAL:C	1:H:129:THR:N	2.71	0.44
1:J:166:LEU:HA	1:J:169:VAL:HG12	2.00	0.44
1:D:16:LYS:HE2	1:D:89:VAL:HG11	1.99	0.44
1:J:247:LEU:O	1:J:251:ILE:HG13	2.18	0.44
1:C:166:LEU:O	1:C:169:VAL:HG12	2.17	0.44
1:D:235:LEU:O	1:D:239:VAL:HG23	2.18	0.44
1:E:194:PHE:CD1	1:E:194:PHE:C	2.90	0.44
1:F:218:ILE:HB	1:F:219:SER:H	1.43	0.44
1:F:223:ILE:CG2	1:F:224:GLY:N	2.81	0.44
1:I:124:ILE:HG22	1:I:125:ILE:N	2.31	0.44
1:I:226:ALA:O	1:I:227:ILE:C	2.56	0.44
1:B:99:VAL:HB	1:B:103:ASP:HB2	2.00	0.43
1:F:170:SER:HB3	1:F:190:CYS:SG	2.58	0.43
1:G:90:MET:HB3	1:G:104:THR:HG23	1.99	0.43
1:G:247:LEU:O	1:G:250:TYR:HB3	2.18	0.43
1:A:129:THR:C	1:A:131:LEU:H	2.22	0.43
1:E:68:PHE:CD2	1:E:191:LEU:HD23	2.52	0.43
1:F:95:LEU:C	1:F:97:LYS:H	2.20	0.43
1:G:191:LEU:N	1:G:191:LEU:CD1	2.80	0.43
1:H:149:ALA:O	1:H:228:TYR:CE2	2.70	0.43
1:H:190:CYS:O	1:H:193:ALA:HB3	2.17	0.43
1:A:87:ASN:O	1:A:91:SER:HB3	2.18	0.43
1:A:9:LEU:HD11	1:A:172:LEU:HD13	2.00	0.43
1:A:70:ILE:HG13	1:D:189:LEU:HB3	2.00	0.43
1:A:107:ILE:C	1:A:109:ALA:N	2.72	0.43
1:B:46:PHE:HD2	1:B:141:PHE:CE1	2.36	0.43
1:C:13:ALA:O	1:C:16:LYS:HB2	2.18	0.43
1:C:47:THR:HG21	1:E:196:THR:O	2.18	0.43
1:C:192:PHE:CD1	1:C:192:PHE:C	2.90	0.43
1:C:197:SER:O	1:D:131:LEU:HD13	2.18	0.43
1:E:42:ILE:CG2	1:E:208:ILE:HG12	2.42	0.43
1:E:104:THR:O	1:E:107:ILE:HB	2.18	0.43
1:F:141:PHE:CD1	1:F:211:VAL:HG11	2.53	0.43
1:H:83:PHE:O	1:H:87:ASN:ND2	2.51	0.43
1:J:83:PHE:CD2	1:J:112:TRP:CD1	3.07	0.43
1:J:203:VAL:HA	1:J:206:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LYS:C	1:B:107:ILE:HD11	2.38	0.43
1:C:62:ILE:HD11	1:D:48:ILE:HG12	2.00	0.43
1:C:151:MET:HG3	1:C:152:PRO:CD	2.44	0.43
1:C:231:VAL:O	1:C:235:LEU:HG	2.17	0.43
1:D:205:ASN:HA	1:D:208:ILE:HD12	2.00	0.43
1:E:88:MET:HB2	1:E:168:CYS:SG	2.59	0.43
1:F:235:LEU:O	1:F:236:GLY:C	2.55	0.43
1:G:113:VAL:O	1:G:116:LEU:HB3	2.18	0.43
1:G:159:ARG:HE	1:J:131:LEU:HD21	1.84	0.43
1:H:88:MET:HE3	1:H:88:MET:HB3	1.88	0.43
1:I:163:CYS:HB3	1:I:200:GLU:O	2.19	0.43
1:A:158:PHE:HD1	1:A:161:ILE:HD12	1.82	0.43
1:H:158:PHE:HD1	1:I:125:ILE:HG23	1.84	0.43
1:I:6:LEU:HD13	1:I:250:TYR:HA	2.01	0.43
1:J:83:PHE:O	1:J:87:ASN:ND2	2.52	0.43
1:C:179:SER:HB3	1:C:182:ALA:HB3	2.00	0.43
1:D:2:HIS:CE1	1:D:252:LEU:HD22	2.53	0.43
1:E:17:ILE:HG12	1:E:103:ASP:OD1	2.18	0.43
1:E:43:LEU:HD22	1:E:126:PHE:CD2	2.54	0.43
1:J:10:THR:HG23	1:J:93:GLY:CA	2.48	0.43
1:J:148:LYS:HB3	1:J:229:ASN:ND2	2.34	0.43
1:D:194:PHE:HD1	1:D:199:PHE:HB2	1.84	0.43
1:E:169:VAL:CG1	1:E:170:SER:N	2.81	0.43
1:E:209:TYR:CD1	1:E:221:VAL:HG11	2.53	0.43
1:E:243:LEU:O	1:E:243:LEU:HD23	2.19	0.43
1:G:124:ILE:HG12	1:G:214:PHE:CE2	2.54	0.43
1:C:193:ALA:HA	1:D:44:LEU:HD13	1.99	0.43
1:D:29:VAL:O	1:D:32:ALA:HB3	2.19	0.43
1:D:133:ASP:O	1:D:134:LYS:CB	2.67	0.43
1:D:163:CYS:SG	1:D:201:HIS:HD2	2.42	0.43
1:E:223:ILE:HG22	1:E:223:ILE:O	2.19	0.43
1:F:17:ILE:HG23	1:F:18:ASN:N	2.34	0.43
1:F:248:GLY:O	1:F:249:THR:C	2.57	0.43
1:B:217:THR:O	1:B:218:ILE:CB	2.65	0.43
1:C:37:TYR:O	1:C:40:ILE:HB	2.18	0.43
1:D:90:MET:HE1	1:D:107:ILE:HG13	2.01	0.43
1:D:104:THR:CG2	1:D:105:SER:N	2.82	0.43
1:F:61:LYS:HB2	1:F:61:LYS:NZ	2.34	0.43
1:F:107:ILE:HD13	1:F:107:ILE:HA	1.85	0.43
1:G:220:THR:O	1:G:221:VAL:CG1	2.65	0.43
1:I:4:GLU:O	1:I:8:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10:THR:O	1:I:14:ILE:HD12	2.19	0.43
1:A:70:ILE:HD12	1:D:193:ALA:HB2	2.01	0.42
1:B:176:ARG:O	1:B:177:THR:HB	2.19	0.42
1:B:247:LEU:O	1:B:250:TYR:HB3	2.18	0.42
1:C:116:LEU:HD12	1:C:116:LEU:O	2.18	0.42
1:E:74:LEU:HD23	1:E:74:LEU:HA	1.83	0.42
1:F:40:ILE:HD13	1:I:166:LEU:HD21	2.02	0.42
1:J:192:PHE:O	1:J:196:THR:HB	2.18	0.42
1:A:45:ILE:HA	1:A:48:ILE:HD12	2.01	0.42
1:A:83:PHE:HA	1:A:86:ASN:HD22	1.83	0.42
1:A:113:VAL:O	1:A:117:ILE:HG13	2.19	0.42
1:A:174:SER:HA	1:A:183:LYS:HG2	2.01	0.42
1:D:38:VAL:HA	1:D:71:ALA:HB1	2.01	0.42
1:E:254:LYS:O	1:E:256:LYS:N	2.52	0.42
1:I:252:LEU:HA	1:I:252:LEU:HD23	1.74	0.42
1:C:17:ILE:HG12	1:C:103:ASP:CB	2.46	0.42
1:C:28:LEU:HD23	1:C:28:LEU:HA	1.76	0.42
1:E:86:ASN:HA	1:E:89:VAL:HB	2.01	0.42
1:H:37:TYR:CE1	1:J:169:VAL:HG21	2.55	0.42
1:H:139:GLU:O	1:H:143:ASN:ND2	2.52	0.42
1:I:16:LYS:HE2	1:I:89:VAL:HG11	2.01	0.42
1:J:37:TYR:C	1:J:39:GLY:N	2.72	0.42
1:J:170:SER:O	1:J:173:CYS:HB2	2.19	0.42
1:C:227:ILE:HD13	1:C:227:ILE:H	1.84	0.42
1:E:171:VAL:O	1:E:174:SER:OG	2.22	0.42
1:A:102:LYS:HE2	1:A:102:LYS:HB2	1.82	0.42
1:A:186:MET:SD	1:B:77:MET:HG3	2.60	0.42
1:C:94:MET:CE	1:C:95:LEU:HD23	2.50	0.42
1:F:189:LEU:HD13	1:G:70:ILE:HA	2.01	0.42
1:H:37:TYR:CZ	1:J:169:VAL:HG21	2.54	0.42
1:I:180:ASP:O	1:I:183:LYS:HB2	2.20	0.42
1:J:155:ALA:O	1:J:157:PHE:N	2.52	0.42
1:B:148:LYS:HB3	1:B:229:ASN:HD21	1.85	0.42
1:G:254:LYS:CG	1:G:256:LYS:HG2	2.49	0.42
1:H:4:GLU:O	1:H:8:LYS:HG3	2.19	0.42
1:I:13:ALA:HB1	1:I:90:MET:CE	2.49	0.42
1:I:24:LYS:HE3	1:I:110:TYR:CZ	2.53	0.42
1:I:90:MET:O	1:I:91:SER:C	2.58	0.42
1:B:42:ILE:HG21	1:B:208:ILE:HG12	2.02	0.42
1:C:250:TYR:CZ	1:C:254:LYS:HG2	2.53	0.42
1:F:128:GLY:O	1:I:158:PHE:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:LEU:HA	1:H:252:LEU:HD23	1.77	0.42
1:I:119:ALA:O	1:I:120:LEU:C	2.57	0.42
1:B:218:ILE:HG23	1:B:219:SER:C	2.40	0.42
1:D:218:ILE:HG23	1:D:219:SER:O	2.20	0.42
1:F:31:SER:O	1:F:115:ASN:ND2	2.51	0.42
1:G:17:ILE:O	1:G:17:ILE:HD12	2.20	0.42
1:I:217:THR:O	1:I:217:THR:OG1	2.38	0.42
1:J:26:LYS:O	1:J:28:LEU:N	2.53	0.42
1:A:107:ILE:O	1:A:108:TRP:C	2.58	0.42
1:C:151:MET:O	1:C:228:TYR:OH	2.20	0.42
1:D:33:PHE:HD1	1:D:33:PHE:HA	1.75	0.42
1:E:19:LEU:HD12	1:E:19:LEU:O	2.20	0.42
1:F:217:THR:O	1:F:218:ILE:CG2	2.54	0.42
1:G:151:MET:HA	1:G:152:PRO:HD3	1.91	0.42
1:H:76:ILE:HD11	1:H:171:VAL:CG2	2.47	0.42
1:I:60:THR:O	1:I:64:MET:HG3	2.20	0.42
1:A:88:MET:HB2	1:A:168:CYS:SG	2.59	0.42
1:A:162:LEU:HA	1:A:165:ILE:HD12	2.01	0.42
1:E:14:ILE:HG22	1:E:15:ASN:N	2.35	0.42
1:F:9:LEU:HD23	1:F:175:PHE:CE2	2.55	0.42
1:H:72:LEU:HD12	1:H:72:LEU:HA	1.67	0.42
1:H:88:MET:HG3	1:H:245:MET:CB	2.49	0.42
1:I:69:ALA:HB2	1:I:188:PHE:HA	2.01	0.42
1:I:151:MET:HA	1:I:152:PRO:HD3	1.93	0.42
1:A:187:ILE:HG22	1:A:191:LEU:HD13	2.00	0.41
1:D:134:LYS:HB2	1:D:134:LYS:HE3	1.76	0.41
1:H:25:VAL:O	1:H:29:VAL:HG23	2.20	0.41
1:I:107:ILE:HD13	1:I:107:ILE:HA	1.91	0.41
1:J:47:THR:O	1:J:51:LEU:CD1	2.68	0.41
1:A:14:ILE:C	1:A:16:LYS:H	2.23	0.41
1:D:157:PHE:HD2	1:D:158:PHE:CE1	2.38	0.41
1:F:46:PHE:CZ	1:F:208:ILE:HG12	2.55	0.41
1:G:39:GLY:HA2	1:G:207:THR:HG21	2.01	0.41
1:G:85:GLY:C	1:G:87:ASN:N	2.73	0.41
1:G:203:VAL:HA	1:G:206:MET:SD	2.60	0.41
1:H:181:THR:HG23	1:J:185:ILE:HD12	2.02	0.41
1:H:231:VAL:O	1:H:235:LEU:HB2	2.20	0.41
1:I:13:ALA:HB1	1:I:90:MET:HE1	2.02	0.41
1:A:29:VAL:O	1:A:32:ALA:N	2.52	0.41
1:A:123:GLY:O	1:A:127:VAL:HG23	2.19	0.41
1:B:163:CYS:SG	1:B:164:ASN:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ILE:HG21	1:B:220:THR:HG23	2.02	0.41
1:C:83:PHE:O	1:C:85:GLY:N	2.54	0.41
1:F:32:ALA:HA	1:F:114:GLY:O	2.19	0.41
1:G:10:THR:HG22	1:G:14:ILE:HD11	2.03	0.41
1:G:159:ARG:HB3	1:G:199:PHE:HA	2.02	0.41
1:I:9:LEU:HD23	1:I:9:LEU:HA	1.90	0.41
1:I:163:CYS:CB	1:I:200:GLU:O	2.69	0.41
1:D:174:SER:HA	1:D:183:LYS:HG2	2.01	0.41
1:E:218:ILE:HD13	1:G:218:ILE:CA	2.47	0.41
1:F:189:LEU:HB3	1:G:70:ILE:HG13	2.03	0.41
1:J:247:LEU:HG	1:J:251:ILE:HD11	2.02	0.41
1:A:145:ALA:O	1:A:221:VAL:HG11	2.20	0.41
1:A:201:HIS:CE1	1:A:203:VAL:HB	2.56	0.41
1:C:256:LYS:H	1:C:256:LYS:HG3	1.51	0.41
1:D:36:LEU:C	1:D:36:LEU:HD23	2.41	0.41
1:F:215:SER:HB3	1:F:218:ILE:HD11	2.01	0.41
1:G:213:LEU:HD22	1:G:213:LEU:HA	1.89	0.41
1:H:247:LEU:O	1:H:247:LEU:HD12	2.19	0.41
1:I:70:ILE:O	1:I:74:LEU:HG	2.20	0.41
1:A:197:SER:HA	1:B:47:THR:HG21	2.03	0.41
1:B:33:PHE:HD1	1:B:33:PHE:HA	1.69	0.41
1:B:102:LYS:O	1:B:106:LYS:HB2	2.20	0.41
1:C:176:ARG:NE	1:D:77:MET:O	2.53	0.41
1:F:159:ARG:O	1:F:199:PHE:HB3	2.21	0.41
1:H:95:LEU:O	1:H:250:TYR:CE2	2.73	0.41
1:J:83:PHE:CD1	1:J:84:THR:N	2.88	0.41
1:C:6:LEU:HD12	1:C:6:LEU:O	2.20	0.41
1:D:74:LEU:HA	1:D:74:LEU:HD23	1.71	0.41
1:D:155:ALA:O	1:D:157:PHE:N	2.53	0.41
1:D:163:CYS:O	1:D:167:VAL:HG23	2.21	0.41
1:E:119:ALA:HB1	1:E:207:THR:N	2.35	0.41
1:E:148:LYS:HD3	1:E:200:GLU:OE1	2.21	0.41
1:F:110:TYR:HD1	1:F:110:TYR:N	2.19	0.41
1:F:155:ALA:O	1:F:156:LEU:C	2.58	0.41
1:G:218:ILE:O	1:G:219:SER:CB	2.68	0.41
1:G:220:THR:O	1:G:220:THR:OG1	2.39	0.41
1:G:223:ILE:HG22	1:G:224:GLY:N	2.35	0.41
1:H:83:PHE:HZ	1:H:238:ILE:HD11	1.86	0.41
1:I:87:ASN:O	1:I:91:SER:CB	2.61	0.41
1:J:48:ILE:HG22	1:J:49:GLY:N	2.35	0.41
1:B:163:CYS:SG	1:B:201:HIS:HB2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:HD11	1:C:96:ASN:CB	2.50	0.41
1:E:35:GLY:H	1:E:115:ASN:HD22	1.68	0.41
1:E:225:GLY:O	1:E:226:ALA:C	2.59	0.41
1:F:123:GLY:O	1:F:127:VAL:HG23	2.20	0.41
1:F:165:ILE:HD13	1:F:165:ILE:HG21	1.88	0.41
1:G:73:SER:OG	1:G:184:ILE:HG23	2.21	0.41
1:G:75:VAL:HG12	1:G:76:ILE:N	2.34	0.41
1:G:127:VAL:C	1:G:129:THR:H	2.24	0.41
1:J:51:LEU:H	1:J:51:LEU:CD1	2.27	0.41
1:B:40:ILE:HA	1:B:43:LEU:HG	2.02	0.41
1:B:62:ILE:HA	1:B:196:THR:CG2	2.50	0.41
1:C:247:LEU:HG	1:C:251:ILE:HD11	2.02	0.41
1:D:217:THR:O	1:D:218:ILE:HB	2.21	0.41
1:F:164:ASN:O	1:F:168:CYS:HB2	2.20	0.41
1:F:227:ILE:H	1:F:227:ILE:HG12	1.56	0.41
1:G:222:THR:HB	1:G:223:ILE:H	1.61	0.41
1:H:58:PRO:C	1:H:60:THR:H	2.23	0.41
1:H:192:PHE:C	1:H:192:PHE:CD1	2.90	0.41
1:H:213:LEU:HD11	1:H:223:ILE:HG13	2.03	0.41
1:I:33:PHE:HD1	1:I:33:PHE:HA	1.73	0.41
1:I:100:SER:C	1:I:102:LYS:N	2.74	0.41
1:J:132:VAL:CA	1:J:138:ALA:HB2	2.46	0.41
1:J:174:SER:HA	1:J:183:LYS:HG2	2.03	0.41
1:B:83:PHE:CD2	1:B:112:TRP:CD1	3.08	0.41
1:B:169:VAL:HG21	1:E:37:TYR:CE1	2.55	0.41
1:C:31:SER:CB	1:C:114:GLY:HA3	2.51	0.41
1:E:72:LEU:HD12	1:E:72:LEU:HA	1.85	0.41
1:E:83:PHE:CD1	1:E:83:PHE:C	2.94	0.41
1:F:101:ILE:HD12	1:F:101:ILE:N	2.27	0.41
1:H:93:GLY:C	1:H:95:LEU:N	2.72	0.41
1:H:209:TYR:O	1:H:213:LEU:N	2.47	0.41
1:J:84:THR:HG22	1:J:164:ASN:CG	2.41	0.41
1:A:65:GLY:O	1:A:192:PHE:HA	2.21	0.40
1:A:91:SER:OG	1:A:92:ALA:N	2.54	0.40
1:E:151:MET:HA	1:E:152:PRO:HD3	1.96	0.40
1:F:36:LEU:HD12	1:F:122:LEU:HB2	2.02	0.40
1:F:122:LEU:HD23	1:F:207:THR:CG2	2.50	0.40
1:F:179:SER:HB3	1:F:182:ALA:CB	2.51	0.40
1:G:39:GLY:O	1:G:42:ILE:N	2.43	0.40
1:G:240:GLY:O	1:G:244:PHE:HB2	2.21	0.40
1:I:174:SER:HA	1:I:183:LYS:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:203:VAL:O	1:I:206:MET:HB2	2.21	0.40
1:C:161:ILE:HG23	1:C:240:GLY:CA	2.50	0.40
1:E:87:ASN:O	1:E:91:SER:OG	2.28	0.40
1:J:166:LEU:CD1	1:J:194:PHE:HB3	2.50	0.40
1:A:37:TYR:CE1	1:D:169:VAL:HG21	2.56	0.40
1:A:59:MET:O	1:A:62:ILE:HB	2.21	0.40
1:A:84:THR:HG21	1:A:201:HIS:CD2	2.55	0.40
1:C:83:PHE:O	1:C:84:THR:C	2.60	0.40
1:C:162:LEU:HD11	1:D:125:ILE:HG22	2.03	0.40
1:D:9:LEU:HD23	1:D:175:PHE:CE2	2.56	0.40
1:D:207:THR:HA	1:D:210:SER:HB3	2.02	0.40
1:F:148:LYS:HB3	1:F:229:ASN:ND2	2.36	0.40
1:H:34:ALA:CB	1:H:81:GLU:O	2.69	0.40
1:H:240:GLY:HA2	1:H:244:PHE:HD2	1.86	0.40
1:I:36:LEU:HD23	1:I:36:LEU:C	2.40	0.40
1:B:87:ASN:OD1	1:B:238:ILE:HG12	2.22	0.40
1:C:153:PHE:CD2	1:C:232:ALA:HB2	2.56	0.40
1:D:9:LEU:HD21	1:D:88:MET:HE2	2.03	0.40
1:D:66:LEU:HA	1:D:66:LEU:HD23	1.76	0.40
1:E:35:GLY:H	1:E:115:ASN:ND2	2.19	0.40
1:G:157:PHE:O	1:G:161:ILE:HG13	2.20	0.40
1:H:157:PHE:CZ	1:H:239:VAL:HG21	2.56	0.40
1:I:68:PHE:CD2	1:I:195:ILE:HG13	2.56	0.40
1:I:108:TRP:O	1:I:112:TRP:HB2	2.20	0.40
1:J:229:ASN:O	1:J:233:VAL:HG23	2.21	0.40
1:B:238:ILE:O	1:B:242:ALA:HB3	2.20	0.40
1:C:16:LYS:NZ	1:C:81:GLU:OE2	2.39	0.40
1:D:20:LEU:HD11	1:D:110:TYR:CD2	2.57	0.40
1:F:42:ILE:HA	1:F:45:ILE:HG12	2.04	0.40
1:F:166:LEU:HG	1:G:40:ILE:HD13	2.03	0.40
1:G:192:PHE:CE2	1:J:67:SER:OG	2.74	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	254/268 (95%)	205 (81%)	34 (13%)	15 (6%)	1	12
1	B	254/268 (95%)	209 (82%)	35 (14%)	10 (4%)	3	22
1	C	255/268 (95%)	209 (82%)	35 (14%)	11 (4%)	2	20
1	D	254/268 (95%)	217 (85%)	27 (11%)	10 (4%)	3	22
1	E	254/268 (95%)	203 (80%)	38 (15%)	13 (5%)	2	15
1	F	254/268 (95%)	203 (80%)	35 (14%)	16 (6%)	1	10
1	G	254/268 (95%)	206 (81%)	40 (16%)	8 (3%)	4	26
1	H	254/268 (95%)	199 (78%)	39 (15%)	16 (6%)	1	10
1	I	254/268 (95%)	222 (87%)	29 (11%)	3 (1%)	13	49
1	J	254/268 (95%)	208 (82%)	37 (15%)	9 (4%)	3	24
All	All	2541/2680 (95%)	2081 (82%)	349 (14%)	111 (4%)	2	19

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ALA
1	A	108	TRP
1	C	218	ILE
1	D	60	THR
1	D	223	ILE
1	F	193	ALA
1	F	218	ILE
1	F	219	SER
1	F	227	ILE
1	G	143	ASN
1	G	219	SER
1	G	223	ILE
1	H	218	ILE
1	H	224	GLY
1	I	91	SER
1	I	218	ILE
1	J	218	ILE
1	J	220	THR
1	A	89	VAL
1	A	90	MET
1	A	107	ILE
1	A	255	GLU

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Mol	Chain	Res	Type
1	B	56	GLY
1	B	218	ILE
1	C	79	GLY
1	C	162	LEU
1	C	222	THR
1	D	134	LYS
1	D	143	ASN
1	D	218	ILE
1	D	220	THR
1	D	222	THR
1	E	79	GLY
1	E	217	THR
1	E	218	ILE
1	E	222	THR
1	E	255	GLU
1	F	50	GLY
1	F	54	ASP
1	F	59	MET
1	G	142	ALA
1	G	146	ALA
1	G	218	ILE
1	G	224	GLY
1	H	59	MET
1	H	89	VAL
1	H	128	GLY
1	H	221	VAL
1	J	71	ALA
1	A	218	ILE
1	B	90	MET
1	B	97	LYS
1	C	83	PHE
1	C	161	ILE
1	D	156	LEU
1	E	146	ALA
1	F	128	GLY
1	F	226	ALA
1	F	250	TYR
1	H	71	ALA
1	H	142	ALA
1	I	222	THR
1	J	26	LYS
1	J	27	TYR

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Mol	Chain	Res	Type
1	J	155	ALA
1	J	210	SER
1	A	193	ALA
1	A	220	THR
1	B	48	ILE
1	D	221	VAL
1	E	15	ASN
1	E	71	ALA
1	E	155	ALA
1	F	220	THR
1	F	251	ILE
1	H	54	ASP
1	J	133	ASP
1	J	156	LEU
1	A	72	LEU
1	A	152	PRO
1	A	230	LEU
1	B	49	GLY
1	B	79	GLY
1	B	80	THR
1	B	134	LYS
1	B	163	CYS
1	C	14	ILE
1	C	84	THR
1	C	150	SER
1	E	213	LEU
1	F	146	ALA
1	H	154	THR
1	H	193	ALA
1	H	220	THR
1	A	15	ASN
1	A	49	GLY
1	E	14	ILE
1	E	226	ALA
1	F	222	THR
1	H	90	MET
1	H	246	GLY
1	C	221	VAL
1	D	75	VAL
1	H	35	GLY
1	H	223	ILE
1	A	48	ILE

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Mol	Chain	Res	Type
1	E	161	ILE
1	F	124	ILE
1	G	50	GLY
1	C	132	VAL
1	F	239	VAL

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	205/214 (96%)	181 (88%)	24 (12%)	5	23
1	B	206/214 (96%)	178 (86%)	28 (14%)	3	17
1	C	207/214 (97%)	188 (91%)	19 (9%)	9	33
1	D	206/214 (96%)	186 (90%)	20 (10%)	8	31
1	E	206/214 (96%)	179 (87%)	27 (13%)	4	19
1	F	205/214 (96%)	189 (92%)	16 (8%)	12	43
1	G	206/214 (96%)	182 (88%)	24 (12%)	5	23
1	H	206/214 (96%)	178 (86%)	28 (14%)	3	17
1	I	206/214 (96%)	193 (94%)	13 (6%)	18	52
1	J	206/214 (96%)	172 (84%)	34 (16%)	2	10
All	All	2059/2140 (96%)	1826 (89%)	233 (11%)	6	25

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	11	ASN
1	A	19	LEU
1	A	31	SER
1	A	33	PHE
1	A	40	ILE
1	A	47	THR
1	A	60	THR

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Mol	Chain	Res	Type
1	A	70	ILE
1	A	82	LEU
1	A	84	THR
1	A	91	SER
1	A	94	MET
1	A	101	ILE
1	A	134	LYS
1	A	137	VAL
1	A	154	THR
1	A	194	PHE
1	A	202	SER
1	A	217	THR
1	A	220	THR
1	A	235	LEU
1	A	243	LEU
1	A	245	MET
1	B	4	GLU
1	B	30	SER
1	B	33	PHE
1	B	45	ILE
1	B	52	LEU
1	B	53	THR
1	B	67	SER
1	B	76	ILE
1	B	80	THR
1	B	82	LEU
1	B	84	THR
1	B	94	MET
1	B	95	LEU
1	B	99	VAL
1	B	132	VAL
1	B	133	ASP
1	B	134	LYS
1	B	139	GLU
1	B	141	PHE
1	B	144	THR
1	B	163	CYS
1	B	169	VAL
1	B	194	PHE
1	B	199	PHE
1	B	218	ILE
1	B	220	THR

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Mol	Chain	Res	Type
1	B	227	ILE
1	B	255	GLU
1	C	15	ASN
1	C	40	ILE
1	C	42	ILE
1	C	51	LEU
1	C	53	THR
1	C	59	MET
1	C	99	VAL
1	C	101	ILE
1	C	116	LEU
1	C	131	LEU
1	C	132	VAL
1	C	156	LEU
1	C	174	SER
1	C	192	PHE
1	C	194	PHE
1	C	218	ILE
1	C	227	ILE
1	C	249	THR
1	C	256	LYS
1	D	15	ASN
1	D	17	ILE
1	D	33	PHE
1	D	43	LEU
1	D	52	LEU
1	D	63	VAL
1	D	84	THR
1	D	91	SER
1	D	102	LYS
1	D	104	THR
1	D	143	ASN
1	D	161	ILE
1	D	163	CYS
1	D	170	SER
1	D	194	PHE
1	D	195	ILE
1	D	217	THR
1	D	218	ILE
1	D	221	VAL
1	D	245	MET
1	E	10	THR

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Mol	Chain	Res	Type
1	E	26	LYS
1	E	45	ILE
1	E	73	SER
1	E	76	ILE
1	E	80	THR
1	E	94	MET
1	E	99	VAL
1	E	102	LYS
1	E	105	SER
1	E	106	LYS
1	E	132	VAL
1	E	134	LYS
1	E	147	SER
1	E	154	THR
1	E	156	LEU
1	E	194	PHE
1	E	210	SER
1	E	217	THR
1	E	218	ILE
1	E	220	THR
1	E	221	VAL
1	E	222	THR
1	E	243	LEU
1	E	247	LEU
1	E	252	LEU
1	E	255	GLU
1	F	33	PHE
1	F	36	LEU
1	F	73	SER
1	F	94	MET
1	F	97	LYS
1	F	134	LYS
1	F	153	PHE
1	F	169	VAL
1	F	174	SER
1	F	181	THR
1	F	194	PHE
1	F	217	THR
1	F	218	ILE
1	F	220	THR
1	F	223	ILE
1	F	227	ILE

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Mol	Chain	Res	Type
1	G	3	LYS
1	G	4	GLU
1	G	31	SER
1	G	54	ASP
1	G	70	ILE
1	G	73	SER
1	G	101	ILE
1	G	111	SER
1	G	132	VAL
1	G	144	THR
1	G	163	CYS
1	G	170	SER
1	G	176	ARG
1	G	187	ILE
1	G	194	PHE
1	G	196	THR
1	G	213	LEU
1	G	217	THR
1	G	220	THR
1	G	227	ILE
1	G	243	LEU
1	G	245	MET
1	G	247	LEU
1	G	254	LYS
1	H	10	THR
1	H	22	THR
1	H	24	LYS
1	H	33	PHE
1	H	36	LEU
1	H	51	LEU
1	H	72	LEU
1	H	84	THR
1	H	88	MET
1	H	91	SER
1	H	94	MET
1	H	103	ASP
1	H	105	SER
1	H	115	ASN
1	H	116	LEU
1	H	131	LEU
1	H	133	ASP
1	H	134	LYS

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Mol	Chain	Res	Type
1	H	143	ASN
1	H	150	SER
1	H	192	PHE
1	H	194	PHE
1	H	195	ILE
1	H	213	LEU
1	H	218	ILE
1	H	221	VAL
1	H	227	ILE
1	H	235	LEU
1	I	14	ILE
1	I	33	PHE
1	I	40	ILE
1	I	52	LEU
1	I	53	THR
1	I	80	THR
1	I	103	ASP
1	I	163	CYS
1	I	194	PHE
1	I	214	PHE
1	I	217	THR
1	I	218	ILE
1	I	243	LEU
1	J	19	LEU
1	J	30	SER
1	J	36	LEU
1	J	48	ILE
1	J	51	LEU
1	J	52	LEU
1	J	53	THR
1	J	59	MET
1	J	62	ILE
1	J	84	THR
1	J	90	MET
1	J	94	MET
1	J	99	VAL
1	J	101	ILE
1	J	102	LYS
1	J	125	ILE
1	J	129	THR
1	J	132	VAL
1	J	137	VAL

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Mol	Chain	Res	Type
1	J	147	SER
1	J	148	LYS
1	J	150	SER
1	J	154	THR
1	J	156	LEU
1	J	168	CYS
1	J	194	PHE
1	J	196	THR
1	J	213	LEU
1	J	218	ILE
1	J	220	THR
1	J	221	VAL
1	J	251	ILE
1	J	255	GLU
1	J	256	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	B	229	ASN
1	C	2	HIS
1	C	11	ASN
1	C	15	ASN
1	D	87	ASN
1	D	201	HIS
1	E	87	ASN
1	E	115	ASN
1	F	87	ASN
1	G	18	ASN
1	G	86	ASN
1	G	237	ASN
1	H	115	ASN
1	H	143	ASN
1	I	2	HIS
1	J	2	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PG4	I	266	-	12,12,12	1.02	0	11,11,11	1.16	2 (18%)

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	PG4	I	266	-	-	6/10/10/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	266	PG4	C3-O2-C2	2.40	123.70	113.29
2	I	266	PG4	C7-O4-C6	2.20	122.81	113.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	266	PG4	O3-C5-C6-O4
2	I	266	PG4	O1-C1-C2-O2
2	I	266	PG4	O4-C7-C8-O5
2	I	266	PG4	O2-C3-C4-O3
2	I	266	PG4	C1-C2-O2-C3
2	I	266	PG4	C6-C5-O3-C4

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	266	PG4	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	256/268 (95%)	0.38	18 (7%)	16	9	83, 133, 178, 215	0
1	B	256/268 (95%)	0.35	22 (8%)	10	5	70, 135, 181, 243	0
1	C	257/268 (95%)	0.08	11 (4%)	35	22	61, 103, 143, 201	0
1	D	256/268 (95%)	0.19	15 (5%)	22	13	67, 111, 156, 183	0
1	E	256/268 (95%)	0.09	9 (3%)	44	28	59, 101, 140, 181	0
1	F	256/268 (95%)	-0.15	1 (0%)	92	89	41, 70, 108, 162	0
1	G	256/268 (95%)	-0.08	3 (1%)	79	67	50, 92, 133, 175	0
1	H	256/268 (95%)	-0.06	3 (1%)	79	67	48, 91, 135, 170	0
1	I	256/268 (95%)	-0.27	2 (0%)	86	78	35, 64, 97, 148	0
1	J	256/268 (95%)	0.07	9 (3%)	44	28	56, 103, 146, 183	0
All	All	2561/2680 (95%)	0.06	93 (3%)	42	27	35, 100, 157, 243	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	LYS	5.7
1	A	217	THR	5.1
1	B	133	ASP	5.0
1	A	216	PRO	4.6
1	B	13	ALA	4.5
1	B	217	THR	4.5
1	B	216	PRO	4.4
1	B	236	GLY	4.4
1	C	251	ILE	4.3
1	A	179	SER	4.2
1	B	108	TRP	4.1
1	E	135	GLY	4.0
1	D	154	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	237	ASN	3.7
1	J	220	THR	3.6
1	A	199	PHE	3.5
1	J	148	LYS	3.5
1	D	25	VAL	3.4
1	D	223	ILE	3.4
1	A	21	ASN	3.4
1	E	134	LYS	3.4
1	A	214	PHE	3.4
1	E	253	GLY	3.3
1	A	178	ASN	3.2
1	A	212	SER	3.2
1	D	157	PHE	3.2
1	A	133	ASP	3.1
1	E	20	LEU	3.1
1	D	26	LYS	3.1
1	J	69	ALA	3.1
1	D	252	LEU	3.1
1	D	214	PHE	3.0
1	H	24	LYS	2.9
1	H	220	THR	2.9
1	B	181	THR	2.8
1	E	28	LEU	2.8
1	B	97	LYS	2.8
1	B	69	ALA	2.8
1	J	149	ALA	2.8
1	C	249	THR	2.8
1	C	219	SER	2.7
1	C	18	ASN	2.7
1	B	218	ILE	2.7
1	J	147	SER	2.6
1	D	250	TYR	2.6
1	B	178	ASN	2.5
1	B	162	LEU	2.5
1	B	233	VAL	2.5
1	B	14	ILE	2.5
1	B	105	SER	2.4
1	C	30	SER	2.4
1	C	81	GLU	2.4
1	I	22	THR	2.4
1	F	219	SER	2.4
1	D	213	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	235	LEU	2.4
1	A	200	GLU	2.4
1	B	220	THR	2.4
1	G	179	SER	2.4
1	J	154	THR	2.4
1	A	67	SER	2.4
1	C	214	PHE	2.4
1	A	24	LYS	2.4
1	H	110	TYR	2.4
1	I	254	LYS	2.3
1	J	174	SER	2.3
1	J	67	SER	2.3
1	B	229	ASN	2.3
1	A	215	SER	2.3
1	G	139	GLU	2.3
1	A	173	CYS	2.3
1	E	10	THR	2.3
1	G	181	THR	2.3
1	A	134	LYS	2.3
1	D	24	LYS	2.3
1	B	157	PHE	2.2
1	D	158	PHE	2.2
1	D	181	THR	2.2
1	C	252	LEU	2.2
1	B	67	SER	2.2
1	B	179	SER	2.2
1	B	227	ILE	2.2
1	D	153	PHE	2.1
1	E	31	SER	2.1
1	B	73	SER	2.1
1	D	80	THR	2.1
1	C	26	LYS	2.1
1	E	80	THR	2.1
1	D	254	LYS	2.1
1	J	143	ASN	2.0
1	A	20	LEU	2.0
1	C	127	VAL	2.0
1	C	181	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PG4	I	266	13/13	0.90	0.28	71,89,116,131	0

6.5 Other polymers (i)

There are no such residues in this entry.