Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:17 PM GMT

PDB ID	:	1WYZ
Title	:	X-Ray structure of the putative methyltransferase from Bacteroides thetaiotaomicron VPI-5482 at the resolution 2.5 A. Norteast Structural Genomics Consortium target Btr28
Authors	:	Kuzin, A.P.; Chen, Y.; Forouhar, F.; Vorobiev, S.M.; Acton, T.; Ma, L.-C.; Xiao, R.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2005-02-21
Resolution	:	2.50 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

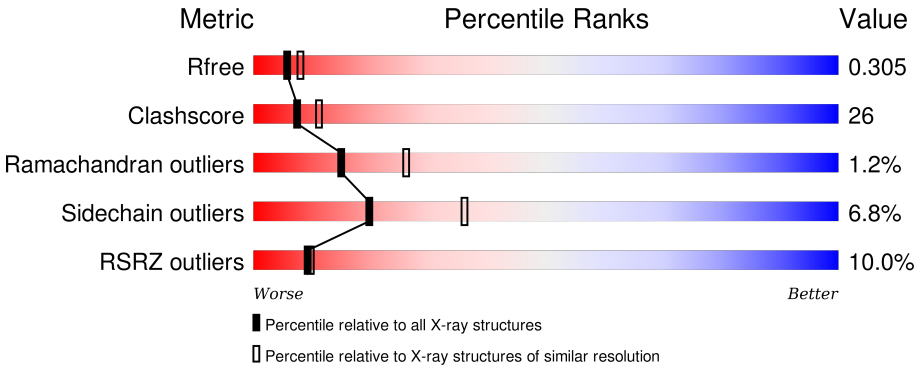
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	242	10% 45% 43% • 8%
1	B	242	7% 54% 35% 5% 6%
1	C	242	12% 50% 40% • 8%
1	D	242	7% 54% 36% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7245 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 putative S-adenosylmethionine-dependent methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	Se	0	0	0
			1765	1134	301	323	4	3			
1	B	227	Total	C	N	O	S	Se	0	0	0
			1796	1154	305	330	4	3			
1	C	223	Total	C	N	O	S	Se	0	0	0
			1762	1134	297	324	4	3			
1	D	227	Total	C	N	O	S	Se	0	0	0
			1796	1154	305	330	4	3			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
A	86	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
A	129	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
A	181	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
A	235	LEU	-	EXPRESSION TAG	UNP Q8A031
A	236	GLU	-	EXPRESSION TAG	UNP Q8A031
A	237	HIS	-	EXPRESSION TAG	UNP Q8A031
A	238	HIS	-	EXPRESSION TAG	UNP Q8A031
A	239	HIS	-	EXPRESSION TAG	UNP Q8A031
A	240	HIS	-	EXPRESSION TAG	UNP Q8A031
A	241	HIS	-	EXPRESSION TAG	UNP Q8A031
A	242	HIS	-	EXPRESSION TAG	UNP Q8A031
B	1	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
B	86	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
B	129	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
B	181	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
B	235	LEU	-	EXPRESSION TAG	UNP Q8A031
B	236	GLU	-	EXPRESSION TAG	UNP Q8A031
B	237	HIS	-	EXPRESSION TAG	UNP Q8A031
B	238	HIS	-	EXPRESSION TAG	UNP Q8A031
B	239	HIS	-	EXPRESSION TAG	UNP Q8A031

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Chain	Residue	Modelled	Actual	Comment	Reference
B	240	HIS	-	EXPRESSION TAG	UNP Q8A031
B	241	HIS	-	EXPRESSION TAG	UNP Q8A031
B	242	HIS	-	EXPRESSION TAG	UNP Q8A031
C	1	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
C	86	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
C	129	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
C	181	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
C	235	LEU	-	EXPRESSION TAG	UNP Q8A031
C	236	GLU	-	EXPRESSION TAG	UNP Q8A031
C	237	HIS	-	EXPRESSION TAG	UNP Q8A031
C	238	HIS	-	EXPRESSION TAG	UNP Q8A031
C	239	HIS	-	EXPRESSION TAG	UNP Q8A031
C	240	HIS	-	EXPRESSION TAG	UNP Q8A031
C	241	HIS	-	EXPRESSION TAG	UNP Q8A031
C	242	HIS	-	EXPRESSION TAG	UNP Q8A031
D	1	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
D	86	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
D	129	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
D	181	MSE	MET	MODIFIED RESIDUES	UNP Q8A031
D	235	LEU	-	EXPRESSION TAG	UNP Q8A031
D	236	GLU	-	EXPRESSION TAG	UNP Q8A031
D	237	HIS	-	EXPRESSION TAG	UNP Q8A031
D	238	HIS	-	EXPRESSION TAG	UNP Q8A031
D	239	HIS	-	EXPRESSION TAG	UNP Q8A031
D	240	HIS	-	EXPRESSION TAG	UNP Q8A031
D	241	HIS	-	EXPRESSION TAG	UNP Q8A031
D	242	HIS	-	EXPRESSION TAG	UNP Q8A031

- Molecule 2 is water.

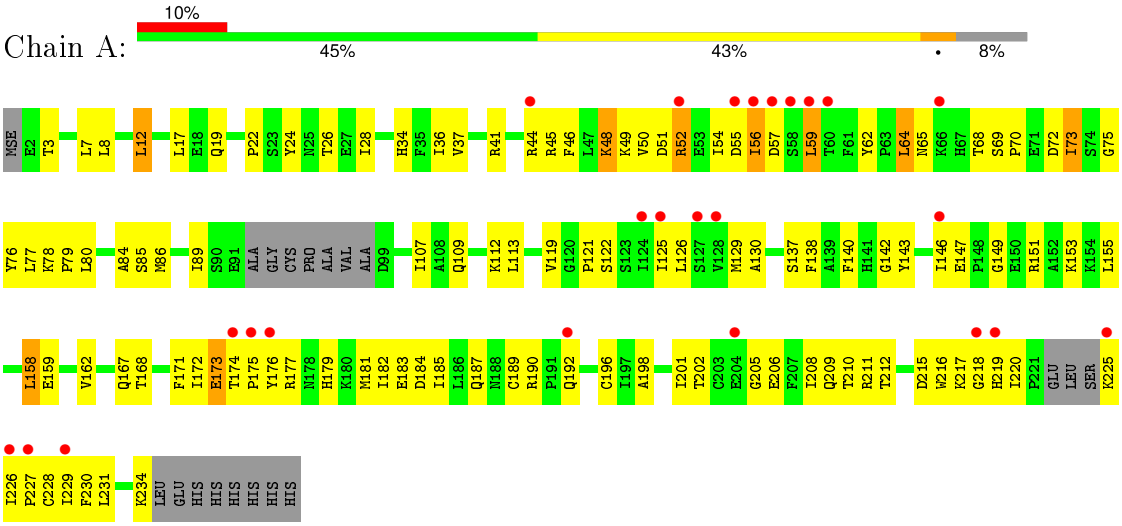
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	34	Total O 34 34	0	0
2	B	38	Total O 38 38	0	0
2	C	28	Total O 28 28	0	0
2	D	26	Total O 26 26	0	0

3 Residue-property plots (i)

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

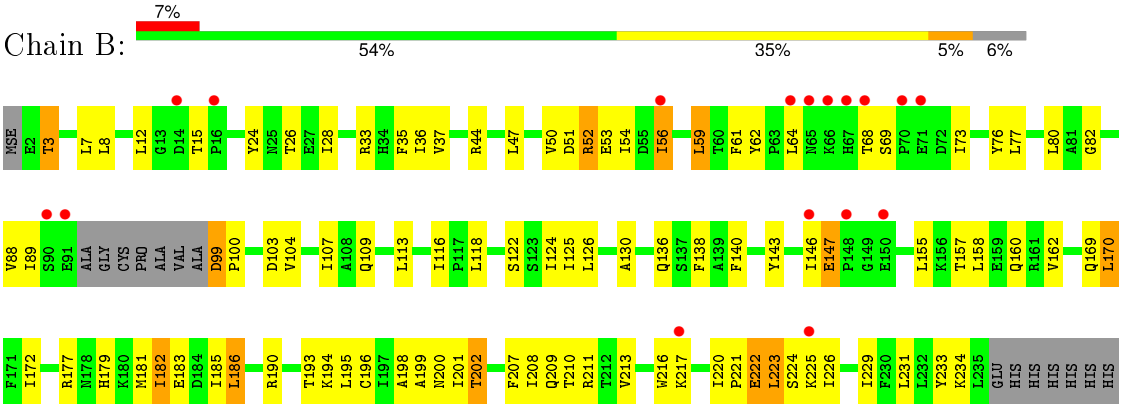
- Molecule 1: putative S-adenosylmethionine-dependent methyltransferase

Chain A:



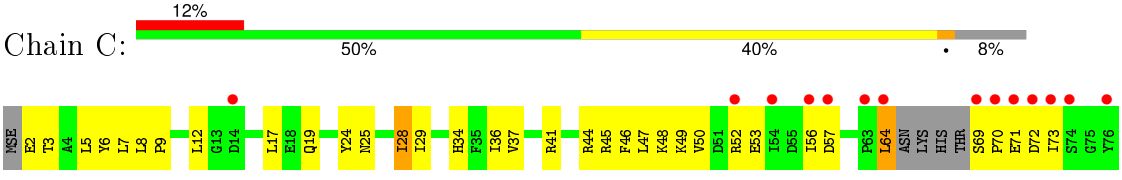
- Molecule 1: putative S-adenosylmethionine-dependent methyltransferase

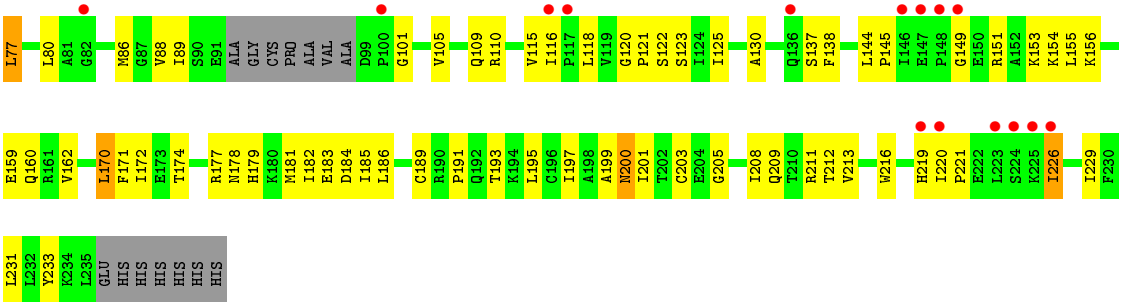
Chain B:



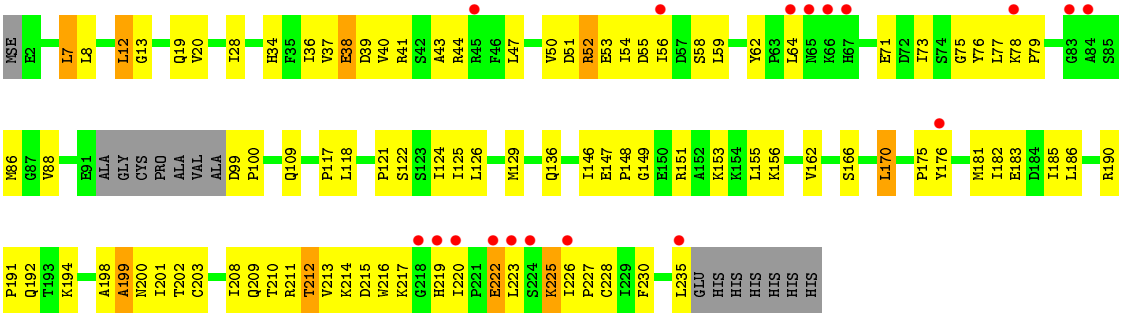
- Molecule 1: putative S-adenosylmethionine-dependent methyltransferase

Chain C:





• Molecule 1: putative S-adenosylmethionine-dependent methyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.78Å 101.54Å 108.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.74 – 2.50 28.74 – 2.49	Depositor EDS
% Data completeness (in resolution range)	88.3 (28.74-2.50) 97.1 (28.74-2.49)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.89 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.293 0.242 , 0.305	Depositor DCC
R_{free} test set	1623 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 71.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 62876 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7245	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.39	0/1798	0.66	2/2428 (0.1%)
1	B	0.40	0/1830	0.65	0/2473
1	C	0.41	0/1794	0.68	1/2423 (0.0%)
1	D	0.39	0/1830	0.64	0/2473
All	All	0.40	0/7252	0.66	3/9797 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	GLY	N-CA-C	-7.15	95.22	113.10
1	C	205	GLY	N-CA-C	-7.15	95.22	113.10
1	A	234	LYS	N-CA-C	6.44	128.38	111.00

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	1765	0	1808	121	0
1	B	1796	0	1842	99	0
1	C	1762	0	1808	89	0
1	D	1796	0	1842	86	0
2	A	34	0	0	1	0
2	B	38	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	0	1	0
2	D	26	0	0	1	0
All	All	7245	0	7300	369	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 26.

All (369) 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:C:44:ARG:HG3	1:C:56:ILE:CD1	1.54	1.37
1:C:44:ARG:CG	1:C:56:ILE:HD11	1.64	1.28
1:A:36:ILE:HD13	1:A:62:TYR:HB2	1.37	1.05
1:A:73:ILE:HB	1:A:107:ILE:HD12	1.44	1.00
1:B:36:ILE:HD13	1:B:62:TYR:HB2	1.44	0.98
1:A:181:MSE:HE2	1:A:185:ILE:HG12	1.49	0.93
1:B:36:ILE:HD11	1:B:76:TYR:HB3	1.53	0.89
1:A:155:LEU:HD22	1:A:185:ILE:HD13	1.55	0.89
1:A:146:ILE:H	1:A:146:ILE:HD12	1.38	0.88
1:C:200:ASN:HB3	1:C:203:CYS:HB2	1.58	0.84
1:D:146:ILE:HD12	1:D:146:ILE:H	1.42	0.84
1:A:36:ILE:HD11	1:A:76:TYR:HB3	1.60	0.83
1:A:159:GLU:HG2	1:A:190:ARG:HH12	1.40	0.82
1:A:73:ILE:CB	1:A:107:ILE:HD12	2.10	0.81
1:A:70:PRO:HA	1:A:107:ILE:HD11	1.61	0.81
1:A:226:ILE:HG23	1:A:227:PRO:HD2	1.61	0.81
1:D:122:SER:HB3	1:D:125:ILE:HG12	1.62	0.80
1:D:201:ILE:HD12	1:D:208:ILE:HD11	1.64	0.79
1:D:8:LEU:HD21	1:D:28:ILE:HD11	1.65	0.79
1:A:210:THR:H	1:C:109:GLN:NE2	1.79	0.79
1:B:211:ARG:HB2	1:B:216:TRP:NE1	1.98	0.78
1:B:122:SER:HB2	1:D:125:ILE:HD13	1.64	0.78
1:B:26:THR:HG23	1:B:50:VAL:HG22	1.66	0.77
1:B:181:MSE:HE3	1:B:185:ILE:HG13	1.67	0.76
1:A:181:MSE:HE3	1:A:184:ASP:HB2	1.65	0.76
1:A:44:ARG:HD3	1:A:56:ILE:HD12	1.68	0.75
1:D:12:LEU:HD13	1:D:121:PRO:HG2	1.68	0.75
1:C:155:LEU:HD11	1:C:181:MSE:HE1	1.67	0.75
1:B:210:THR:H	1:D:109:GLN:NE2	1.83	0.75
1:D:201:ILE:O	1:D:202:THR:HB	1.86	0.75
1:C:44:ARG:HG3	1:C:56:ILE:HD11	0.77	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:MSE:HE2	1:C:185:ILE:HG12	1.68	0.74
1:A:51:ASP:HB3	1:A:54:ILE:HG12	1.69	0.74
1:B:146:ILE:HD12	1:B:146:ILE:H	1.52	0.74
1:B:130:ALA:HB3	1:B:208:ILE:HG21	1.69	0.74
1:C:37:VAL:HG12	1:C:89:ILE:CG2	2.19	0.72
1:A:36:ILE:CD1	1:A:62:TYR:HB2	2.18	0.72
1:C:181:MSE:HE3	1:C:184:ASP:HB2	1.71	0.72
1:D:199:ALA:HB1	1:D:226:ILE:HD13	1.72	0.72
1:A:212:THR:HG23	1:A:215:ASP:H	1.56	0.71
1:D:222:GLU:HG2	1:D:223:LEU:H	1.55	0.71
1:C:28:ILE:HD13	1:C:29:ILE:N	2.06	0.71
1:D:200:ASN:HD21	1:D:226:ILE:HG21	1.56	0.70
1:A:182:ILE:HD12	1:A:183:GLU:N	2.07	0.69
1:B:8:LEU:HD21	1:B:28:ILE:HD11	1.74	0.69
1:D:198:ALA:HB1	1:D:201:ILE:HD11	1.75	0.68
1:A:17:LEU:HD13	1:A:49:LYS:HD2	1.76	0.68
1:A:125:ILE:HD13	1:C:122:SER:HB2	1.76	0.68
1:A:36:ILE:CD1	1:A:76:TYR:HB3	2.23	0.68
1:A:155:LEU:HD11	1:A:181:MSE:HE1	1.76	0.67
1:A:48:LYS:NZ	1:A:48:LYS:HA	2.09	0.67
1:C:25:ASN:HA	1:C:28:ILE:HD12	1.75	0.66
1:B:109:GLN:NE2	1:D:210:THR:H	1.92	0.66
1:A:68:THR:CG2	1:A:73:ILE:HD11	2.24	0.66
1:D:182:ILE:HD12	1:D:183:GLU:N	2.10	0.66
1:A:192:GLN:NE2	1:A:192:GLN:HA	2.10	0.66
1:B:220:ILE:HG13	1:B:221:PRO:HD2	1.78	0.66
1:B:36:ILE:CD1	1:B:76:TYR:HB3	2.25	0.66
1:B:44:ARG:HG3	1:B:56:ILE:CD1	2.27	0.65
1:A:19:GLN:HA	1:C:24:TYR:HB2	1.78	0.65
1:D:194:LYS:HE3	1:D:235:LEU:HG	1.78	0.65
1:B:221:PRO:HG2	1:B:223:LEU:HD23	1.80	0.64
1:A:192:GLN:HA	1:A:192:GLN:HE21	1.62	0.64
1:C:70:PRO:HA	1:C:73:ILE:HD12	1.79	0.64
1:C:44:ARG:CD	1:C:56:ILE:HD11	2.28	0.64
1:B:36:ILE:HD13	1:B:62:TYR:CB	2.26	0.64
1:A:181:MSE:HE2	1:A:185:ILE:CG1	2.26	0.64
1:B:69:SER:O	1:B:73:ILE:HD12	1.98	0.64
1:B:103:ASP:O	1:B:107:ILE:HG12	1.98	0.64
1:D:8:LEU:HD23	1:D:118:LEU:HD12	1.79	0.63
1:A:68:THR:OG1	1:A:73:ILE:HD11	1.98	0.63
1:C:179:HIS:HA	1:C:182:ILE:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ILE:HD13	1:B:183:GLU:N	2.15	0.62
1:D:222:GLU:HG2	1:D:223:LEU:N	2.14	0.62
1:B:7:LEU:HD23	1:D:129:MSE:HB3	1.81	0.62
1:C:155:LEU:HD22	1:C:185:ILE:HD13	1.82	0.62
1:B:182:ILE:O	1:B:186:LEU:HG	1.99	0.62
1:D:79:PRO:HG2	1:D:86:MSE:SE	2.50	0.61
1:D:44:ARG:HG2	1:D:56:ILE:HD11	1.82	0.61
1:B:3:THR:HG21	2:B:271:HOH:O	2.00	0.60
1:D:226:ILE:HD12	1:D:226:ILE:O	2.01	0.60
1:A:54:ILE:HD12	2:A:268:HOH:O	2.01	0.60
1:C:34:HIS:HB3	1:C:86:MSE:HE3	1.83	0.60
1:B:68:THR:HG23	1:B:73:ILE:HD11	1.84	0.60
1:B:200:ASN:OD1	1:B:226:ILE:HG12	2.01	0.60
1:B:56:ILE:HA	1:B:59:LEU:HD21	1.84	0.59
1:C:25:ASN:O	1:C:28:ILE:HD13	2.02	0.59
1:A:73:ILE:CG2	1:A:107:ILE:HD12	2.33	0.59
1:A:159:GLU:HG2	1:A:190:ARG:NH1	2.17	0.59
1:A:112:LYS:O	1:A:112:LYS:HG2	2.02	0.59
1:A:70:PRO:HA	1:A:107:ILE:CD1	2.30	0.59
1:B:35:PHE:HD2	1:B:89:ILE:HD11	1.66	0.59
1:C:156:LYS:O	1:C:160:GLN:HG3	2.02	0.58
1:B:199:ALA:O	1:B:201:ILE:HD12	2.02	0.58
1:A:155:LEU:HD22	1:A:185:ILE:CD1	2.30	0.58
1:A:209:GLN:HA	1:C:109:GLN:HE22	1.67	0.58
1:B:209:GLN:HA	1:D:109:GLN:HE22	1.69	0.58
1:D:186:LEU:HD22	1:D:213:VAL:HG13	1.85	0.58
1:A:41:ARG:O	1:A:45:ARG:HG3	2.03	0.58
1:B:190:ARG:NH2	1:C:2:GLU:HG3	2.19	0.57
1:C:64:LEU:O	1:C:64:LEU:HD13	2.03	0.57
1:A:122:SER:HB2	1:C:125:ILE:HD13	1.85	0.57
1:B:122:SER:CB	1:D:125:ILE:HD13	2.35	0.57
1:A:225:LYS:O	1:A:226:ILE:HG12	2.05	0.57
1:B:155:LEU:HD11	1:B:181:MSE:HE1	1.85	0.57
1:B:124:ILE:HD11	1:B:140:PHE:CE1	2.40	0.57
1:C:171:PHE:HZ	1:C:185:ILE:HD11	1.70	0.56
1:D:34:HIS:HB2	1:D:86:MSE:HG2	1.87	0.56
1:A:155:LEU:CD2	1:A:185:ILE:HD13	2.32	0.56
1:B:37:VAL:O	1:B:64:LEU:HD23	2.06	0.56
1:A:80:LEU:HD23	1:A:113:LEU:HD13	1.87	0.56
1:C:145:PRO:O	1:C:151:ARG:HB2	2.06	0.56
1:A:70:PRO:CA	1:A:107:ILE:HD11	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HD22	1:B:217:LYS:HD3	1.88	0.55
1:A:37:VAL:HG12	1:A:89:ILE:HB	1.88	0.55
1:A:201:ILE:HG22	1:A:202:THR:HG23	1.89	0.55
1:B:130:ALA:CB	1:B:208:ILE:HG21	2.37	0.55
1:A:46:PHE:O	1:A:50:VAL:HG23	2.05	0.55
1:B:64:LEU:HD13	1:B:104:VAL:HG21	1.88	0.55
1:A:69:SER:HB3	1:A:72:ASP:OD2	2.06	0.55
1:A:225:LYS:HG2	1:A:226:ILE:H	1.72	0.55
1:B:181:MSE:HE3	1:B:185:ILE:CG1	2.34	0.55
1:A:26:THR:HG23	1:A:50:VAL:HG12	1.88	0.55
1:D:225:LYS:H	1:D:225:LYS:HD3	1.71	0.55
1:A:8:LEU:HD21	1:A:28:ILE:HD11	1.89	0.55
1:D:7:LEU:HB2	1:D:117:PRO:HA	1.89	0.55
1:A:174:THR:HG22	1:A:177:ARG:HB2	1.89	0.55
1:C:211:ARG:NH1	1:C:219:HIS:HB2	2.22	0.54
1:C:28:ILE:HD13	1:C:29:ILE:H	1.71	0.54
1:D:191:PRO:O	1:D:212:THR:HG23	2.08	0.54
1:B:37:VAL:HG12	1:B:89:ILE:HD13	1.89	0.54
1:B:231:LEU:N	1:B:231:LEU:HD12	2.21	0.54
1:A:192:GLN:CA	1:A:192:GLN:HE21	2.20	0.54
1:B:221:PRO:HG2	1:B:223:LEU:CD2	2.37	0.54
1:A:146:ILE:CD1	1:A:146:ILE:H	2.10	0.54
1:D:155:LEU:HD11	1:D:181:MSE:HE1	1.88	0.53
1:B:24:TYR:CD2	1:D:19:GLN:HG3	2.42	0.53
1:D:8:LEU:CD2	1:D:28:ILE:HD11	2.37	0.53
1:B:64:LEU:CD1	1:B:100:PRO:HB2	2.38	0.53
1:A:226:ILE:HG23	1:A:227:PRO:CD	2.36	0.53
1:D:223:LEU:HD23	1:D:226:ILE:HD11	1.90	0.53
1:B:89:ILE:HD12	1:B:89:ILE:N	2.24	0.53
1:B:15:THR:HG21	1:B:202:THR:HG23	1.90	0.53
1:A:48:LYS:HZ3	1:A:48:LYS:HA	1.74	0.53
1:A:183:GLU:O	1:A:187:GLN:HG2	2.09	0.53
1:A:220:ILE:O	1:A:220:ILE:HG23	2.09	0.53
1:C:193:THR:O	1:C:213:VAL:HG23	2.09	0.53
1:C:181:MSE:HE2	1:C:185:ILE:CG1	2.38	0.52
1:B:146:ILE:N	1:B:146:ILE:HD12	2.23	0.52
1:B:8:LEU:HD23	1:B:118:LEU:HD12	1.90	0.52
1:B:44:ARG:HG3	1:B:56:ILE:HD11	1.91	0.52
1:B:59:LEU:HD13	1:B:59:LEU:N	2.23	0.52
1:D:211:ARG:HB2	1:D:216:TRP:CE2	2.45	0.52
1:D:149:GLY:O	1:D:153:LYS:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:HG13	1:A:126:LEU:N	2.24	0.52
1:A:140:PHE:CZ	1:A:142:GLY:HA2	2.45	0.52
1:D:13:GLY:HA3	1:D:203:CYS:SG	2.49	0.52
1:B:182:ILE:HA	1:B:185:ILE:HD12	1.92	0.52
1:D:52:ARG:H	1:D:52:ARG:CD	2.22	0.52
1:B:190:ARG:HB2	1:B:193:THR:OG1	2.10	0.52
1:C:64:LEU:HD22	1:C:64:LEU:C	2.30	0.52
1:B:99:ASP:OD2	1:D:136:GLN:NE2	2.43	0.52
1:A:229:ILE:HG22	1:A:230:PHE:N	2.25	0.52
1:D:170:LEU:HD12	1:D:170:LEU:N	2.25	0.52
1:C:36:ILE:HD12	1:C:36:ILE:H	1.75	0.51
1:B:193:THR:O	1:B:213:VAL:HG23	2.11	0.51
1:C:36:ILE:N	1:C:36:ILE:HD12	2.25	0.51
1:C:56:ILE:HD12	1:C:56:ILE:O	2.11	0.51
1:B:7:LEU:N	1:B:7:LEU:HD12	2.26	0.51
1:C:105:VAL:HG13	1:C:115:VAL:HG11	1.93	0.51
1:B:47:LEU:O	1:B:50:VAL:HG12	2.10	0.50
1:B:52:ARG:HH11	1:B:52:ARG:HG2	1.75	0.50
1:B:207:PHE:O	1:B:208:ILE:HD13	2.10	0.50
1:A:3:THR:HA	1:A:85:SER:OG	2.10	0.50
1:D:201:ILE:HD12	1:D:208:ILE:CD1	2.38	0.50
1:A:172:ILE:HG22	1:A:229:ILE:HG13	1.92	0.50
1:A:52:ARG:HG2	1:A:52:ARG:HH11	1.76	0.50
1:B:8:LEU:CD2	1:B:28:ILE:HD11	2.41	0.50
1:A:125:ILE:HD13	1:C:122:SER:CB	2.40	0.50
1:A:129:MSE:HB3	1:C:7:LEU:HD23	1.94	0.50
1:A:73:ILE:HB	1:A:107:ILE:CD1	2.29	0.50
1:D:181:MSE:HE2	1:D:185:ILE:HG13	1.93	0.50
1:C:182:ILE:O	1:C:186:LEU:HG	2.12	0.50
1:D:36:ILE:HB	1:D:88:VAL:HG22	1.93	0.50
1:D:38:GLU:HA	1:D:64:LEU:O	2.12	0.50
1:A:75:GLY:HA2	1:A:78:LYS:HE3	1.92	0.50
1:D:146:ILE:CD1	1:D:146:ILE:H	2.18	0.49
1:A:211:ARG:HD2	1:A:216:TRP:CD2	2.47	0.49
1:C:162:VAL:HG13	1:C:233:TYR:CD1	2.47	0.49
1:D:99:ASP:HB3	1:D:100:PRO:HD3	1.94	0.49
1:B:122:SER:HB3	1:B:125:ILE:HG13	1.94	0.49
1:C:25:ASN:O	1:C:28:ILE:CD1	2.60	0.49
1:A:201:ILE:HD12	1:A:229:ILE:HD13	1.93	0.49
1:B:7:LEU:N	1:B:7:LEU:CD1	2.74	0.49
1:C:174:THR:HG23	1:C:177:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ARG:HG3	1:D:190:ARG:HH11	1.76	0.49
1:A:73:ILE:HD13	1:A:73:ILE:N	2.28	0.49
1:C:12:LEU:HD13	1:C:121:PRO:HB2	1.95	0.49
1:A:44:ARG:NH2	1:A:59:LEU:HD13	2.27	0.49
1:C:69:SER:O	1:C:73:ILE:HG13	2.13	0.49
1:C:199:ALA:O	1:C:201:ILE:HG13	2.12	0.49
1:D:199:ALA:HB1	1:D:226:ILE:CD1	2.41	0.49
1:B:24:TYR:CB	1:D:19:GLN:HA	2.43	0.49
1:C:46:PHE:CD2	1:C:89:ILE:HD12	2.48	0.49
1:D:76:TYR:O	1:D:86:MSE:HE1	2.14	0.48
1:A:229:ILE:HD12	1:A:229:ILE:N	2.27	0.48
1:D:75:GLY:HA2	1:D:78:LYS:HE3	1.95	0.48
1:C:231:LEU:N	1:C:231:LEU:HD12	2.28	0.48
1:B:138:PHE:HB2	1:B:170:LEU:HD11	1.94	0.48
1:B:136:GLN:HG3	2:B:276:HOH:O	2.13	0.48
1:B:233:TYR:CG	1:B:234:LYS:N	2.81	0.48
1:D:37:VAL:HG11	1:D:43:ALA:HB1	1.96	0.48
1:D:214:LYS:O	1:D:217:LYS:HB2	2.13	0.48
1:C:44:ARG:HG3	1:C:56:ILE:HD13	1.76	0.48
1:B:143:TYR:CZ	1:B:172:ILE:HD12	2.49	0.48
1:A:122:SER:CB	1:C:125:ILE:HD13	2.44	0.48
1:C:24:TYR:O	1:C:28:ILE:HG23	2.14	0.47
1:D:36:ILE:CG2	1:D:64:LEU:HD12	2.43	0.47
1:B:125:ILE:HD12	1:B:125:ILE:C	2.35	0.47
1:B:47:LEU:HA	1:B:50:VAL:HG12	1.96	0.47
1:C:9:PRO:HG3	1:C:120:GLY:HA3	1.95	0.47
1:B:125:ILE:HD12	1:B:126:LEU:N	2.30	0.47
1:C:156:LYS:HG2	1:C:160:GLN:HE21	1.78	0.47
1:D:47:LEU:HA	1:D:50:VAL:HG12	1.95	0.47
1:C:220:ILE:HD12	1:C:221:PRO:HD2	1.96	0.47
1:B:162:VAL:HG23	1:B:169:GLN:HG2	1.96	0.47
1:B:109:GLN:HE22	1:D:209:GLN:HA	1.79	0.47
1:B:24:TYR:HB2	1:D:19:GLN:HA	1.97	0.47
1:D:225:LYS:N	1:D:225:LYS:HD3	2.29	0.47
1:B:172:ILE:CG2	1:B:229:ILE:HG13	2.45	0.47
1:B:56:ILE:CD1	1:B:61:PHE:HE2	2.28	0.47
1:B:88:VAL:C	1:B:89:ILE:HD12	2.35	0.47
1:D:212:THR:HG22	1:D:215:ASP:H	1.80	0.47
1:C:123:SER:HB2	1:C:201:ILE:HD12	1.96	0.47
1:D:40:VAL:HG13	1:D:41:ARG:N	2.29	0.47
1:B:44:ARG:HG3	1:B:56:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:THR:O	1:B:160:GLN:HB2	2.15	0.46
1:C:36:ILE:HB	1:C:88:VAL:HG22	1.98	0.46
1:A:68:THR:OG1	1:A:73:ILE:CD1	2.62	0.46
1:D:125:ILE:HG13	1:D:126:LEU:N	2.29	0.46
1:D:51:ASP:HB3	1:D:54:ILE:HG12	1.96	0.46
1:D:99:ASP:HB3	1:D:100:PRO:CD	2.46	0.46
1:D:192:GLN:HA	1:D:192:GLN:NE2	2.31	0.46
1:B:147:GLU:HG3	1:B:147:GLU:O	2.16	0.46
1:C:191:PRO:O	1:C:212:THR:HG22	2.16	0.46
1:C:195:LEU:HD12	1:C:231:LEU:O	2.15	0.46
1:D:52:ARG:HH11	1:D:52:ARG:HG2	1.81	0.46
1:D:146:ILE:HD12	1:D:146:ILE:N	2.22	0.46
1:D:147:GLU:OE2	1:D:148:PRO:HD2	2.16	0.45
1:A:225:LYS:HG2	1:A:226:ILE:N	2.31	0.45
1:B:183:GLU:O	1:B:186:LEU:HD12	2.16	0.45
1:A:231:LEU:HD12	1:A:231:LEU:N	2.32	0.45
1:A:48:LYS:HZ2	1:A:48:LYS:HA	1.79	0.45
1:A:140:PHE:O	1:C:137:SER:HA	2.16	0.45
1:A:109:GLN:OE1	1:C:209:GLN:HA	2.17	0.45
1:C:181:MSE:HE2	1:C:185:ILE:CD1	2.46	0.45
1:A:212:THR:HG22	1:A:215:ASP:HB2	1.98	0.45
1:B:64:LEU:HD13	1:B:104:VAL:CG2	2.46	0.45
1:A:201:ILE:CD1	1:A:229:ILE:HD13	2.46	0.45
1:D:73:ILE:O	1:D:77:LEU:HD13	2.17	0.45
1:A:225:LYS:CG	1:A:226:ILE:H	2.29	0.45
1:D:182:ILE:HA	1:D:185:ILE:HD12	1.98	0.45
1:A:226:ILE:CG2	1:A:227:PRO:HD2	2.40	0.45
1:D:235:LEU:O	1:D:235:LEU:HD23	2.17	0.45
1:A:109:GLN:NE2	1:C:209:GLN:HA	2.32	0.45
1:A:55:ASP:C	1:A:57:ASP:H	2.20	0.45
1:D:175:PRO:HG3	1:D:227:PRO:HA	1.98	0.45
1:A:216:TRP:O	1:A:217:LYS:C	2.55	0.44
1:C:211:ARG:HB2	1:C:216:TRP:CE2	2.52	0.44
1:A:149:GLY:O	1:A:153:LYS:HG3	2.17	0.44
1:A:76:TYR:O	1:A:86:MSE:HE1	2.17	0.44
1:B:211:ARG:HB2	1:B:216:TRP:CE2	2.51	0.44
1:D:52:ARG:NE	1:D:52:ARG:H	2.15	0.44
1:C:226:ILE:H	1:C:226:ILE:HD13	1.82	0.44
1:C:5:LEU:HB2	1:C:80:LEU:CD2	2.47	0.44
1:B:35:PHE:CD2	1:B:89:ILE:HD11	2.50	0.44
1:C:138:PHE:HB2	1:C:170:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:LEU:CD2	1:D:226:ILE:HD11	2.47	0.44
1:A:158:LEU:O	1:A:162:VAL:HG23	2.17	0.44
1:C:144:LEU:HD22	1:C:154:LYS:HD3	2.00	0.44
1:A:147:GLU:HG3	1:A:147:GLU:O	2.17	0.44
1:A:137:SER:C	1:A:167:GLN:HG3	2.38	0.44
1:A:12:LEU:HD13	1:A:121:PRO:HG2	2.00	0.44
1:C:44:ARG:CG	1:C:56:ILE:CD1	2.47	0.43
1:A:73:ILE:O	1:A:77:LEU:HD13	2.18	0.43
1:C:48:LYS:HE2	1:C:56:ILE:HG21	1.99	0.43
1:C:211:ARG:HH12	1:C:219:HIS:HB2	1.83	0.43
1:C:149:GLY:O	1:C:153:LYS:HB2	2.18	0.43
1:A:179:HIS:O	1:A:182:ILE:HG13	2.17	0.43
1:D:34:HIS:HD2	1:D:62:TYR:OH	2.02	0.43
1:A:22:PRO:HG2	1:A:119:VAL:HB	2.00	0.43
1:A:181:MSE:HE2	1:A:185:ILE:CD1	2.49	0.43
1:C:28:ILE:HG13	1:C:118:LEU:HD11	2.00	0.43
1:D:182:ILE:O	1:D:186:LEU:HG	2.19	0.43
1:C:178:ASN:O	1:C:182:ILE:HG23	2.19	0.43
1:A:80:LEU:HA	1:A:84:ALA:O	2.17	0.43
1:C:201:ILE:HG13	1:C:201:ILE:H	1.68	0.43
1:C:9:PRO:CG	1:C:120:GLY:HA3	2.48	0.43
1:B:146:ILE:CD1	1:B:146:ILE:H	2.25	0.43
1:A:52:ARG:HG2	1:A:52:ARG:NH1	2.34	0.43
1:D:37:VAL:HG11	1:D:43:ALA:CB	2.48	0.43
1:B:80:LEU:HD23	1:B:113:LEU:HD13	2.01	0.43
1:D:223:LEU:HD22	1:D:228:CYS:SG	2.58	0.43
1:C:69:SER:OG	1:C:71:GLU:HG2	2.18	0.43
1:B:195:LEU:HD12	1:B:231:LEU:O	2.19	0.43
1:A:26:THR:HG23	1:A:50:VAL:CG1	2.48	0.43
1:A:159:GLU:O	1:A:162:VAL:HB	2.19	0.43
1:A:109:GLN:NE2	1:A:109:GLN:HA	2.34	0.43
1:C:197:ILE:O	1:C:208:ILE:HA	2.19	0.43
1:A:174:THR:OG1	1:A:175:PRO:HD2	2.19	0.42
1:A:109:GLN:HE21	1:A:109:GLN:HA	1.84	0.42
1:C:8:LEU:HD13	1:C:29:ILE:HG12	2.01	0.42
1:B:28:ILE:HG12	1:B:118:LEU:HD11	2.00	0.42
1:D:170:LEU:HA	1:D:230:PHE:O	2.19	0.42
1:B:125:ILE:HD11	2:B:272:HOH:O	2.20	0.42
1:B:179:HIS:NE2	1:B:222:GLU:O	2.52	0.42
1:A:155:LEU:CD2	1:A:185:ILE:CD1	2.96	0.42
1:A:190:ARG:NH1	1:A:190:ARG:HG3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:HA	1:C:24:TYR:CB	2.47	0.42
1:B:73:ILE:HG21	1:B:104:VAL:HA	2.01	0.42
1:A:143:TYR:CE2	1:A:172:ILE:HD11	2.54	0.42
1:A:78:LYS:HB2	1:A:79:PRO:HD3	2.01	0.42
1:A:198:ALA:O	1:A:228:CYS:HB2	2.20	0.42
1:D:222:GLU:H	1:D:222:GLU:CD	2.23	0.42
1:C:8:LEU:HD22	1:C:28:ILE:HD11	2.02	0.42
1:B:196:CYS:HB3	1:B:231:LEU:HB2	2.01	0.42
1:C:47:LEU:HA	1:C:50:VAL:HG12	2.01	0.42
1:A:171:PHE:CZ	1:A:185:ILE:HD11	2.54	0.42
1:A:211:ARG:HD3	1:A:215:ASP:O	2.20	0.42
1:C:159:GLU:OE2	1:C:189:CYS:HB3	2.19	0.42
1:B:51:ASP:HB3	1:B:54:ILE:CD1	2.50	0.42
1:C:172:ILE:HG22	1:C:229:ILE:HG13	2.02	0.42
1:B:182:ILE:HD13	1:B:182:ILE:C	2.40	0.42
1:D:162:VAL:O	1:D:166:SER:HA	2.19	0.42
1:A:28:ILE:C	1:A:28:ILE:HD12	2.40	0.41
1:A:24:TYR:HB2	1:C:19:GLN:HA	2.01	0.41
1:D:20:VAL:HG11	1:D:202:THR:HG21	2.02	0.41
1:A:138:PHE:HB3	1:A:168:THR:HB	2.02	0.41
1:B:201:ILE:O	1:B:202:THR:HG22	2.19	0.41
1:D:156:LYS:HG3	2:D:249:HOH:O	2.19	0.41
1:D:226:ILE:HD12	1:D:226:ILE:C	2.41	0.41
1:C:77:LEU:O	1:C:80:LEU:HB3	2.21	0.41
1:A:218:GLY:O	1:A:219:HIS:HB2	2.19	0.41
1:C:156:LYS:HD2	2:C:252:HOH:O	2.20	0.41
1:B:33:ARG:CD	1:B:59:LEU:HD12	2.51	0.41
1:C:130:ALA:HB3	1:C:208:ILE:HG21	2.03	0.41
1:A:138:PHE:CB	1:A:168:THR:HB	2.51	0.41
1:C:6:TYR:HA	1:C:116:ILE:HG23	2.03	0.41
1:A:196:CYS:HB3	1:A:231:LEU:HB2	2.02	0.41
1:C:17:LEU:HD13	1:C:49:LYS:HE2	2.02	0.41
1:B:122:SER:HB2	1:D:125:ILE:CD1	2.43	0.41
1:B:198:ALA:HB1	1:B:208:ILE:HD12	2.03	0.41
1:B:44:ARG:HG3	1:B:56:ILE:CG1	2.50	0.41
1:A:130:ALA:HB3	1:A:208:ILE:HG21	2.03	0.41
1:D:124:ILE:N	1:D:124:ILE:HD12	2.36	0.41
1:C:182:ILE:HG13	1:C:183:GLU:N	2.35	0.41
1:B:193:THR:HG22	1:B:194:LYS:N	2.36	0.41
1:B:33:ARG:HD3	1:B:59:LEU:HD12	2.03	0.40
1:D:55:ASP:OD2	1:D:58:SER:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:HG13	1:B:56:ILE:O	2.20	0.40
1:B:56:ILE:CD1	1:B:61:PHE:CE2	3.03	0.40
1:D:211:ARG:HD2	1:D:216:TRP:CE3	2.56	0.40
1:D:52:ARG:CZ	1:D:52:ARG:HB2	2.51	0.40
1:A:109:GLN:HE21	1:A:109:GLN:CA	2.34	0.40
1:A:159:GLU:CG	1:A:190:ARG:HH12	2.21	0.40
1:C:41:ARG:O	1:C:45:ARG:HB2	2.21	0.40
1:A:185:ILE:O	1:A:189:CYS:HB2	2.22	0.40
1:A:173:GLU:OE2	1:A:177:ARG:HB3	2.22	0.40
1:A:64:LEU:HD13	1:A:65:ASN:N	2.37	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	217/242 (90%)	197 (91%)	17 (8%)	3 (1%)	14	24
1	B	223/242 (92%)	201 (90%)	18 (8%)	4 (2%)	11	18
1	C	217/242 (90%)	196 (90%)	19 (9%)	2 (1%)	21	37
1	D	223/242 (92%)	201 (90%)	20 (9%)	2 (1%)	21	37
All	All	880/968 (91%)	795 (90%)	74 (8%)	11 (1%)	15	26

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	B	82	GLY
1	C	101	GLY
1	C	200	ASN
1	A	56	ILE

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Mol	Chain	Res	Type
1	A	206	GLU
1	B	222	GLU
1	B	223	LEU
1	B	225	LYS
1	D	199	ALA
1	D	39	ASP

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	196/207 (95%)	185 (94%)	11 (6%)	26	47
1	B	200/207 (97%)	183 (92%)	17 (8%)	13	25
1	C	196/207 (95%)	185 (94%)	11 (6%)	26	47
1	D	200/207 (97%)	185 (92%)	15 (8%)	17	31
All	All	792/828 (96%)	738 (93%)	54 (7%)	20	36

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	12	LEU
1	A	34	HIS
1	A	48	LYS
1	A	52	ARG
1	A	64	LEU
1	A	73	ILE
1	A	151	ARG
1	A	158	LEU
1	A	173	GLU
1	A	176	TYR
1	B	3	THR
1	B	12	LEU
1	B	52	ARG
1	B	53	GLU

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Mol	Chain	Res	Type
1	B	56	ILE
1	B	59	LEU
1	B	77	LEU
1	B	99	ASP
1	B	116	ILE
1	B	147	GLU
1	B	158	LEU
1	B	170	LEU
1	B	177	ARG
1	B	182	ILE
1	B	186	LEU
1	B	202	THR
1	B	224	SER
1	C	3	THR
1	C	28	ILE
1	C	52	ARG
1	C	53	GLU
1	C	57	ASP
1	C	64	LEU
1	C	72	ASP
1	C	77	LEU
1	C	110	ARG
1	C	170	LEU
1	C	226	ILE
1	D	7	LEU
1	D	12	LEU
1	D	38	GLU
1	D	52	ARG
1	D	53	GLU
1	D	59	LEU
1	D	71	GLU
1	D	151	ARG
1	D	170	LEU
1	D	176	TYR
1	D	212	THR
1	D	219	HIS
1	D	220	ILE
1	D	222	GLU
1	D	225	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	136	GLN
1	A	187	GLN
1	A	188	ASN
1	A	192	GLN
1	B	109	GLN
1	B	136	GLN
1	B	179	HIS
1	B	187	GLN
1	B	188	ASN
1	B	192	GLN
1	C	109	GLN
1	C	160	GLN
1	C	192	GLN
1	D	34	HIS
1	D	109	GLN
1	D	111	GLN
1	D	136	GLN
1	D	179	HIS
1	D	188	ASN
1	D	192	GLN
1	D	200	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	220/242 (90%)	0.59	25 (11%) 7 6	21, 44, 99, 126	0
1	B	224/242 (92%)	0.42	17 (7%) 17 18	15, 41, 84, 153	0
1	C	220/242 (90%)	0.72	29 (13%) 4 4	16, 45, 85, 123	0
1	D	224/242 (92%)	0.40	18 (8%) 15 16	16, 42, 82, 116	0
All	All	888/968 (91%)	0.53	89 (10%) 9 10	15, 43, 88, 153	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	67	HIS	10.1
1	A	226	ILE	9.7
1	A	176	TYR	7.2
1	B	66	LYS	6.6
1	A	59	LEU	6.2
1	C	225	LYS	5.7
1	C	71	GLU	5.6
1	D	84	ALA	5.4
1	B	146	ILE	5.1
1	A	57	ASP	5.1
1	B	68	THR	4.8
1	A	56	ILE	4.8
1	C	70	PRO	4.8
1	D	83	GLY	4.5
1	C	57	ASP	4.4
1	D	65	ASN	4.4
1	D	64	LEU	4.2
1	D	66	LYS	4.2
1	C	64	LEU	4.2
1	C	63	PRO	4.1
1	A	60	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	14	ASP	3.8
1	C	73	ILE	3.8
1	A	204	GLU	3.8
1	D	220	ILE	3.8
1	D	219	HIS	3.7
1	C	220	ILE	3.7
1	C	56	ILE	3.6
1	C	219	HIS	3.5
1	A	227	PRO	3.5
1	C	148	PRO	3.5
1	A	229	ILE	3.4
1	C	226	ILE	3.4
1	D	218	GLY	3.3
1	A	125	ILE	3.2
1	A	218	GLY	3.2
1	C	149	GLY	3.2
1	C	100	PRO	3.1
1	C	52	ARG	3.1
1	D	67	HIS	3.1
1	B	217	LYS	3.1
1	D	226	ILE	3.1
1	B	148	PRO	3.0
1	D	235	LEU	3.0
1	B	150	GLU	3.0
1	B	91	GLU	3.0
1	A	219	HIS	2.9
1	A	58	SER	2.9
1	C	223	LEU	2.9
1	C	146	ILE	2.8
1	C	147	GLU	2.8
1	B	65	ASN	2.8
1	A	175	PRO	2.7
1	A	66	LYS	2.7
1	C	72	ASP	2.7
1	D	56	ILE	2.6
1	B	56	ILE	2.6
1	A	128	VAL	2.6
1	C	224	SER	2.5
1	C	76	TYR	2.5
1	D	45	ARG	2.4
1	B	225	LYS	2.4
1	B	16	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	44	ARG	2.4
1	C	69	SER	2.4
1	D	224	SER	2.4
1	D	222	GLU	2.4
1	A	52	ARG	2.3
1	B	64	LEU	2.3
1	C	54	ILE	2.3
1	C	82	GLY	2.3
1	A	124	ILE	2.2
1	A	174	THR	2.2
1	B	71	GLU	2.2
1	C	74	SER	2.2
1	A	225	LYS	2.2
1	C	136	GLN	2.1
1	D	176	TYR	2.1
1	D	78	LYS	2.1
1	A	146	ILE	2.1
1	D	223	LEU	2.1
1	B	70	PRO	2.1
1	C	116	ILE	2.1
1	A	55	ASP	2.1
1	A	127	SER	2.1
1	B	14	ASP	2.0
1	A	192	GLN	2.0
1	C	117	PRO	2.0
1	B	90	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.