Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:02 PM GMT

PDB ID	:	3SO4
Title	:	Methionine-adenosyltransferase from Entamoeba histolytica
Authors	:	Merritt, E.A.; Medical Structural Genomics of Pathogenic Protozoa (MSGPP)
Deposited on	:	2011-06-29
Resolution	:	3.18 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:

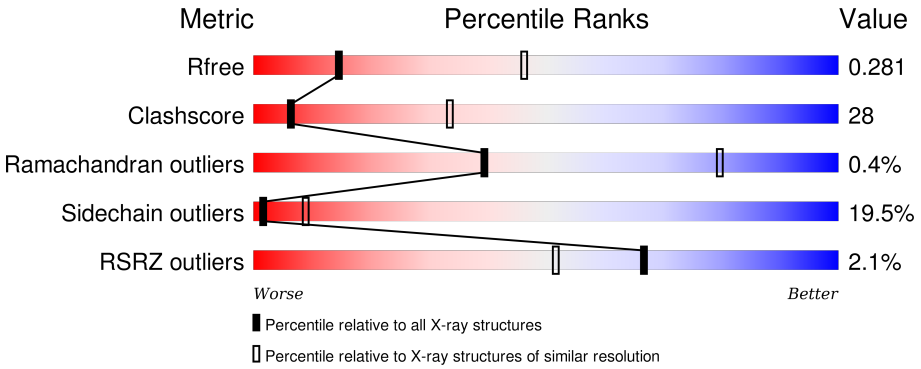
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.18 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	1115 (3.22-3.14)
Clashscore	102246	1125 (3.20-3.16)
Ramachandran outliers	100387	1105 (3.20-3.16)
Sidechain outliers	100360	1104 (3.20-3.16)
RSRZ outliers	91569	1120 (3.22-3.14)

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	415	54% 29% 8% 9%
1	B	415	50% 32% 9% 9%
1	C	415	3% 54% 27% 10% 9%
1	D	415	2% 53% 32% 6% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	400	-	-	-	X
2	ACT	C	400	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11498 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 Methionine-adenosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2858	1804	487	549	18			
1	B	379	Total	C	N	O	S	0	0	0
			2881	1818	491	554	18			
1	C	379	Total	C	N	O	S	0	0	0
			2865	1807	490	550	18			
1	D	379	Total	C	N	O	S	0	0	0
			2874	1815	491	550	18			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	EXPRESSION TAG	UNP C4M272
A	-16	ALA	-	EXPRESSION TAG	UNP C4M272
A	-15	HIS	-	EXPRESSION TAG	UNP C4M272
A	-14	HIS	-	EXPRESSION TAG	UNP C4M272
A	-13	HIS	-	EXPRESSION TAG	UNP C4M272
A	-12	HIS	-	EXPRESSION TAG	UNP C4M272
A	-11	HIS	-	EXPRESSION TAG	UNP C4M272
A	-10	HIS	-	EXPRESSION TAG	UNP C4M272
A	-9	MET	-	EXPRESSION TAG	UNP C4M272
A	-8	GLY	-	EXPRESSION TAG	UNP C4M272
A	-7	THR	-	EXPRESSION TAG	UNP C4M272
A	-6	LEU	-	EXPRESSION TAG	UNP C4M272
A	-5	GLU	-	EXPRESSION TAG	UNP C4M272
A	-4	ALA	-	EXPRESSION TAG	UNP C4M272
A	-3	GLN	-	EXPRESSION TAG	UNP C4M272
A	-2	THR	-	EXPRESSION TAG	UNP C4M272
A	-1	GLN	-	EXPRESSION TAG	UNP C4M272
A	0	GLY	-	EXPRESSION TAG	UNP C4M272
A	1	PRO	-	EXPRESSION TAG	UNP C4M272
A	2	GLY	-	EXPRESSION TAG	UNP C4M272
A	3	SER	-	EXPRESSION TAG	UNP C4M272

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	EXPRESSION TAG	UNP C4M272
B	-16	ALA	-	EXPRESSION TAG	UNP C4M272
B	-15	HIS	-	EXPRESSION TAG	UNP C4M272
B	-14	HIS	-	EXPRESSION TAG	UNP C4M272
B	-13	HIS	-	EXPRESSION TAG	UNP C4M272
B	-12	HIS	-	EXPRESSION TAG	UNP C4M272
B	-11	HIS	-	EXPRESSION TAG	UNP C4M272
B	-10	HIS	-	EXPRESSION TAG	UNP C4M272
B	-9	MET	-	EXPRESSION TAG	UNP C4M272
B	-8	GLY	-	EXPRESSION TAG	UNP C4M272
B	-7	THR	-	EXPRESSION TAG	UNP C4M272
B	-6	LEU	-	EXPRESSION TAG	UNP C4M272
B	-5	GLU	-	EXPRESSION TAG	UNP C4M272
B	-4	ALA	-	EXPRESSION TAG	UNP C4M272
B	-3	GLN	-	EXPRESSION TAG	UNP C4M272
B	-2	THR	-	EXPRESSION TAG	UNP C4M272
B	-1	GLN	-	EXPRESSION TAG	UNP C4M272
B	0	GLY	-	EXPRESSION TAG	UNP C4M272
B	1	PRO	-	EXPRESSION TAG	UNP C4M272
B	2	GLY	-	EXPRESSION TAG	UNP C4M272
B	3	SER	-	EXPRESSION TAG	UNP C4M272
C	-17	MET	-	EXPRESSION TAG	UNP C4M272
C	-16	ALA	-	EXPRESSION TAG	UNP C4M272
C	-15	HIS	-	EXPRESSION TAG	UNP C4M272
C	-14	HIS	-	EXPRESSION TAG	UNP C4M272
C	-13	HIS	-	EXPRESSION TAG	UNP C4M272
C	-12	HIS	-	EXPRESSION TAG	UNP C4M272
C	-11	HIS	-	EXPRESSION TAG	UNP C4M272
C	-10	HIS	-	EXPRESSION TAG	UNP C4M272
C	-9	MET	-	EXPRESSION TAG	UNP C4M272
C	-8	GLY	-	EXPRESSION TAG	UNP C4M272
C	-7	THR	-	EXPRESSION TAG	UNP C4M272
C	-6	LEU	-	EXPRESSION TAG	UNP C4M272
C	-5	GLU	-	EXPRESSION TAG	UNP C4M272
C	-4	ALA	-	EXPRESSION TAG	UNP C4M272
C	-3	GLN	-	EXPRESSION TAG	UNP C4M272
C	-2	THR	-	EXPRESSION TAG	UNP C4M272
C	-1	GLN	-	EXPRESSION TAG	UNP C4M272
C	0	GLY	-	EXPRESSION TAG	UNP C4M272
C	1	PRO	-	EXPRESSION TAG	UNP C4M272
C	2	GLY	-	EXPRESSION TAG	UNP C4M272
C	3	SER	-	EXPRESSION TAG	UNP C4M272

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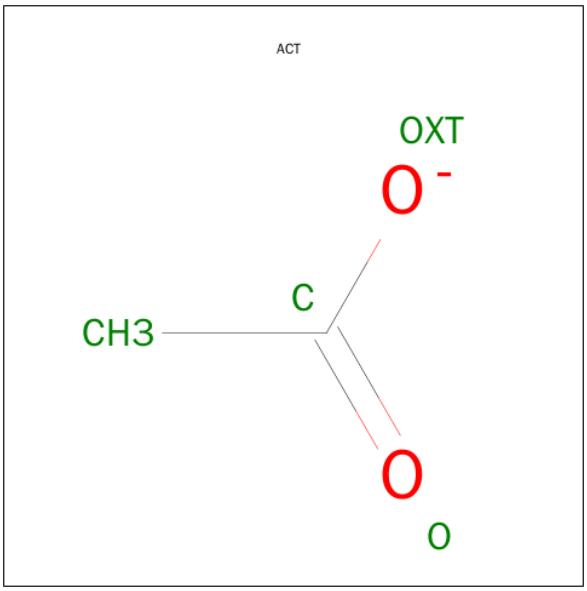
Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	MET	-	EXPRESSION TAG	UNP C4M272
D	-16	ALA	-	EXPRESSION TAG	UNP C4M272
D	-15	HIS	-	EXPRESSION TAG	UNP C4M272
D	-14	HIS	-	EXPRESSION TAG	UNP C4M272
D	-13	HIS	-	EXPRESSION TAG	UNP C4M272
D	-12	HIS	-	EXPRESSION TAG	UNP C4M272
D	-11	HIS	-	EXPRESSION TAG	UNP C4M272
D	-10	HIS	-	EXPRESSION TAG	UNP C4M272
D	-9	MET	-	EXPRESSION TAG	UNP C4M272
D	-8	GLY	-	EXPRESSION TAG	UNP C4M272
D	-7	THR	-	EXPRESSION TAG	UNP C4M272
D	-6	LEU	-	EXPRESSION TAG	UNP C4M272
D	-5	GLU	-	EXPRESSION TAG	UNP C4M272
D	-4	ALA	-	EXPRESSION TAG	UNP C4M272
D	-3	GLN	-	EXPRESSION TAG	UNP C4M272
D	-2	THR	-	EXPRESSION TAG	UNP C4M272
D	-1	GLN	-	EXPRESSION TAG	UNP C4M272
D	0	GLY	-	EXPRESSION TAG	UNP C4M272
D	1	PRO	-	EXPRESSION TAG	UNP C4M272
D	2	GLY	-	EXPRESSION TAG	UNP C4M272
D	3	SER	-	EXPRESSION TAG	UNP C4M272

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

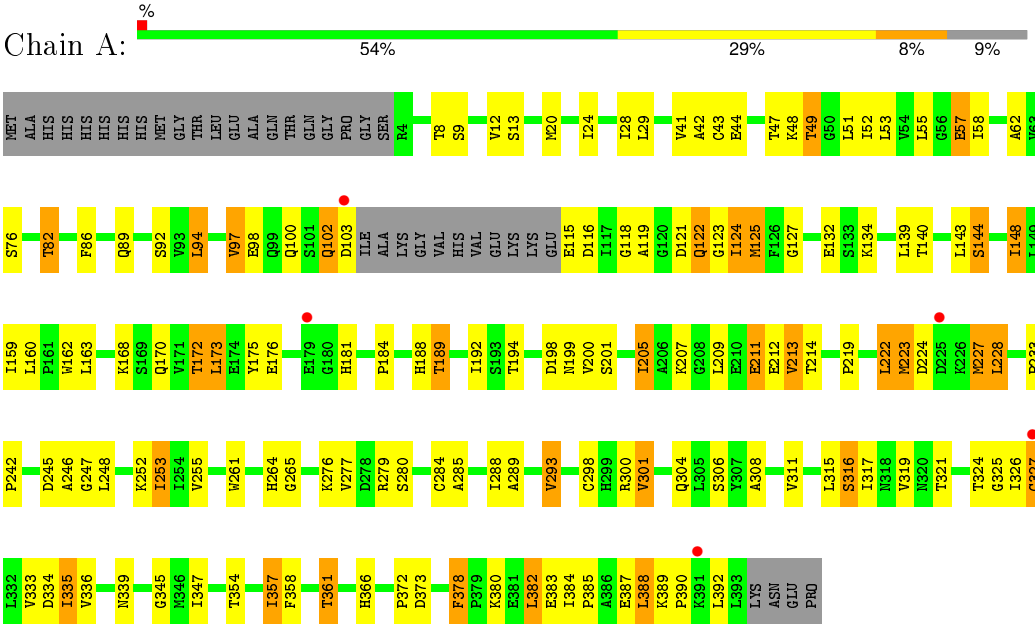
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0

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.

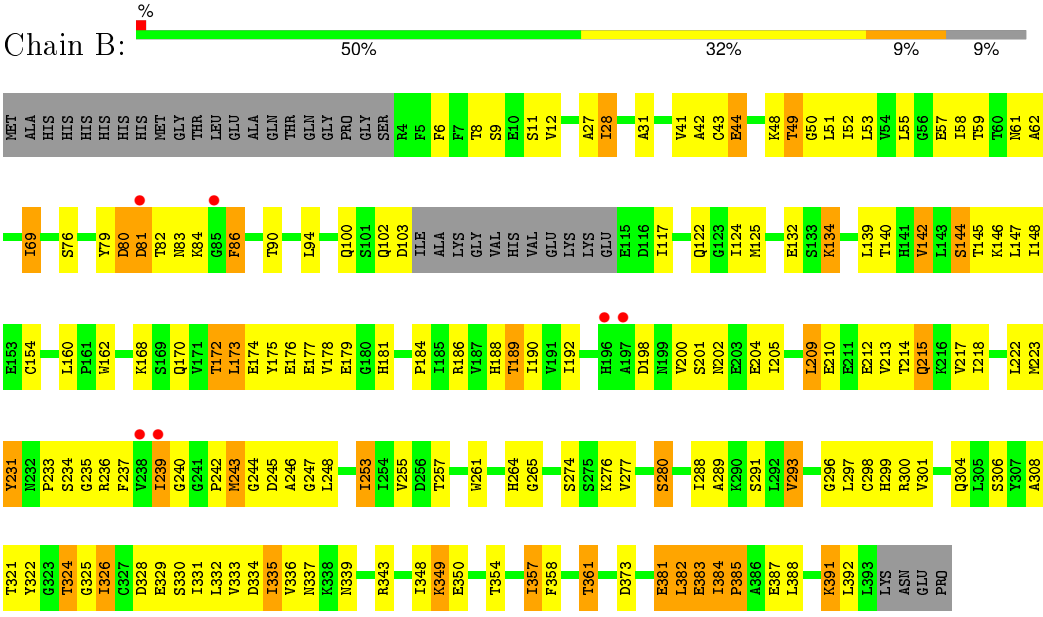
- Molecule 1: Methionine-adenosyltransferase

Chain A:



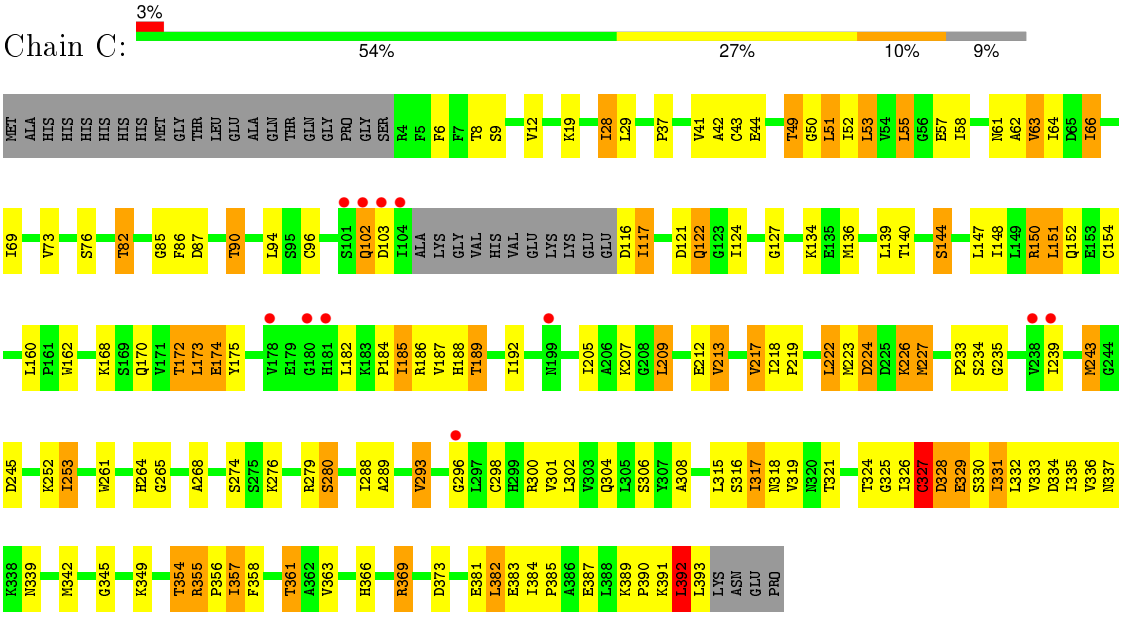
- Molecule 1: Methionine-adenosyltransferase

Chain B:



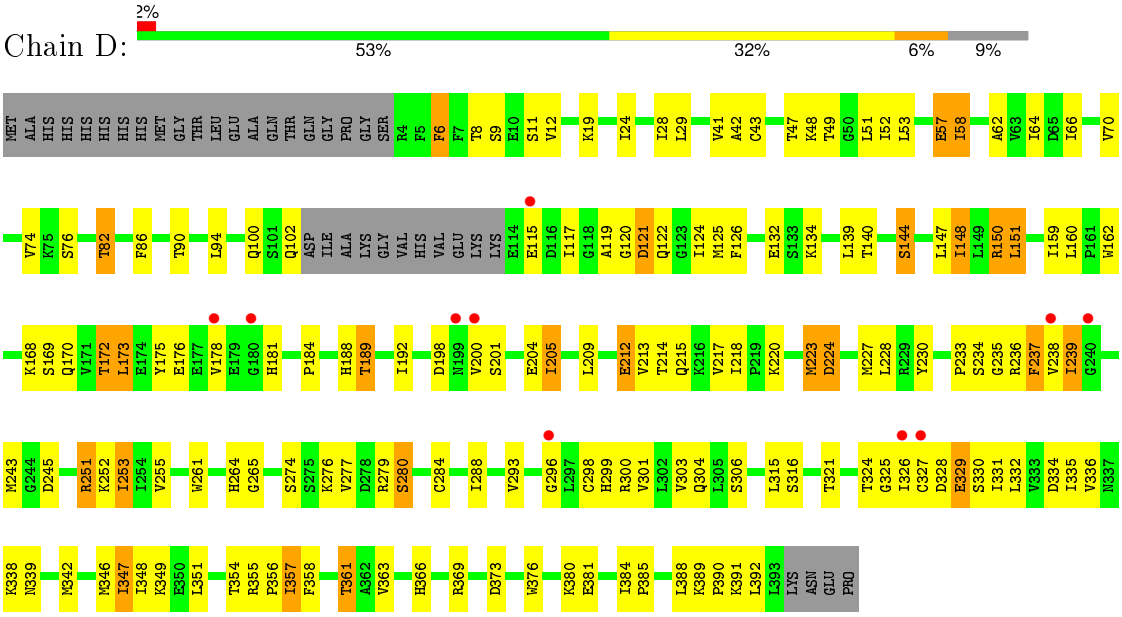
• Molecule 1: Methionine-adenosyltransferase

Chain C:



• Molecule 1: Methionine-adenosyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.49Å 113.16Å 220.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.18 29.92 – 3.18	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-3.18) 91.3 (29.92-3.18)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0095	Depositor
R, R_{free}	0.228 , 0.284 0.230 , 0.281	Depositor DCC
R_{free} test set	1295 reflections (5.86%)	DCC
Wilson B-factor (Å^2)	76.0	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 23419 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11498	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.44	0/2914	0.69	2/3952 (0.1%)
1	B	0.46	0/2937	0.72	1/3978 (0.0%)
1	C	0.43	0/2921	0.70	1/3959 (0.0%)
1	D	0.42	0/2930	0.68	1/3969 (0.0%)
All	All	0.44	0/11702	0.70	5/15858 (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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	LEU	CA-CB-CG	5.73	128.47	115.30
1	C	55	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	213	VAL	CB-CA-C	-5.60	100.76	111.40
1	D	224	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	B	343	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	ILE	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	2858	0	2785	150	0
1	B	2881	0	2830	182	0
1	C	2865	0	2799	180	0
1	D	2874	0	2824	161	0
2	A	4	0	3	1	0
2	B	4	0	3	0	0
2	C	4	0	3	2	0
2	D	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	11498	0	11250	630	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 28.

All (630) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:O	1:A:213:VAL:HG22	1.24	1.29
1:A:213:VAL:CG2	1:A:214:THR:H	1.37	1.28
1:D:47:THR:CG2	1:D:52:ILE:HD13	1.63	1.27
1:A:213:VAL:HG23	1:A:214:THR:N	1.26	1.20
1:C:326:ILE:HD12	1:C:327:CYS:N	1.58	1.16
1:A:327:CYS:SG	1:A:388:LEU:CD2	2.36	1.13
1:D:47:THR:HG21	1:D:52:ILE:HD13	1.24	1.10
1:B:209:LEU:H	1:B:209:LEU:HD23	1.02	1.10
1:B:385:PRO:CG	1:B:388:LEU:HD12	1.81	1.09
1:B:385:PRO:HG2	1:B:388:LEU:CD1	1.81	1.08
1:B:205:ILE:O	1:B:209:LEU:CD2	2.00	1.08
1:A:331:ILE:O	1:A:335:ILE:HD13	1.51	1.07
1:D:181:HIS:ND1	1:D:299:HIS:ND1	2.01	1.06
1:C:187:VAL:HB	1:C:227:MET:HE1	1.38	1.05
1:B:205:ILE:O	1:B:209:LEU:HD23	1.52	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:OD2	1:A:236:ARG:NH2	1.91	1.04
1:B:385:PRO:HG2	1:B:388:LEU:HD12	1.07	1.03
1:C:224:ASP:OD2	1:C:226:LYS:HB2	1.58	1.03
1:C:392:LEU:HD23	1:C:393:LEU:H	1.25	1.01
1:D:173:LEU:HD12	1:D:173:LEU:O	1.61	1.00
1:B:308:ALA:HB2	1:B:315:LEU:HD23	1.43	1.00
1:C:327:CYS:SG	1:C:328:ASP:N	2.32	1.00
1:A:248:LEU:HD23	1:B:248:LEU:HD23	1.44	1.00
1:D:147:LEU:HD12	1:D:217:VAL:HG21	1.45	0.98
1:B:209:LEU:HD23	1:B:209:LEU:N	1.73	0.97
1:A:327:CYS:SG	1:A:388:LEU:HD23	2.04	0.97
1:D:173:LEU:C	1:D:173:LEU:HD12	1.85	0.97
1:A:209:LEU:O	1:A:213:VAL:CG2	2.11	0.97
1:C:117:ILE:O	1:C:117:ILE:HG23	1.64	0.96
1:D:173:LEU:HD11	1:D:175:TYR:CE1	1.99	0.96
1:D:299:HIS:CD2	1:D:392:LEU:HD11	2.01	0.95
1:D:391:LYS:HG3	1:D:392:LEU:H	1.29	0.94
1:C:173:LEU:HD11	1:C:175:TYR:CE1	2.01	0.94
1:A:385:PRO:O	1:A:388:LEU:HD12	1.66	0.94
1:B:63:VAL:HG11	1:C:63:VAL:HG11	1.49	0.93
1:C:37:PRO:HB3	1:C:354:THR:HG23	1.51	0.93
1:C:213:VAL:O	1:C:217:VAL:HG12	1.66	0.92
1:C:174:GLU:HG3	1:C:175:TYR:N	1.84	0.92
1:C:326:ILE:HD12	1:C:327:CYS:H	1.21	0.91
1:B:209:LEU:O	1:B:213:VAL:HG22	1.69	0.91
1:B:298:CYS:SG	1:B:301:VAL:HG22	2.10	0.91
1:A:335:ILE:HD13	1:A:335:ILE:H	1.35	0.91
1:A:388:LEU:H	1:A:388:LEU:HD12	1.33	0.91
1:B:188:HIS:ND1	1:B:189:THR:HG22	1.87	0.90
1:A:327:CYS:SG	1:A:388:LEU:HD21	2.08	0.90
1:D:298:CYS:SG	1:D:301:VAL:HG22	2.12	0.90
1:C:187:VAL:HB	1:C:227:MET:CE	2.01	0.89
1:B:209:LEU:H	1:B:209:LEU:CD2	1.86	0.88
1:D:299:HIS:HD2	1:D:392:LEU:HD11	1.32	0.88
1:D:48:LYS:HG3	1:D:49:THR:N	1.88	0.88
1:B:213:VAL:O	1:B:217:VAL:HG13	1.71	0.88
1:D:47:THR:HG21	1:D:52:ILE:CD1	2.02	0.87
1:C:55:LEU:HD11	1:D:48:LYS:CB	2.04	0.87
1:C:117:ILE:HG21	1:C:345:GLY:CA	2.04	0.87
1:D:173:LEU:HD11	1:D:175:TYR:CD1	2.11	0.86
1:B:209:LEU:CD2	1:B:209:LEU:N	2.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ARG:NH1	1:A:212:GLU:O	2.09	0.85
1:D:173:LEU:C	1:D:173:LEU:CD1	2.44	0.85
1:B:150:ARG:NH1	1:B:212:GLU:O	2.10	0.85
1:B:49:THR:HG22	1:B:50:GLY:N	1.87	0.85
1:D:150:ARG:NH1	1:D:212:GLU:O	2.11	0.84
1:C:150:ARG:NH1	1:C:212:GLU:O	2.10	0.84
1:A:213:VAL:HG23	1:A:214:THR:H	0.72	0.84
1:A:213:VAL:CG2	1:A:214:THR:N	2.01	0.84
1:C:117:ILE:HG21	1:C:345:GLY:HA3	1.60	0.84
1:A:385:PRO:O	1:A:388:LEU:CD1	2.26	0.83
1:C:173:LEU:HD12	1:C:173:LEU:C	1.99	0.82
1:C:384:ILE:HG23	1:C:385:PRO:HD2	1.61	0.82
1:D:47:THR:CG2	1:D:52:ILE:CD1	2.55	0.82
1:A:124:ILE:HD11	1:B:8:THR:O	1.78	0.82
1:C:37:PRO:HB3	1:C:354:THR:CG2	2.08	0.82
1:C:28:ILE:HD11	1:C:66:ILE:HG23	1.63	0.81
1:B:205:ILE:O	1:B:209:LEU:HD21	1.78	0.81
1:C:336:VAL:HG12	1:C:342:MET:HE3	1.61	0.80
1:B:41:VAL:HG13	1:B:58:ILE:HG22	1.63	0.80
1:A:335:ILE:CD1	1:A:335:ILE:N	2.45	0.79
1:D:336:VAL:HG12	1:D:342:MET:HE1	1.65	0.79
1:D:47:THR:HG22	1:D:52:ILE:HD13	1.64	0.79
1:D:48:LYS:CG	1:D:49:THR:H	1.95	0.79
1:A:200:VAL:HG11	1:A:205:ILE:HG12	1.63	0.79
1:B:151:LEU:HD21	1:B:192:ILE:HD11	1.63	0.79
1:A:308:ALA:HB2	1:A:315:LEU:HD13	1.66	0.78
1:D:120:GLY:O	1:D:121:ASP:HB2	1.83	0.77
1:A:335:ILE:H	1:A:335:ILE:CD1	1.97	0.77
1:A:388:LEU:HD12	1:A:388:LEU:N	2.00	0.77
1:C:173:LEU:HD12	1:C:173:LEU:O	1.82	0.77
1:C:151:LEU:HD21	1:C:192:ILE:HD11	1.65	0.77
1:C:252:LYS:NZ	2:C:400:ACT:H3	2.00	0.77
1:D:209:LEU:O	1:D:213:VAL:HG22	1.85	0.77
1:D:151:LEU:HD21	1:D:192:ILE:HD11	1.67	0.77
1:C:147:LEU:HD12	1:C:217:VAL:HG11	1.66	0.76
1:B:384:ILE:HG13	1:B:385:PRO:HD2	1.67	0.76
1:A:41:VAL:HG13	1:A:58:ILE:HG22	1.68	0.76
1:D:48:LYS:CG	1:D:49:THR:N	2.48	0.76
1:D:188:HIS:ND1	1:D:189:THR:HG22	2.00	0.76
1:B:298:CYS:SG	1:B:301:VAL:CG2	2.73	0.76
1:B:218:ILE:HB	1:B:223:MET:HE1	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:PRO:CD	1:B:388:LEU:HD12	2.16	0.75
1:B:139:LEU:HA	1:B:142:VAL:HG23	1.68	0.75
1:C:61:ASN:OD1	1:C:102:GLN:NE2	2.19	0.75
1:C:252:LYS:HZ1	2:C:400:ACT:H3	1.51	0.74
1:A:172:THR:HG21	1:B:315:LEU:HD13	1.69	0.74
1:C:298:CYS:SG	1:C:301:VAL:CG2	2.76	0.74
1:B:178:VAL:O	1:B:179:GLU:CG	2.36	0.73
1:A:159:ILE:O	1:A:160:LEU:HD12	1.89	0.73
1:A:53:LEU:HD22	1:B:53:LEU:HD22	1.69	0.73
1:C:41:VAL:HG13	1:C:58:ILE:HG22	1.69	0.73
1:D:332:LEU:HA	1:D:335:ILE:HD13	1.70	0.73
1:A:124:ILE:CD1	1:B:8:THR:O	2.36	0.72
1:C:188:HIS:ND1	1:C:189:THR:HG22	2.03	0.72
1:C:336:VAL:CG1	1:C:342:MET:CE	2.68	0.72
1:C:53:LEU:HD22	1:D:53:LEU:HD22	1.71	0.72
1:C:209:LEU:O	1:C:213:VAL:HG13	1.90	0.72
1:B:201:SER:O	1:B:205:ILE:HG23	1.90	0.71
1:B:134:LYS:HD3	1:B:134:LYS:O	1.88	0.71
1:D:299:HIS:CD2	1:D:392:LEU:CD1	2.74	0.71
1:D:336:VAL:HG12	1:D:342:MET:CE	2.20	0.71
1:B:322:TYR:O	1:B:324:THR:HG22	1.91	0.71
1:C:187:VAL:CB	1:C:227:MET:HE1	2.19	0.71
1:A:331:ILE:O	1:A:335:ILE:CD1	2.33	0.71
1:B:173:LEU:HD11	1:B:175:TYR:CE1	2.26	0.71
1:D:200:VAL:HG11	1:D:205:ILE:HD11	1.72	0.71
1:D:298:CYS:SG	1:D:301:VAL:CG2	2.78	0.70
1:C:28:ILE:CD1	1:C:66:ILE:HG23	2.21	0.70
1:B:82:THR:HB	1:D:82:THR:HG21	1.73	0.70
1:A:284:CYS:HB2	1:A:347:ILE:HD12	1.72	0.70
1:C:173:LEU:HD11	1:C:175:TYR:CD1	2.26	0.70
1:C:28:ILE:HD12	1:C:66:ILE:HD13	1.72	0.70
1:D:384:ILE:CG2	1:D:388:LEU:HD12	2.22	0.70
1:C:117:ILE:HG21	1:C:345:GLY:N	2.07	0.70
1:C:174:GLU:HG2	1:C:185:ILE:HG23	1.72	0.70
1:B:49:THR:CG2	1:B:50:GLY:N	2.54	0.70
1:B:140:THR:O	1:B:144:SER:OG	2.10	0.70
1:B:49:THR:HG22	1:B:50:GLY:H	1.56	0.69
1:D:355:ARG:O	1:D:357:ILE:HD13	1.92	0.69
1:C:173:LEU:C	1:C:173:LEU:CD1	2.61	0.69
1:D:326:ILE:HD12	1:D:327:CYS:N	2.07	0.69
1:C:140:THR:O	1:C:144:SER:OG	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:VAL:HG23	1:A:214:THR:CA	2.21	0.69
1:D:47:THR:HG22	1:D:52:ILE:HA	1.74	0.69
1:C:326:ILE:CD1	1:C:327:CYS:N	2.48	0.69
1:C:355:ARG:NH2	1:C:373:ASP:OD1	2.26	0.69
1:A:188:HIS:ND1	1:A:189:THR:HG22	2.08	0.69
1:C:160:LEU:HD22	1:C:162:TRP:CZ2	2.27	0.68
1:D:200:VAL:HG21	1:D:205:ILE:HG12	1.76	0.68
1:B:66:ILE:O	1:B:69:ILE:HG23	1.92	0.68
1:A:284:CYS:SG	1:A:347:ILE:HD11	2.33	0.68
1:D:140:THR:O	1:D:144:SER:OG	2.10	0.68
1:B:82:THR:OG1	1:D:90:THR:HG21	1.94	0.68
1:B:81:ASP:HB2	1:B:84:LYS:HG3	1.75	0.68
1:A:140:THR:O	1:A:144:SER:OG	2.11	0.67
1:A:48:LYS:O	1:A:242:PRO:O	2.12	0.67
1:A:284:CYS:SG	1:A:347:ILE:CD1	2.82	0.67
1:C:317:ILE:HD12	1:C:318:ASN:N	2.07	0.67
1:A:57:GLU:OE2	1:B:244:GLY:O	2.11	0.67
1:B:63:VAL:HG11	1:C:63:VAL:CG1	2.23	0.67
1:B:139:LEU:HA	1:B:142:VAL:CG2	2.25	0.67
1:C:392:LEU:HD23	1:C:393:LEU:N	2.05	0.66
1:B:48:LYS:O	1:B:242:PRO:O	2.13	0.66
1:A:151:LEU:HD23	1:A:163:LEU:HD21	1.78	0.66
1:B:247:GLY:C	1:B:248:LEU:HD12	2.15	0.66
1:C:55:LEU:HD11	1:D:48:LYS:HB2	1.76	0.66
1:D:385:PRO:HD2	1:D:388:LEU:HD12	1.77	0.66
1:C:28:ILE:CD1	1:C:66:ILE:HD13	2.26	0.66
1:C:317:ILE:HD11	1:C:333:VAL:HG13	1.76	0.66
1:B:349:LYS:HG3	1:B:350:GLU:N	2.10	0.66
1:B:213:VAL:HG23	1:B:214:THR:N	2.11	0.66
1:C:336:VAL:HG12	1:C:342:MET:CE	2.26	0.65
1:B:160:LEU:HD22	1:B:162:TRP:CZ2	2.30	0.65
1:C:298:CYS:SG	1:C:301:VAL:HG22	2.36	0.65
1:A:94:LEU:HD21	1:C:51:LEU:HD13	1.79	0.65
1:D:148:ILE:CD1	1:D:169:SER:OG	2.44	0.65
1:B:28:ILE:HD11	1:B:66:ILE:HG23	1.79	0.64
1:C:85:GLY:HA2	1:C:243:MET:HE3	1.78	0.64
1:C:384:ILE:CG2	1:C:385:PRO:HD2	2.28	0.64
1:A:308:ALA:CB	1:A:315:LEU:HD13	2.27	0.64
1:D:215:GLN:O	1:D:220:LYS:NZ	2.27	0.64
1:B:297:LEU:HD11	1:B:335:ILE:CD1	2.28	0.63
1:B:6:PHE:CE2	1:B:174:GLU:HG3	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:VAL:O	1:C:369:ARG:NH1	2.31	0.63
1:B:289:ALA:O	1:B:293:VAL:HG12	1.99	0.63
1:C:174:GLU:HG2	1:C:185:ILE:HG12	1.81	0.63
1:A:326:ILE:HD12	1:A:327:CYS:N	2.14	0.62
1:B:190:ILE:HD12	1:B:227:MET:CE	2.29	0.62
1:C:289:ALA:O	1:C:293:VAL:HG12	1.98	0.62
1:B:148:ILE:HA	1:B:151:LEU:HD12	1.81	0.62
1:B:9:SER:HB2	1:B:140:THR:HG23	1.79	0.62
1:A:289:ALA:O	1:A:293:VAL:HG12	1.98	0.62
1:C:253:ILE:HD12	1:C:264:HIS:CE1	2.34	0.62
1:B:177:GLU:HG3	1:B:177:GLU:O	1.97	0.62
1:C:328:ASP:O	1:C:331:ILE:HG22	1.99	0.62
1:D:329:GLU:O	1:D:332:LEU:HD23	2.00	0.62
1:A:162:TRP:HB2	1:A:200:VAL:HG21	1.80	0.61
1:B:139:LEU:CA	1:B:142:VAL:HG23	2.31	0.61
1:C:301:VAL:HG12	1:C:302:LEU:N	2.15	0.61
1:D:384:ILE:HG23	1:D:388:LEU:HD12	1.82	0.61
1:B:27:ALA:C	1:B:69:ILE:HD11	2.21	0.61
1:A:162:TRP:HB2	1:A:200:VAL:CG2	2.31	0.61
1:C:304:GLN:HE22	1:D:8:THR:H	1.48	0.61
1:D:389:LYS:CB	1:D:390:PRO:HD3	2.30	0.61
1:C:187:VAL:CB	1:C:227:MET:CE	2.77	0.61
1:D:253:ILE:HD12	1:D:264:HIS:CE1	2.35	0.61
1:D:159:ILE:O	1:D:160:LEU:HD12	2.01	0.61
1:B:160:LEU:HD22	1:B:162:TRP:CE2	2.36	0.61
1:A:12:VAL:C	1:A:148:ILE:CD1	2.69	0.61
1:B:41:VAL:HG13	1:B:58:ILE:CG2	2.29	0.61
1:D:42:ALA:HB2	1:D:276:LYS:HE2	1.83	0.61
1:A:41:VAL:HG13	1:A:58:ILE:CG2	2.31	0.60
1:C:336:VAL:CG1	1:C:342:MET:HE1	2.31	0.60
1:B:80:ASP:OD1	1:B:84:LYS:NZ	2.34	0.60
1:B:332:LEU:HA	1:B:335:ILE:HG23	1.82	0.60
1:C:41:VAL:HG13	1:C:58:ILE:CG2	2.31	0.60
1:C:140:THR:HG21	1:C:261:TRP:HE1	1.67	0.60
1:C:321:THR:HG21	1:C:325:GLY:N	2.17	0.60
1:B:321:THR:HG21	1:B:325:GLY:N	2.17	0.60
1:D:119:ALA:HB1	1:D:277:VAL:HG11	1.83	0.60
1:B:257:THR:HG21	1:B:264:HIS:HE2	1.67	0.60
1:C:187:VAL:HG12	1:C:227:MET:HE2	1.83	0.59
1:C:55:LEU:HD11	1:D:48:LYS:HB3	1.82	0.59
1:C:12:VAL:HG12	1:C:168:LYS:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ALA:HB2	1:C:276:LYS:HE2	1.84	0.59
1:C:148:ILE:HA	1:C:151:LEU:HD12	1.84	0.59
1:A:140:THR:HG21	1:A:261:TRP:HE1	1.67	0.59
1:D:9:SER:HB2	1:D:140:THR:HG23	1.83	0.59
1:A:361:THR:HG23	1:A:366:HIS:CE1	2.36	0.59
1:D:293:VAL:O	1:D:293:VAL:CG2	2.50	0.59
1:D:147:LEU:HD12	1:D:217:VAL:CG2	2.24	0.59
1:B:178:VAL:O	1:B:179:GLU:HG2	2.03	0.59
1:D:140:THR:HG21	1:D:261:TRP:HE1	1.68	0.59
1:B:42:ALA:HB2	1:B:276:LYS:HE2	1.85	0.59
1:C:87:ASP:CG	1:C:90:THR:HG23	2.23	0.59
1:A:253:ILE:HD12	1:A:264:HIS:CE1	2.37	0.59
1:B:83:ASN:O	1:B:239:ILE:HG21	2.03	0.59
1:A:13:SER:N	1:A:148:ILE:HD13	2.17	0.59
1:B:213:VAL:HG23	1:B:214:THR:H	1.68	0.59
1:C:279:ARG:HH21	1:C:361:THR:HG21	1.68	0.59
1:C:147:LEU:HD12	1:C:217:VAL:CG1	2.32	0.58
1:A:279:ARG:HH21	1:A:361:THR:HG21	1.67	0.58
1:C:361:THR:HG23	1:C:366:HIS:CE1	2.38	0.58
1:A:44:GLU:OE2	1:B:248:LEU:HD13	2.03	0.58
1:B:65:ASP:O	1:B:69:ILE:HG22	2.03	0.58
1:B:297:LEU:O	1:B:326:ILE:HG22	2.04	0.58
1:C:174:GLU:HG2	1:C:185:ILE:CG2	2.33	0.58
1:C:189:THR:OG1	1:D:315:LEU:HD11	2.03	0.58
1:D:293:VAL:HG22	1:D:293:VAL:O	2.03	0.58
1:A:207:LYS:O	1:A:211:GLU:HG3	2.04	0.58
1:A:48:LYS:CG	1:A:49:THR:N	2.62	0.58
1:C:382:LEU:N	1:C:382:LEU:CD1	2.67	0.58
1:C:384:ILE:HG22	1:C:385:PRO:O	2.04	0.58
1:D:11:SER:HB3	1:D:148:ILE:HD13	1.85	0.57
1:C:9:SER:HB2	1:C:140:THR:HG23	1.85	0.57
1:D:279:ARG:HH21	1:D:361:THR:HG21	1.67	0.57
1:B:253:ILE:HD12	1:B:264:HIS:CE1	2.40	0.57
1:D:363:VAL:O	1:D:369:ARG:NH2	2.37	0.57
1:A:9:SER:HB2	1:A:140:THR:HG23	1.85	0.57
1:C:391:LYS:O	1:C:392:LEU:HB2	2.03	0.57
1:C:392:LEU:CD2	1:C:393:LEU:H	2.11	0.57
1:D:160:LEU:HD23	1:D:162:TRP:CZ2	2.39	0.57
1:B:213:VAL:O	1:B:217:VAL:CG1	2.49	0.57
1:C:354:THR:O	1:C:354:THR:CG2	2.53	0.57
1:D:361:THR:HG23	1:D:366:HIS:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD21	1:C:51:LEU:CD1	2.34	0.56
1:B:140:THR:HG21	1:B:261:TRP:HE1	1.70	0.56
1:D:198:ASP:OD1	1:D:236:ARG:NH2	2.38	0.56
1:C:37:PRO:CB	1:C:354:THR:HG23	2.30	0.56
1:C:139:LEU:HD22	1:C:184:PRO:HG3	1.87	0.56
1:B:339:ASN:ND2	1:B:382:LEU:HB3	2.20	0.56
1:C:87:ASP:HB3	1:C:90:THR:HG23	1.88	0.56
1:B:198:ASP:OD1	1:B:236:ARG:NH2	2.38	0.56
1:D:358:PHE:O	1:D:361:THR:HG22	2.05	0.56
1:A:331:ILE:HG22	1:A:335:ILE:HD11	1.87	0.56
1:C:288:ILE:HD11	1:C:342:MET:HE2	1.86	0.56
1:D:339:ASN:O	1:D:380:LYS:NZ	2.37	0.56
1:B:329:GLU:O	1:B:333:VAL:HG23	2.06	0.56
1:D:181:HIS:CG	1:D:299:HIS:HD1	2.14	0.55
1:A:42:ALA:HB2	1:A:276:LYS:HE2	1.88	0.55
1:B:178:VAL:O	1:B:179:GLU:HG3	2.05	0.55
1:A:12:VAL:HG12	1:A:168:LYS:HG3	1.88	0.55
1:A:223:MET:HG3	1:A:227:MET:HE3	1.88	0.55
1:A:48:LYS:HG2	1:A:49:THR:N	2.20	0.55
1:D:70:VAL:O	1:D:74:VAL:HG23	2.07	0.55
1:A:357:ILE:HG21	1:A:373:ASP:HB3	1.88	0.55
1:B:202:ASN:O	1:B:205:ILE:HG13	2.07	0.55
1:A:53:LEU:HD12	1:A:94:LEU:HB2	1.88	0.55
1:C:117:ILE:HG21	1:C:345:GLY:H	1.70	0.55
1:B:139:LEU:HD22	1:B:184:PRO:HG3	1.87	0.55
1:A:124:ILE:O	1:A:265:GLY:HA3	2.06	0.55
1:B:190:ILE:HD12	1:B:227:MET:HE1	1.88	0.55
1:B:213:VAL:CG2	1:B:214:THR:H	2.20	0.54
1:D:391:LYS:HG3	1:D:392:LEU:N	2.10	0.54
1:B:82:THR:HB	1:D:82:THR:CG2	2.37	0.54
1:D:148:ILE:HA	1:D:151:LEU:HD12	1.89	0.54
1:B:326:ILE:HG13	1:B:326:ILE:O	2.08	0.54
1:A:321:THR:HG21	1:A:325:GLY:N	2.23	0.54
1:B:385:PRO:HD2	1:B:388:LEU:HD12	1.89	0.54
1:A:382:LEU:N	1:A:382:LEU:CD1	2.71	0.54
1:A:378:PHE:N	1:A:378:PHE:CD1	2.75	0.54
1:A:339:ASN:ND2	1:A:382:LEU:HB3	2.23	0.54
1:C:127:GLY:O	1:C:302:LEU:HD12	2.07	0.54
1:B:173:LEU:C	1:B:173:LEU:HD12	2.28	0.54
1:B:124:ILE:HG23	1:B:265:GLY:CA	2.38	0.54
1:D:53:LEU:HD12	1:D:94:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ARG:O	1:C:321:THR:HG23	2.08	0.54
1:D:181:HIS:ND1	1:D:299:HIS:CE1	2.74	0.54
1:A:213:VAL:HG22	1:A:214:THR:H	1.57	0.53
1:C:116:ASP:O	1:C:117:ILE:HG22	2.08	0.53
1:C:117:ILE:CG2	1:C:117:ILE:O	2.41	0.53
1:D:300:ARG:O	1:D:321:THR:HG23	2.08	0.53
1:A:82:THR:HG21	1:C:82:THR:CG2	2.38	0.53
1:A:139:LEU:HD22	1:A:184:PRO:HG3	1.89	0.53
1:A:139:LEU:O	1:A:143:LEU:HD12	2.08	0.53
1:A:55:LEU:HD12	1:A:55:LEU:C	2.29	0.53
1:A:358:PHE:O	1:A:361:THR:HG22	2.08	0.53
1:A:82:THR:CG2	1:C:82:THR:HG21	2.39	0.53
1:A:335:ILE:HD12	1:A:335:ILE:N	2.21	0.53
1:D:213:VAL:HG23	1:D:214:THR:H	1.73	0.53
1:C:358:PHE:O	1:C:361:THR:HG22	2.08	0.53
1:B:162:TRP:CB	1:B:200:VAL:HG11	2.39	0.53
1:C:205:ILE:CG2	1:C:209:LEU:HD22	2.38	0.53
1:B:304:GLN:O	1:B:304:GLN:HG2	2.08	0.53
1:A:162:TRP:CB	1:A:200:VAL:CG2	2.86	0.53
1:C:308:ALA:HB2	1:C:315:LEU:HD22	1.90	0.53
1:D:351:LEU:HD13	1:D:376:TRP:HB3	1.91	0.53
1:B:53:LEU:HD12	1:B:94:LEU:HB2	1.91	0.53
1:A:284:CYS:CB	1:A:347:ILE:HD12	2.38	0.53
1:A:162:TRP:CB	1:A:200:VAL:HG21	2.39	0.52
1:B:321:THR:HG21	1:B:325:GLY:CA	2.39	0.52
1:C:124:ILE:HG23	1:C:265:GLY:CA	2.39	0.52
1:D:321:THR:HG21	1:D:325:GLY:N	2.25	0.52
1:C:268:ALA:HB3	1:D:251:ARG:CZ	2.39	0.52
1:D:24:ILE:O	1:D:28:ILE:HD12	2.09	0.52
1:D:332:LEU:HA	1:D:335:ILE:CD1	2.37	0.52
1:C:187:VAL:O	1:C:227:MET:HE2	2.09	0.52
1:D:173:LEU:CD1	1:D:175:TYR:CD1	2.88	0.52
1:C:288:ILE:HD11	1:C:342:MET:CE	2.40	0.52
1:B:382:LEU:CD1	1:B:382:LEU:N	2.73	0.52
1:D:296:GLY:O	1:D:392:LEU:HB2	2.09	0.52
1:D:384:ILE:CG2	1:D:385:PRO:HD2	2.39	0.52
1:B:81:ASP:C	1:B:83:ASN:N	2.63	0.52
1:D:57:GLU:O	1:D:58:ILE:HG22	2.10	0.52
1:B:213:VAL:CG2	1:B:214:THR:N	2.72	0.52
1:C:116:ASP:C	1:C:117:ILE:HG22	2.30	0.52
1:A:335:ILE:HG22	1:A:339:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:THR:HG21	1:B:315:LEU:CD1	2.38	0.52
1:D:209:LEU:O	1:D:213:VAL:CG2	2.56	0.52
1:A:284:CYS:SG	1:A:347:ILE:HD12	2.49	0.52
1:C:317:ILE:CG1	1:C:333:VAL:HG13	2.40	0.52
1:D:124:ILE:HG23	1:D:265:GLY:CA	2.40	0.52
1:D:213:VAL:HG23	1:D:214:THR:N	2.25	0.52
1:B:296:GLY:O	1:B:392:LEU:HB2	2.10	0.52
1:B:209:LEU:HB2	1:B:231:TYR:CE1	2.46	0.51
1:C:187:VAL:CG1	1:C:227:MET:HE2	2.41	0.51
1:C:173:LEU:CD1	1:C:175:TYR:CD1	2.93	0.51
1:A:300:ARG:O	1:A:321:THR:HG23	2.09	0.51
1:D:299:HIS:HD2	1:D:392:LEU:CD1	2.12	0.51
1:D:391:LYS:CG	1:D:392:LEU:H	2.07	0.51
1:B:124:ILE:HG23	1:B:265:GLY:HA2	1.93	0.51
1:D:57:GLU:C	1:D:58:ILE:CG2	2.79	0.51
1:D:200:VAL:CG2	1:D:205:ILE:HG12	2.40	0.51
1:A:29:LEU:HD13	1:A:41:VAL:HB	1.92	0.51
1:B:66:ILE:HA	1:B:69:ILE:CG2	2.41	0.51
1:A:288:ILE:HD13	1:A:336:VAL:HG13	1.92	0.51
1:C:331:ILE:CG2	1:C:332:LEU:N	2.74	0.51
1:C:205:ILE:HG22	1:C:209:LEU:HD22	1.93	0.50
1:C:357:ILE:HG21	1:C:373:ASP:HB3	1.93	0.50
1:C:315:LEU:HD11	1:D:230:TYR:CE2	2.46	0.50
1:A:199:ASN:C	1:A:199:ASN:OD1	2.49	0.50
1:C:187:VAL:CG1	1:C:227:MET:CE	2.89	0.50
1:D:148:ILE:HD12	1:D:169:SER:OG	2.11	0.50
1:D:192:ILE:HD13	1:D:209:LEU:HD22	1.93	0.50
1:B:209:LEU:O	1:B:213:VAL:CG2	2.53	0.50
1:A:116:ASP:OD1	1:A:116:ASP:C	2.50	0.50
1:C:117:ILE:CG2	1:C:345:GLY:HA3	2.37	0.50
1:A:123:GLY:C	1:A:125:MET:HE3	2.32	0.50
1:A:162:TRP:CG	1:A:200:VAL:HG21	2.47	0.50
1:A:12:VAL:C	1:A:148:ILE:HD13	2.32	0.50
1:B:210:GLU:OE2	1:B:215:GLN:HG2	2.11	0.50
1:D:384:ILE:HG23	1:D:385:PRO:HD2	1.94	0.49
1:D:8:THR:HG23	1:D:172:THR:HG22	1.93	0.49
1:D:218:ILE:HG22	1:D:223:MET:HG3	1.94	0.49
1:A:247:GLY:C	1:A:248:LEU:HD12	2.32	0.49
1:C:321:THR:HG21	1:C:325:GLY:CA	2.42	0.49
1:D:139:LEU:HD22	1:D:184:PRO:HG3	1.93	0.49
1:B:11:SER:HA	1:B:255:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:HA	1:B:335:ILE:CG2	2.42	0.49
1:C:124:ILE:HG23	1:C:265:GLY:HA2	1.95	0.49
1:A:316:SER:O	1:A:317:ILE:HD13	2.13	0.49
1:B:146:LYS:HA	1:B:149:LEU:HD12	1.94	0.49
1:B:61:ASN:OD1	1:B:102:GLN:HB2	2.13	0.49
1:B:59:THR:HG22	1:B:102:GLN:HG3	1.95	0.49
1:C:224:ASP:OD2	1:C:226:LYS:CB	2.45	0.49
1:C:317:ILE:CD1	1:C:333:VAL:HG13	2.42	0.49
1:D:218:ILE:CG2	1:D:223:MET:HG3	2.43	0.49
1:B:300:ARG:O	1:B:321:THR:HG23	2.13	0.48
1:D:119:ALA:HB1	1:D:277:VAL:CG1	2.43	0.48
1:D:148:ILE:HD11	1:D:169:SER:CB	2.42	0.48
1:B:297:LEU:HD11	1:B:335:ILE:HD11	1.95	0.48
1:B:391:LYS:O	1:B:392:LEU:HD12	2.13	0.48
1:A:62:ALA:HB1	1:A:64:ILE:CD1	2.43	0.48
1:D:189:THR:HB	1:D:228:LEU:HB2	1.94	0.48
1:C:302:LEU:HG	1:C:302:LEU:O	2.11	0.48
1:A:159:ILE:O	1:A:160:LEU:CD1	2.59	0.48
1:B:332:LEU:O	1:B:335:ILE:HG23	2.13	0.48
1:A:173:LEU:HD23	1:A:175:TYR:CE1	2.49	0.48
1:C:354:THR:O	1:C:354:THR:HG23	2.12	0.48
1:C:69:ILE:O	1:C:73:VAL:HG23	2.13	0.48
1:B:147:LEU:HD12	1:B:217:VAL:HG21	1.94	0.48
1:B:297:LEU:HD11	1:B:335:ILE:HD13	1.94	0.48
1:A:388:LEU:CD1	1:A:388:LEU:N	2.73	0.48
1:D:385:PRO:HD2	1:D:388:LEU:CD1	2.43	0.48
1:D:357:ILE:HG21	1:D:373:ASP:HB3	1.94	0.48
1:C:160:LEU:HD22	1:C:162:TRP:CE2	2.48	0.48
1:C:321:THR:HG21	1:C:325:GLY:H	1.79	0.48
1:A:12:VAL:HA	1:A:148:ILE:HD11	1.95	0.48
1:B:299:HIS:CD2	1:B:392:LEU:HD23	2.49	0.48
1:D:178:VAL:HG12	1:D:178:VAL:O	2.13	0.48
1:B:384:ILE:CG1	1:B:385:PRO:HD2	2.40	0.48
1:D:296:GLY:O	1:D:391:LYS:HB2	2.14	0.48
1:D:58:ILE:HG12	1:D:58:ILE:O	2.12	0.47
1:C:224:ASP:HB3	1:C:226:LYS:H	1.79	0.47
1:A:248:LEU:HD13	1:B:44:GLU:OE1	2.14	0.47
1:A:62:ALA:HB1	1:A:64:ILE:HD13	1.96	0.47
1:C:253:ILE:HD12	1:C:264:HIS:NE2	2.29	0.47
1:C:87:ASP:CB	1:C:90:THR:HG23	2.43	0.47
1:C:8:THR:HG23	1:C:172:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ILE:HG12	1:B:385:PRO:O	2.15	0.47
1:C:304:GLN:O	1:C:304:GLN:HG2	2.14	0.47
1:C:391:LYS:O	1:C:392:LEU:CB	2.63	0.47
1:A:151:LEU:HD11	1:A:192:ILE:CD1	2.44	0.47
1:D:253:ILE:HD12	1:D:264:HIS:NE2	2.30	0.47
1:B:382:LEU:N	1:B:382:LEU:HD12	2.29	0.47
1:A:339:ASN:O	1:A:380:LYS:NZ	2.42	0.47
1:D:148:ILE:CD1	1:D:169:SER:CB	2.93	0.47
1:D:332:LEU:H	1:D:332:LEU:HD23	1.80	0.47
1:A:140:THR:CG2	1:A:261:TRP:HE1	2.28	0.47
1:D:124:ILE:HG23	1:D:265:GLY:HA2	1.96	0.47
1:B:186:ARG:HA	1:B:222:LEU:HD23	1.97	0.47
1:A:115:GLU:O	1:A:345:GLY:HA3	2.15	0.47
1:D:392:LEU:HA	1:D:392:LEU:HD23	1.69	0.47
1:B:9:SER:CB	1:B:140:THR:HG23	2.42	0.47
1:A:279:ARG:NH2	1:A:361:THR:HG21	2.30	0.47
1:B:102:GLN:O	1:B:103:ASP:C	2.53	0.47
1:C:121:ASP:OD1	1:C:122:GLN:N	2.48	0.47
1:B:357:ILE:HG21	1:B:373:ASP:HB3	1.97	0.47
1:B:90:THR:HB	1:D:243:MET:HE1	1.95	0.47
1:D:243:MET:HE2	1:D:243:MET:HB2	1.67	0.47
1:D:62:ALA:HB1	1:D:64:ILE:CD1	2.45	0.47
1:B:81:ASP:OD1	1:B:83:ASN:OD1	2.33	0.46
1:D:279:ARG:NH2	1:D:361:THR:HG21	2.30	0.46
1:C:49:THR:HG22	1:C:50:GLY:N	2.30	0.46
1:D:391:LYS:CG	1:D:392:LEU:N	2.75	0.46
1:A:315:LEU:HD11	1:B:230:TYR:CE2	2.50	0.46
1:D:162:TRP:CZ3	1:D:205:ILE:HD13	2.50	0.46
1:C:182:LEU:CD1	1:C:300:ARG:HD2	2.44	0.46
1:D:148:ILE:HD11	1:D:169:SER:OG	2.15	0.46
1:B:48:LYS:CG	1:B:49:THR:N	2.75	0.46
1:D:8:THR:OG1	1:D:172:THR:HB	2.16	0.46
1:A:12:VAL:CA	1:A:148:ILE:CD1	2.92	0.46
1:C:321:THR:HG21	1:C:325:GLY:HA3	1.96	0.46
1:A:132:GLU:OE2	1:A:175:TYR:OH	2.24	0.46
1:B:79:TYR:HB3	1:B:86:PHE:O	2.15	0.46
1:C:335:ILE:HD11	1:C:385:PRO:HD3	1.97	0.46
1:D:9:SER:CB	1:D:140:THR:HG23	2.46	0.46
1:A:20:MET:HE1	1:A:47:THR:HG21	1.97	0.46
1:A:311:VAL:HG21	1:B:230:TYR:CE1	2.50	0.46
1:A:372:PRO:HA	1:A:378:PHE:HZ	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ILE:HD13	1:B:336:VAL:HG13	1.98	0.46
1:D:48:LYS:HG3	1:D:49:THR:H	1.57	0.46
1:C:329:GLU:O	1:C:333:VAL:HG23	2.15	0.46
1:A:121:ASP:OD1	1:A:122:GLN:N	2.48	0.46
1:A:82:THR:HG21	1:C:82:THR:HG21	1.97	0.46
1:D:284:CYS:SG	1:D:347:ILE:HD13	2.56	0.46
1:C:326:ILE:HD12	1:C:327:CYS:CA	2.42	0.46
1:B:201:SER:HG	1:B:204:GLU:H	1.59	0.46
1:B:81:ASP:CB	1:B:84:LYS:HG3	2.42	0.46
1:C:317:ILE:C	1:C:317:ILE:HD12	2.36	0.45
1:A:124:ILE:C	1:A:125:MET:HG3	2.37	0.45
1:C:339:ASN:HD21	1:C:383:GLU:HG2	1.81	0.45
1:C:186:ARG:NH1	1:C:226:LYS:O	2.49	0.45
1:D:298:CYS:HG	1:D:301:VAL:HG22	1.76	0.45
1:B:358:PHE:HA	1:B:361:THR:OG1	2.16	0.45
1:B:147:LEU:O	1:B:151:LEU:HD12	2.16	0.45
1:C:9:SER:CB	1:C:140:THR:HG23	2.47	0.45
1:C:218:ILE:CG2	1:C:223:MET:HG3	2.46	0.45
1:B:8:THR:OG1	1:B:172:THR:HB	2.17	0.45
1:C:8:THR:HA	1:C:172:THR:HA	1.99	0.45
1:A:219:PRO:HG2	1:A:222:LEU:HD22	1.99	0.45
1:B:218:ILE:CB	1:B:223:MET:HE1	2.44	0.45
1:B:274:SER:O	1:B:280:SER:OG	2.33	0.45
1:B:247:GLY:O	1:B:248:LEU:HD12	2.16	0.45
1:B:12:VAL:HG12	1:B:168:LYS:HG3	1.99	0.45
1:A:151:LEU:HD11	1:A:192:ILE:HD12	1.99	0.45
1:A:298:CYS:SG	1:A:301:VAL:HG12	2.57	0.45
1:C:8:THR:OG1	1:C:172:THR:HB	2.17	0.44
1:D:284:CYS:HB2	1:D:347:ILE:HD13	1.98	0.44
1:D:29:LEU:HD13	1:D:41:VAL:HB	1.98	0.44
1:B:237:PHE:HE1	1:B:240:GLY:HA3	1.82	0.44
1:D:120:GLY:O	1:D:121:ASP:CB	2.56	0.44
1:D:140:THR:CG2	1:D:261:TRP:HE1	2.30	0.44
1:D:201:SER:O	1:D:204:GLU:N	2.50	0.44
1:C:174:GLU:CG	1:C:185:ILE:HG23	2.42	0.44
1:D:336:VAL:CG1	1:D:342:MET:CE	2.93	0.44
1:A:9:SER:CB	1:A:140:THR:HG23	2.47	0.44
1:C:321:THR:CG2	1:C:325:GLY:H	2.30	0.44
1:A:327:CYS:HG	1:A:388:LEU:CD2	2.23	0.44
1:B:63:VAL:CG1	1:C:63:VAL:CG1	2.94	0.44
1:C:140:THR:CG2	1:C:261:TRP:HE1	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ILE:O	1:B:332:LEU:C	2.56	0.44
1:C:279:ARG:NH2	1:C:361:THR:HG21	2.31	0.44
1:D:57:GLU:C	1:D:58:ILE:HG22	2.38	0.44
1:B:210:GLU:OE2	1:B:215:GLN:CG	2.65	0.44
1:C:218:ILE:HG22	1:C:223:MET:HG3	1.98	0.44
1:A:253:ILE:HD12	1:A:264:HIS:NE2	2.33	0.44
1:D:326:ILE:HD12	1:D:327:CYS:CA	2.47	0.44
1:A:321:THR:HG21	1:A:325:GLY:CA	2.48	0.44
1:A:8:THR:OG1	1:A:172:THR:HB	2.18	0.44
1:C:87:ASP:CG	1:C:90:THR:CG2	2.86	0.44
1:C:139:LEU:HD21	1:C:222:LEU:HD21	2.00	0.44
1:D:62:ALA:HB1	1:D:64:ILE:HD13	2.00	0.44
1:A:118:GLY:O	1:A:119:ALA:C	2.57	0.44
1:A:124:ILE:HD12	1:B:8:THR:O	2.17	0.43
1:B:140:THR:CG2	1:B:261:TRP:HE1	2.30	0.43
1:B:257:THR:HG21	1:B:264:HIS:NE2	2.31	0.43
1:A:213:VAL:O	1:A:214:THR:C	2.56	0.43
1:A:200:VAL:CG1	1:A:205:ILE:HG12	2.41	0.43
1:B:178:VAL:HG23	1:B:178:VAL:O	2.17	0.43
1:B:132:GLU:OE2	1:B:175:TYR:OH	2.24	0.43
1:A:55:LEU:HD11	1:B:246:ALA:HB1	2.00	0.43
1:A:124:ILE:HD11	1:A:304:GLN:NE2	2.32	0.43
1:D:132:GLU:OE2	1:D:175:TYR:OH	2.24	0.43
1:D:8:THR:HA	1:D:172:THR:HA	1.99	0.43
1:C:55:LEU:HD13	1:C:96:CYS:HB3	2.01	0.43
1:B:8:THR:HA	1:B:172:THR:HA	2.00	0.43
1:D:200:VAL:HG13	1:D:200:VAL:O	2.17	0.43
1:C:382:LEU:N	1:C:382:LEU:HD12	2.32	0.43
1:A:389:LYS:N	1:A:390:PRO:CD	2.81	0.43
1:A:335:ILE:HD13	1:A:335:ILE:N	2.08	0.43
1:B:315:LEU:HD12	1:B:315:LEU:C	2.38	0.43
1:B:134:LYS:C	1:B:134:LYS:HD3	2.30	0.43
1:B:381:GLU:C	1:B:382:LEU:HD12	2.39	0.43
1:A:246:ALA:HB1	1:B:55:LEU:CD1	2.49	0.43
1:D:237:PHE:C	1:D:237:PHE:CD1	2.92	0.43
1:D:331:ILE:HD12	1:D:331:ILE:N	2.34	0.43
1:C:62:ALA:HB1	1:C:64:ILE:CD1	2.49	0.43
1:C:308:ALA:HB2	1:C:315:LEU:HD13	2.01	0.43
1:D:126:PHE:CE1	1:D:304:GLN:HB2	2.53	0.43
1:A:97:VAL:CG2	1:A:98:GLU:N	2.79	0.43
1:B:243:MET:HE1	1:D:90:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:GLU:O	1:B:383:GLU:HG2	2.18	0.43
1:B:391:LYS:C	1:B:392:LEU:HD12	2.39	0.43
1:A:8:THR:HA	1:A:172:THR:HA	2.01	0.43
1:B:139:LEU:O	1:B:142:VAL:HG23	2.19	0.43
1:C:274:SER:O	1:C:280:SER:OG	2.33	0.43
1:A:82:THR:HG23	1:C:82:THR:HG21	2.01	0.42
1:D:233:PRO:C	1:D:235:GLY:H	2.23	0.42
1:D:6:PHE:N	1:D:6:PHE:CD2	2.86	0.42
1:D:47:THR:HG22	1:D:52:ILE:CD1	2.40	0.42
1:A:248:LEU:HD23	1:B:248:LEU:CD2	2.31	0.42
1:D:200:VAL:O	1:D:200:VAL:CG1	2.68	0.42
1:D:12:VAL:HG12	1:D:168:LYS:HG3	2.00	0.42
1:A:189:THR:HB	1:A:228:LEU:HB2	2.00	0.42
1:B:162:TRP:HB3	1:B:200:VAL:HG11	2.01	0.42
1:A:384:ILE:HG22	1:A:388:LEU:HD13	2.00	0.42
1:A:82:THR:HG21	1:C:82:THR:HG23	2.00	0.42
1:D:237:PHE:C	1:D:237:PHE:HD1	2.23	0.42
1:C:62:ALA:HB1	1:C:64:ILE:HD13	2.02	0.42
1:D:274:SER:O	1:D:280:SER:OG	2.33	0.42
1:C:296:GLY:O	1:C:392:LEU:HB2	2.19	0.42
1:B:315:LEU:HD12	1:B:316:SER:N	2.35	0.42
1:C:147:LEU:O	1:C:151:LEU:HD12	2.20	0.42
1:B:27:ALA:CB	1:B:69:ILE:HD11	2.49	0.42
1:A:24:ILE:O	1:A:28:ILE:HD12	2.20	0.42
1:B:62:ALA:HB1	1:B:64:ILE:CD1	2.49	0.42
1:A:233:PRO:C	1:A:235:GLY:H	2.23	0.42
1:A:252:LYS:HB3	1:A:255:VAL:HG22	2.00	0.42
1:C:29:LEU:HD13	1:C:41:VAL:HB	2.02	0.42
1:B:322:TYR:O	1:B:324:THR:CG2	2.65	0.42
1:B:253:ILE:HD12	1:B:264:HIS:NE2	2.34	0.42
1:B:291:SER:HB3	1:B:382:LEU:HD11	2.02	0.42
1:C:315:LEU:HD11	1:D:230:TYR:CZ	2.54	0.42
1:B:62:ALA:HB1	1:B:64:ILE:HD13	2.00	0.42
1:A:51:LEU:HD13	1:C:94:LEU:HD21	2.01	0.42
1:C:336:VAL:HG11	1:C:342:MET:HE1	2.02	0.42
1:A:200:VAL:CG1	1:A:201:SER:N	2.83	0.42
1:A:200:VAL:HG12	1:A:201:SER:O	2.20	0.42
1:D:148:ILE:CD1	1:D:169:SER:HB3	2.50	0.42
1:A:207:LYS:O	1:A:211:GLU:CG	2.66	0.41
1:D:238:VAL:HG13	1:D:239:ILE:HG12	2.01	0.41
1:D:288:ILE:CG2	1:D:303:VAL:HG21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LEU:O	1:C:213:VAL:CG1	2.64	0.41
1:B:139:LEU:C	1:B:142:VAL:HG23	2.41	0.41
1:C:336:VAL:CG1	1:C:342:MET:HE3	2.31	0.41
1:B:90:THR:HB	1:D:243:MET:CE	2.50	0.41
1:C:233:PRO:C	1:C:235:GLY:H	2.24	0.41
1:B:322:TYR:C	1:B:324:THR:CG2	2.89	0.41
1:C:154:CYS:HB3	1:C:160:LEU:HB2	2.02	0.41
1:A:163:LEU:HD11	1:A:194:THR:HG21	2.03	0.41
1:C:219:PRO:HG2	1:C:222:LEU:HD22	2.01	0.41
1:B:94:LEU:HD22	1:C:96:CYS:HB2	2.02	0.41
1:B:321:THR:CG2	1:B:325:GLY:N	2.83	0.41
1:C:328:ASP:O	1:C:331:ILE:N	2.50	0.41
1:B:201:SER:OG	1:B:204:GLU:CB	2.69	0.41
1:D:391:LYS:O	1:D:392:LEU:HD23	2.21	0.41
1:A:94:LEU:N	1:A:94:LEU:HD23	2.36	0.41
1:C:301:VAL:CG1	1:C:302:LEU:N	2.82	0.41
1:B:297:LEU:CD1	1:B:335:ILE:HD13	2.51	0.41
1:B:332:LEU:CA	1:B:335:ILE:HG23	2.50	0.41
1:D:125:MET:HE2	1:D:277:VAL:C	2.41	0.41
1:D:284:CYS:CB	1:D:347:ILE:HD13	2.51	0.41
1:B:209:LEU:CA	1:B:213:VAL:HG22	2.51	0.41
1:B:231:TYR:N	1:B:231:TYR:CD2	2.89	0.41
1:A:252:LYS:NZ	2:A:400:ACT:H3	2.36	0.41
1:B:28:ILE:O	1:B:31:ALA:HB3	2.21	0.40
1:B:154:CYS:HB3	1:B:160:LEU:HB2	2.02	0.40
1:A:127:GLY:HA3	1:A:285:ALA:HB1	2.03	0.40
1:A:319:VAL:O	1:A:319:VAL:CG2	2.69	0.40
1:C:227:MET:HE2	1:C:227:MET:HB2	1.93	0.40
1:C:173:LEU:HD13	1:C:174:GLU:O	2.20	0.40
1:D:339:ASN:ND2	1:D:339:ASN:N	2.68	0.40
1:C:389:LYS:CB	1:C:390:PRO:HD3	2.51	0.40
1:B:209:LEU:HG	1:B:231:TYR:CD1	2.57	0.40
1:D:326:ILE:HD12	1:D:326:ILE:C	2.41	0.40
1:B:28:ILE:N	1:B:69:ILE:HD11	2.36	0.40
1:C:308:ALA:CB	1:C:315:LEU:HD13	2.51	0.40
1:D:252:LYS:HB3	1:D:255:VAL:HG22	2.02	0.40
1:B:233:PRO:C	1:B:235:GLY:H	2.23	0.40
1:A:92:SER:OG	1:C:51:LEU:HD12	2.21	0.40
1:D:192:ILE:CD1	1:D:209:LEU:HD22	2.51	0.40
1:D:355:ARG:HA	1:D:356:PRO:HD3	1.98	0.40
1:C:318:ASN:OD1	1:C:319:VAL:N	2.55	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	375/415 (90%)	352 (94%)	22 (6%)	1 (0%)	46 84
1	B	375/415 (90%)	351 (94%)	24 (6%)	0	100 100
1	C	375/415 (90%)	349 (93%)	22 (6%)	4 (1%)	17 62
1	D	375/415 (90%)	349 (93%)	25 (7%)	1 (0%)	46 84
All	All	1500/1660 (90%)	1401 (93%)	93 (6%)	6 (0%)	39 80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	121	ASP
1	A	102	GLN
1	C	327	CYS
1	C	392	LEU
1	C	117	ILE
1	C	356	PRO

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	306/351 (87%)	248 (81%)	58 (19%)	2 10
1	B	312/351 (89%)	249 (80%)	63 (20%)	1 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	308/351 (88%)	241 (78%)	67 (22%)	1 6
1	D	310/351 (88%)	257 (83%)	53 (17%)	2 12
All	All	1236/1404 (88%)	995 (80%)	241 (20%)	2 9

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	CYS
1	A	49	THR
1	A	52	ILE
1	A	57	GLU
1	A	68	LYS
1	A	76	SER
1	A	82	THR
1	A	86	PHE
1	A	89	GLN
1	A	94	LEU
1	A	97	VAL
1	A	100	GLN
1	A	102	GLN
1	A	103	ASP
1	A	122	GLN
1	A	124	ILE
1	A	125	MET
1	A	134	LYS
1	A	144	SER
1	A	148	ILE
1	A	150	ARG
1	A	152	GLN
1	A	170	GLN
1	A	172	THR
1	A	176	GLU
1	A	181	HIS
1	A	189	THR
1	A	205	ILE
1	A	211	GLU
1	A	222	LEU
1	A	223	MET
1	A	224	ASP
1	A	227	MET
1	A	228	LEU

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Mol	Chain	Res	Type
1	A	245	ASP
1	A	253	ILE
1	A	277	VAL
1	A	280	SER
1	A	293	VAL
1	A	301	VAL
1	A	306	SER
1	A	316	SER
1	A	324	THR
1	A	327	CYS
1	A	329	GLU
1	A	330	SER
1	A	333	VAL
1	A	334	ASP
1	A	335	ILE
1	A	354	THR
1	A	357	ILE
1	A	361	THR
1	A	378	PHE
1	A	382	LEU
1	A	383	GLU
1	A	387	GLU
1	A	388	LEU
1	A	392	LEU
1	B	28	ILE
1	B	43	CYS
1	B	44	GLU
1	B	49	THR
1	B	51	LEU
1	B	52	ILE
1	B	57	GLU
1	B	63	VAL
1	B	69	ILE
1	B	76	SER
1	B	80	ASP
1	B	81	ASP
1	B	86	PHE
1	B	100	GLN
1	B	117	ILE
1	B	122	GLN
1	B	125	MET
1	B	134	LYS

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Mol	Chain	Res	Type
1	B	142	VAL
1	B	144	SER
1	B	145	THR
1	B	150	ARG
1	B	151	LEU
1	B	152	GLN
1	B	170	GLN
1	B	172	THR
1	B	173	LEU
1	B	176	GLU
1	B	181	HIS
1	B	189	THR
1	B	209	LEU
1	B	215	GLN
1	B	227	MET
1	B	231	TYR
1	B	234	SER
1	B	243	MET
1	B	245	ASP
1	B	253	ILE
1	B	277	VAL
1	B	280	SER
1	B	293	VAL
1	B	306	SER
1	B	315	LEU
1	B	316	SER
1	B	324	THR
1	B	326	ILE
1	B	328	ASP
1	B	330	SER
1	B	334	ASP
1	B	335	ILE
1	B	337	ASN
1	B	348	ILE
1	B	349	LYS
1	B	354	THR
1	B	357	ILE
1	B	361	THR
1	B	381	GLU
1	B	382	LEU
1	B	383	GLU
1	B	384	ILE

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Mol	Chain	Res	Type
1	B	385	PRO
1	B	387	GLU
1	B	391	LYS
1	C	6	PHE
1	C	19	LYS
1	C	28	ILE
1	C	43	CYS
1	C	44	GLU
1	C	49	THR
1	C	51	LEU
1	C	52	ILE
1	C	53	LEU
1	C	57	GLU
1	C	63	VAL
1	C	66	ILE
1	C	76	SER
1	C	82	THR
1	C	86	PHE
1	C	90	THR
1	C	102	GLN
1	C	103	ASP
1	C	122	GLN
1	C	134	LYS
1	C	136	MET
1	C	144	SER
1	C	150	ARG
1	C	151	LEU
1	C	152	GLN
1	C	170	GLN
1	C	172	THR
1	C	173	LEU
1	C	174	GLU
1	C	185	ILE
1	C	189	THR
1	C	207	LYS
1	C	209	LEU
1	C	213	VAL
1	C	217	VAL
1	C	222	LEU
1	C	224	ASP
1	C	226	LYS
1	C	227	MET

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Mol	Chain	Res	Type
1	C	234	SER
1	C	239	ILE
1	C	243	MET
1	C	245	ASP
1	C	253	ILE
1	C	280	SER
1	C	293	VAL
1	C	306	SER
1	C	316	SER
1	C	317	ILE
1	C	324	THR
1	C	327	CYS
1	C	328	ASP
1	C	329	GLU
1	C	330	SER
1	C	331	ILE
1	C	334	ASP
1	C	337	ASN
1	C	349	LYS
1	C	354	THR
1	C	355	ARG
1	C	357	ILE
1	C	361	THR
1	C	369	ARG
1	C	381	GLU
1	C	382	LEU
1	C	387	GLU
1	C	392	LEU
1	D	6	PHE
1	D	19	LYS
1	D	43	CYS
1	D	51	LEU
1	D	57	GLU
1	D	58	ILE
1	D	66	ILE
1	D	76	SER
1	D	82	THR
1	D	86	PHE
1	D	100	GLN
1	D	102	GLN
1	D	115	GLU
1	D	117	ILE

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Mol	Chain	Res	Type
1	D	122	GLN
1	D	134	LYS
1	D	144	SER
1	D	148	ILE
1	D	150	ARG
1	D	151	LEU
1	D	170	GLN
1	D	172	THR
1	D	173	LEU
1	D	176	GLU
1	D	189	THR
1	D	205	ILE
1	D	212	GLU
1	D	223	MET
1	D	224	ASP
1	D	227	MET
1	D	234	SER
1	D	237	PHE
1	D	239	ILE
1	D	245	ASP
1	D	251	ARG
1	D	253	ILE
1	D	280	SER
1	D	306	SER
1	D	316	SER
1	D	324	THR
1	D	328	ASP
1	D	329	GLU
1	D	330	SER
1	D	334	ASP
1	D	338	LYS
1	D	346	MET
1	D	347	ILE
1	D	348	ILE
1	D	349	LYS
1	D	354	THR
1	D	357	ILE
1	D	361	THR
1	D	381	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	339	ASN
1	B	83	ASN
1	B	122	GLN
1	B	215	GLN
1	B	339	ASN
1	C	304	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	A	400	-	1,3,3	1.47	0	0,3,3	0.00	-
2	ACT	B	400	-	1,3,3	1.09	0	0,3,3	0.00	-
2	ACT	C	400	-	1,3,3	1.42	0	0,3,3	0.00	-
2	ACT	D	400	-	1,3,3	1.44	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACT	A	400	-	-	0/0/0/0	0/0/0/0
2	ACT	B	400	-	-	0/0/0/0	0/0/0/0
2	ACT	C	400	-	-	0/0/0/0	0/0/0/0
2	ACT	D	400	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	ACT	1	0
2	C	400	ACT	2	0

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	379/415 (91%)	-0.16	5 (1%)	79	67	47, 68, 99, 129	0
1	B	379/415 (91%)	-0.12	6 (1%)	74	62	44, 73, 108, 124	0
1	C	379/415 (91%)	0.03	11 (2%)	55	40	49, 80, 119, 139	0
1	D	379/415 (91%)	0.07	10 (2%)	59	45	54, 89, 122, 142	0
All	All	1516/1660 (91%)	-0.05	32 (2%)	67	52	44, 76, 114, 142	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103	ASP	5.2
1	D	199	ASN	4.5
1	A	327	CYS	4.1
1	C	104	ILE	4.1
1	D	200	VAL	3.1
1	C	238	VAL	3.0
1	B	238	VAL	3.0
1	B	239	ILE	3.0
1	D	327	CYS	3.0
1	C	181	HIS	2.9
1	D	238	VAL	2.9
1	D	326	ILE	2.9
1	D	178	VAL	2.9
1	C	178	VAL	2.8
1	C	180	GLY	2.8
1	D	296	GLY	2.7
1	C	239	ILE	2.6
1	B	196	HIS	2.6
1	A	103	ASP	2.5
1	C	296	GLY	2.5
1	D	180	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	197	ALA	2.5
1	B	81	ASP	2.4
1	D	115	GLU	2.4
1	D	240	GLY	2.4
1	C	101	SER	2.4
1	C	102	GLN	2.3
1	C	199	ASN	2.2
1	B	85	GLY	2.2
1	A	391	LYS	2.2
1	A	179	GLU	2.1
1	A	225	ASP	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)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ACT	C	400	4/4	0.94	0.38	3.87	43,47,47,48	0
2	ACT	B	400	4/4	0.97	0.35	3.36	31,32,32,35	0
2	ACT	A	400	4/4	0.94	0.30	1.72	39,40,41,43	0
2	ACT	D	400	4/4	0.93	0.21	-0.06	35,37,38,40	0

6.5 Other polymers (i)

There are no such residues in this entry.