Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:11 AM GMT

PDB ID	:	2ZVI
Title	:	Crystal structure of 2,3-diketo-5-methylthiopentyl-1-phosphate enolase from Bacillus subtilis
Authors	:	Tamura, H.; Yadani, T.; Kai, Y.; Inoue, T.; Matsumura, H.
Deposited on	:	2008-11-07
Resolution	:	2.30 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:

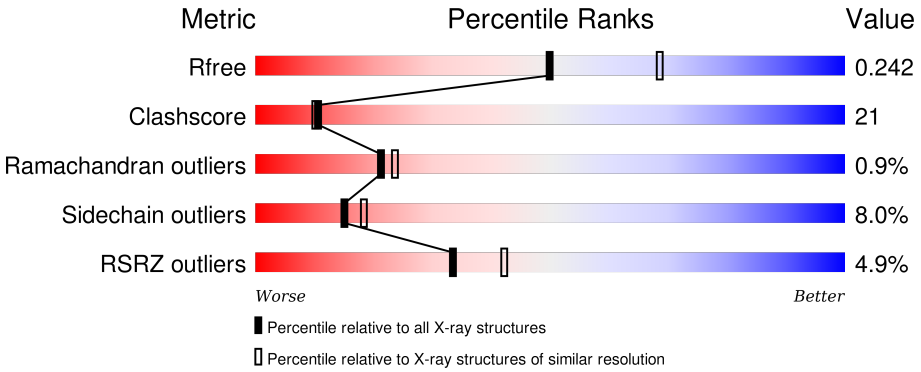
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	425	2% 61% 28% • 7%
1	B	425	5% 58% 30% 5% 7%
1	C	425	7% 56% 31% • 9%
1	D	425	3% 55% 31% 5% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12253 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 2,3-diketo-5-methylthiopentyl-1-phosphate enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3031	1946	515	561	9			
1	B	396	Total	C	N	O	S	0	0	0
			3024	1941	515	559	9			
1	C	385	Total	C	N	O	S	0	0	0
			2936	1885	503	539	9			
1	D	388	Total	C	N	O	S	0	0	0
			2954	1896	506	544	8			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP O31666
A	-9	GLY	-	EXPRESSION TAG	UNP O31666
A	-8	SER	-	EXPRESSION TAG	UNP O31666
A	-7	SER	-	EXPRESSION TAG	UNP O31666
A	-6	HIS	-	EXPRESSION TAG	UNP O31666
A	-5	HIS	-	EXPRESSION TAG	UNP O31666
A	-4	HIS	-	EXPRESSION TAG	UNP O31666
A	-3	HIS	-	EXPRESSION TAG	UNP O31666
A	-2	HIS	-	EXPRESSION TAG	UNP O31666
A	-1	HIS	-	EXPRESSION TAG	UNP O31666
A	0	SER	-	EXPRESSION TAG	UNP O31666
A	1	SER	-	EXPRESSION TAG	UNP O31666
A	2	GLY	-	EXPRESSION TAG	UNP O31666
A	3	LEU	-	EXPRESSION TAG	UNP O31666
A	4	VAL	-	EXPRESSION TAG	UNP O31666
A	5	PRO	-	EXPRESSION TAG	UNP O31666
A	6	ARG	-	EXPRESSION TAG	UNP O31666
A	7	GLY	-	EXPRESSION TAG	UNP O31666
A	8	SER	-	EXPRESSION TAG	UNP O31666
A	9	HIS	-	EXPRESSION TAG	UNP O31666
B	-10	MET	-	EXPRESSION TAG	UNP O31666

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLY	-	EXPRESSION TAG	UNP O31666
B	-8	SER	-	EXPRESSION TAG	UNP O31666
B	-7	SER	-	EXPRESSION TAG	UNP O31666
B	-6	HIS	-	EXPRESSION TAG	UNP O31666
B	-5	HIS	-	EXPRESSION TAG	UNP O31666
B	-4	HIS	-	EXPRESSION TAG	UNP O31666
B	-3	HIS	-	EXPRESSION TAG	UNP O31666
B	-2	HIS	-	EXPRESSION TAG	UNP O31666
B	-1	HIS	-	EXPRESSION TAG	UNP O31666
B	0	SER	-	EXPRESSION TAG	UNP O31666
B	1	SER	-	EXPRESSION TAG	UNP O31666
B	2	GLY	-	EXPRESSION TAG	UNP O31666
B	3	LEU	-	EXPRESSION TAG	UNP O31666
B	4	VAL	-	EXPRESSION TAG	UNP O31666
B	5	PRO	-	EXPRESSION TAG	UNP O31666
B	6	ARG	-	EXPRESSION TAG	UNP O31666
B	7	GLY	-	EXPRESSION TAG	UNP O31666
B	8	SER	-	EXPRESSION TAG	UNP O31666
B	9	HIS	-	EXPRESSION TAG	UNP O31666
C	-10	MET	-	EXPRESSION TAG	UNP O31666
C	-9	GLY	-	EXPRESSION TAG	UNP O31666
C	-8	SER	-	EXPRESSION TAG	UNP O31666
C	-7	SER	-	EXPRESSION TAG	UNP O31666
C	-6	HIS	-	EXPRESSION TAG	UNP O31666
C	-5	HIS	-	EXPRESSION TAG	UNP O31666
C	-4	HIS	-	EXPRESSION TAG	UNP O31666
C	-3	HIS	-	EXPRESSION TAG	UNP O31666
C	-2	HIS	-	EXPRESSION TAG	UNP O31666
C	-1	HIS	-	EXPRESSION TAG	UNP O31666
C	0	SER	-	EXPRESSION TAG	UNP O31666
C	1	SER	-	EXPRESSION TAG	UNP O31666
C	2	GLY	-	EXPRESSION TAG	UNP O31666
C	3	LEU	-	EXPRESSION TAG	UNP O31666
C	4	VAL	-	EXPRESSION TAG	UNP O31666
C	5	PRO	-	EXPRESSION TAG	UNP O31666
C	6	ARG	-	EXPRESSION TAG	UNP O31666
C	7	GLY	-	EXPRESSION TAG	UNP O31666
C	8	SER	-	EXPRESSION TAG	UNP O31666
C	9	HIS	-	EXPRESSION TAG	UNP O31666
D	-10	MET	-	EXPRESSION TAG	UNP O31666
D	-9	GLY	-	EXPRESSION TAG	UNP O31666
D	-8	SER	-	EXPRESSION TAG	UNP O31666

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	SER	-	EXPRESSION TAG	UNP O31666
D	-6	HIS	-	EXPRESSION TAG	UNP O31666
D	-5	HIS	-	EXPRESSION TAG	UNP O31666
D	-4	HIS	-	EXPRESSION TAG	UNP O31666
D	-3	HIS	-	EXPRESSION TAG	UNP O31666
D	-2	HIS	-	EXPRESSION TAG	UNP O31666
D	-1	HIS	-	EXPRESSION TAG	UNP O31666
D	0	SER	-	EXPRESSION TAG	UNP O31666
D	1	SER	-	EXPRESSION TAG	UNP O31666
D	2	GLY	-	EXPRESSION TAG	UNP O31666
D	3	LEU	-	EXPRESSION TAG	UNP O31666
D	4	VAL	-	EXPRESSION TAG	UNP O31666
D	5	PRO	-	EXPRESSION TAG	UNP O31666
D	6	ARG	-	EXPRESSION TAG	UNP O31666
D	7	GLY	-	EXPRESSION TAG	UNP O31666
D	8	SER	-	EXPRESSION TAG	UNP O31666
D	9	HIS	-	EXPRESSION TAG	UNP O31666

- Molecule 2 is water.

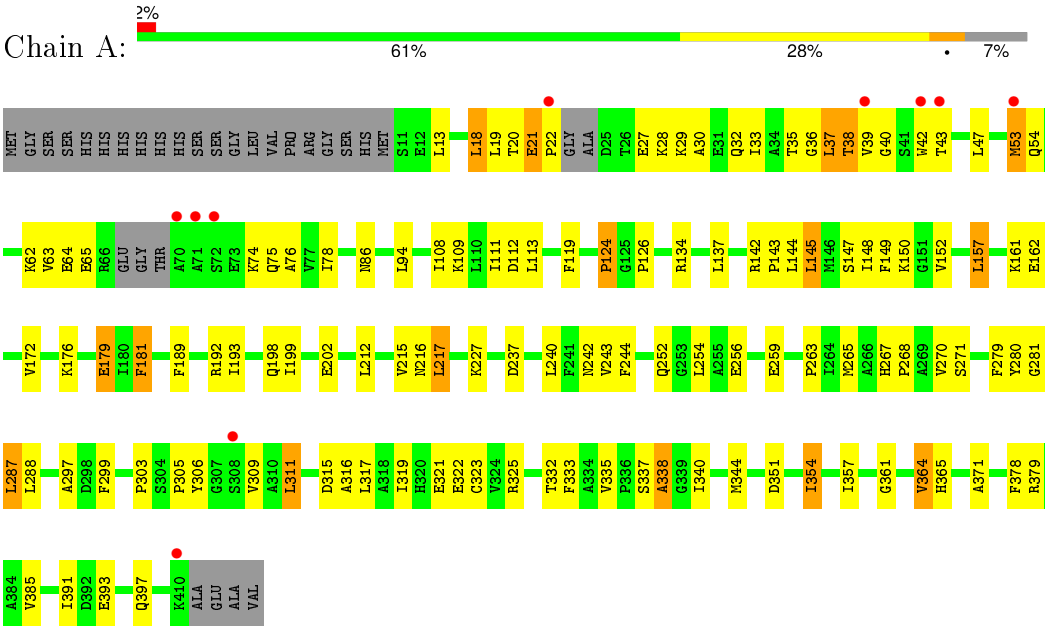
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	80	Total O 80 80	0	0
2	B	70	Total O 70 70	0	0
2	C	62	Total O 62 62	0	0
2	D	96	Total O 96 96	0	0

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.

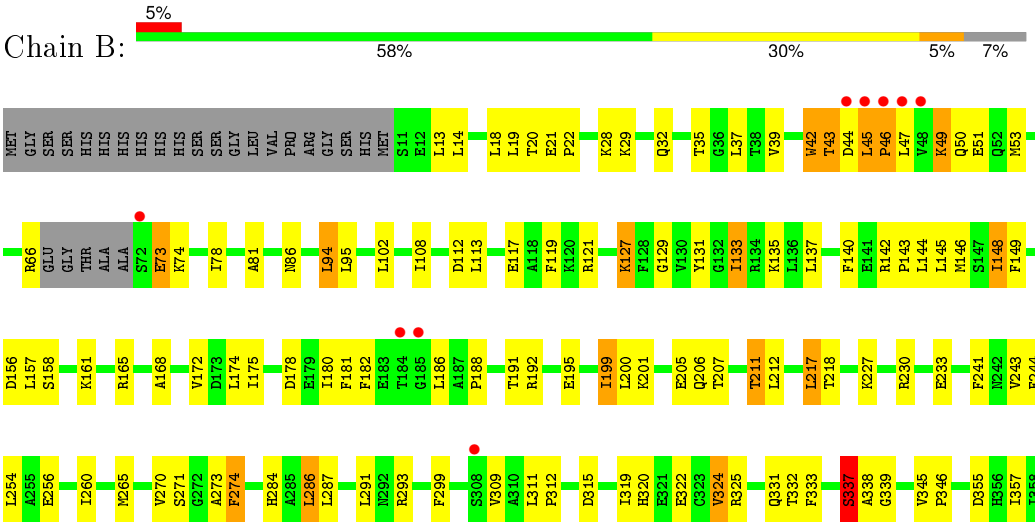
- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase

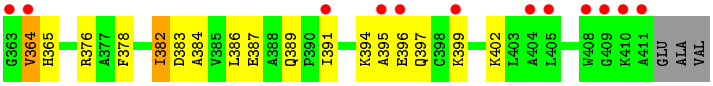
Chain A:



- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase

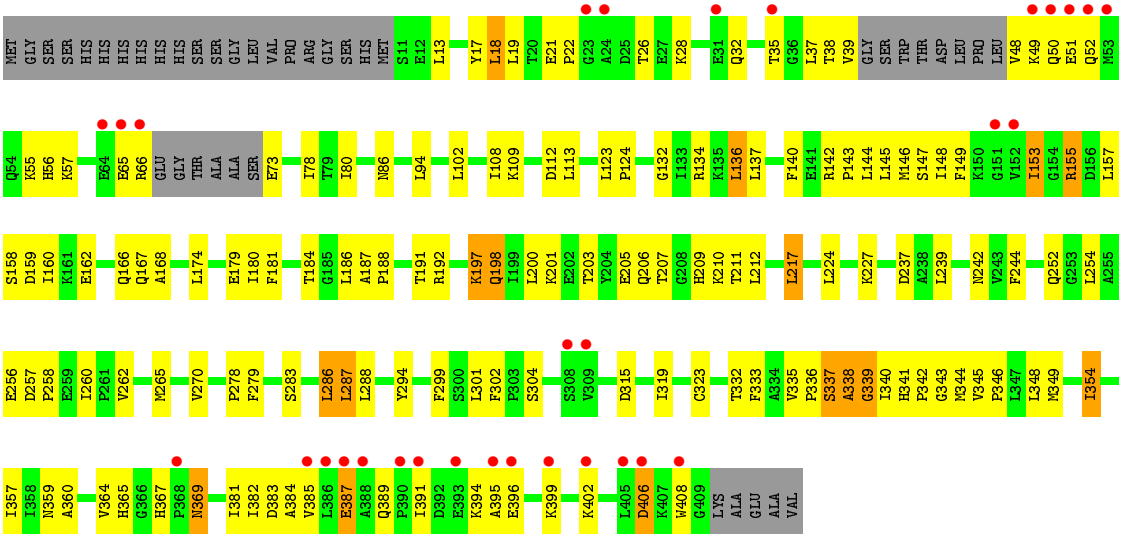
Chain B:





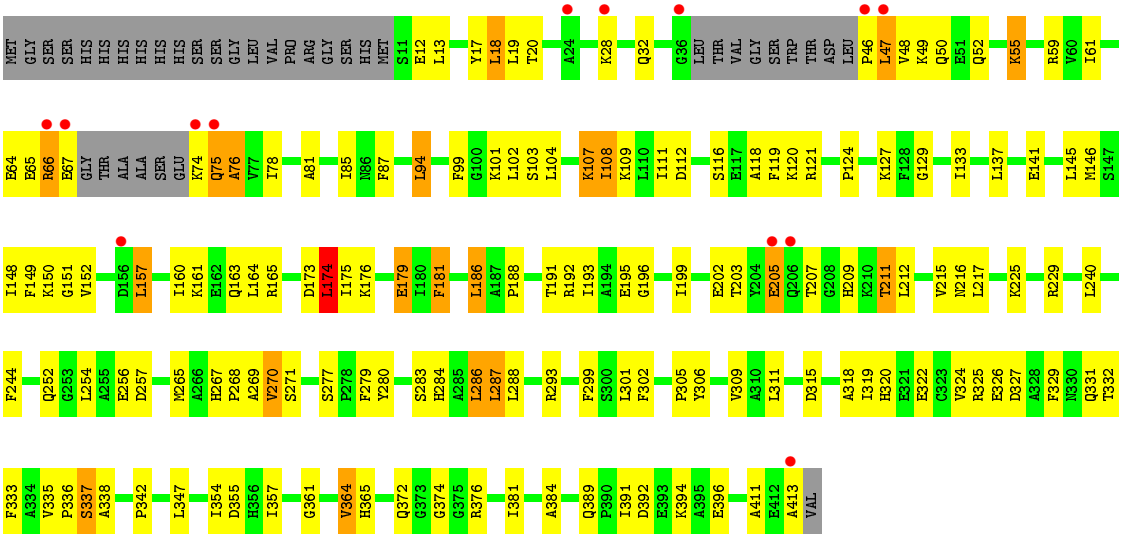
- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase

Chain C:



- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.33Å 91.47Å 106.97Å 90.00° 90.82° 90.00°	Depositor
Resolution (Å)	30.50 – 2.30 30.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.50-2.30) 95.1 (30.50-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.75 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.242 0.201 , 0.242	Depositor DCC
R_{free} test set	3267 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.6	EDS
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 64711 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12253	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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	0.36	0/3093	0.63	0/4180
1	B	0.35	0/3087	0.63	1/4175 (0.0%)
1	C	0.34	0/2995	0.63	1/4046 (0.0%)
1	D	0.35	0/3014	0.64	2/4073 (0.0%)
All	All	0.35	0/12189	0.63	4/16474 (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	C	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	D	337	SER	N-CA-C	5.64	126.23	111.00
1	D	174	LEU	CA-CB-CG	5.57	128.12	115.30
1	C	217	LEU	CA-CB-CG	5.23	127.32	115.30
1	B	337	SER	N-CA-C	5.20	125.03	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	336	PRO	Peptide
1	C	338	ALA	Peptide
1	C	339	GLY	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	3031	0	3054	116	0
1	B	3024	0	3033	152	0
1	C	2936	0	2949	121	0
1	D	2954	0	2965	131	0
2	A	80	0	0	3	0
2	B	70	0	0	4	0
2	C	62	0	0	1	0
2	D	96	0	0	4	0
All	All	12253	0	12001	511	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 21.

All (511) 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:B:146:MET:HE2	1:B:174:LEU:HD11	1.29	1.12
1:B:325:ARG:HD3	1:C:166:GLN:HE22	1.16	1.09
1:B:386:LEU:HD23	1:C:186:LEU:HD21	1.33	1.09
1:B:45:LEU:HD13	1:B:53:MET:HE1	1.37	1.06
1:C:391:ILE:HD12	1:C:391:ILE:H	1.24	0.98
1:D:75:GLN:N	1:D:75:GLN:HE21	1.60	0.98
1:B:152:VAL:HG13	1:B:153:ILE:HD12	1.43	0.98
1:A:38:THR:HG21	1:A:58:GLY:H	1.26	0.96
1:B:142:ARG:HG2	1:B:382:ILE:HD11	1.48	0.95
1:B:13:LEU:HD21	1:B:94:LEU:HD23	1.47	0.95
1:C:207:THR:HG23	1:C:209:HIS:H	1.33	0.93
1:A:38:THR:HG23	1:A:39:VAL:HG23	1.51	0.90
1:D:207:THR:HG23	1:D:209:HIS:H	1.35	0.90
1:B:325:ARG:HD3	1:C:166:GLN:NE2	1.87	0.90
1:D:75:GLN:H	1:D:75:GLN:NE2	1.69	0.90
1:D:61:ILE:HD11	1:D:81:ALA:HB2	1.53	0.89
1:B:37:LEU:HD11	1:B:102:LEU:HG	1.57	0.86
1:B:311:LEU:HD21	1:B:315:ASP:HB2	1.57	0.86
1:D:47:LEU:HA	1:D:50:GLN:HB2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ILE:HD12	1:B:149:PHE:H	1.43	0.84
1:A:306:TYR:HB2	1:A:344:MET:HE3	1.61	0.83
1:C:384:ALA:HB2	1:C:394:LYS:HG3	1.62	0.82
1:D:19:LEU:CD2	1:D:108:ILE:HG12	2.11	0.81
1:C:212:LEU:HD22	1:C:237:ASP:HB3	1.63	0.81
1:A:112:ASP:HA	1:A:286:LEU:HG	1.64	0.80
1:B:378:PHE:O	1:B:382:ILE:HG23	1.82	0.80
1:B:61:ILE:HD11	1:B:81:ALA:HB2	1.64	0.80
1:C:340:ILE:HA	1:C:344:MET:HE3	1.64	0.79
1:C:396:GLU:HA	1:C:402:LYS:HE2	1.65	0.79
1:A:378:PHE:O	1:A:382:ILE:HG22	1.82	0.79
1:C:13:LEU:HD21	1:C:94:LEU:HD23	1.64	0.78
1:D:124:PRO:HB3	1:D:256:GLU:HG2	1.65	0.78
1:A:21:GLU:HB2	1:A:22:PRO:HD3	1.66	0.78
1:B:137:LEU:HD21	1:B:212:LEU:HG	1.66	0.77
1:A:38:THR:HG21	1:A:58:GLY:N	2.00	0.76
1:B:152:VAL:HG22	1:B:153:ILE:H	1.50	0.76
1:D:203:THR:O	1:D:207:THR:HG22	1.85	0.75
1:C:142:ARG:HD2	1:C:143:PRO:O	1.87	0.75
1:B:383:ASP:O	1:B:387:GLU:HG3	1.86	0.75
1:B:127:LYS:HE3	1:B:260:ILE:O	1.86	0.75
1:C:158:SER:O	1:C:162:GLU:HG3	1.87	0.74
1:B:131:TYR:HB2	1:D:48:VAL:HG22	1.68	0.74
1:A:142:ARG:CG	1:A:382:ILE:HD11	2.17	0.74
1:D:152:VAL:HG11	1:D:181:PHE:CG	2.24	0.73
1:C:349:MET:SD	1:C:385:VAL:HG21	2.28	0.73
1:C:340:ILE:HD13	1:C:348:LEU:HD11	1.71	0.72
1:B:311:LEU:CD2	1:B:315:ASP:HB2	2.18	0.72
1:D:75:GLN:N	1:D:75:GLN:NE2	2.28	0.72
1:C:402:LYS:O	1:C:406:ASP:HB2	1.90	0.72
1:D:326:GLU:HG3	2:D:454:HOH:O	1.88	0.72
1:D:309:VAL:HB	1:D:338:ALA:HB1	1.71	0.71
1:B:127:LYS:HE2	2:B:419:HOH:O	1.92	0.70
1:D:193:ILE:HG12	1:D:215:VAL:HG21	1.73	0.70
1:D:75:GLN:H	1:D:75:GLN:HE21	1.28	0.70
1:C:28:LYS:HE2	1:C:32:GLN:NE2	2.06	0.70
1:C:132:GLY:O	1:C:136:LEU:HD22	1.92	0.70
1:C:35:THR:HG22	1:C:57:LYS:HZ3	1.57	0.69
1:C:188:PRO:HG2	1:C:191:THR:OG1	1.92	0.69
1:A:382:ILE:HD13	1:A:382:ILE:C	2.13	0.69
1:B:152:VAL:CG1	1:B:153:ILE:HD12	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:PRO:O	1:C:381:ILE:HD13	1.92	0.68
1:B:230:ARG:O	1:B:233:GLU:HG2	1.92	0.68
1:C:252:GLN:O	1:C:256:GLU:HG3	1.93	0.68
1:C:13:LEU:HD21	1:C:94:LEU:CD2	2.24	0.68
1:A:147:SER:HB2	1:A:172:VAL:HG11	1.76	0.68
1:C:217:LEU:CD1	1:C:224:LEU:HD22	2.23	0.67
1:A:337:SER:O	1:A:340:ILE:HG13	1.94	0.67
1:C:142:ARG:HG2	1:C:143:PRO:HD2	1.76	0.67
1:A:13:LEU:HD11	1:A:113:LEU:HD22	1.76	0.67
1:A:142:ARG:HD2	1:A:143:PRO:O	1.95	0.66
1:C:35:THR:HG22	1:C:57:LYS:NZ	2.11	0.66
1:C:109:LYS:NZ	1:C:283:SER:HA	2.10	0.66
1:C:227:LYS:HD3	2:C:475:HOH:O	1.95	0.66
1:C:304:SER:HB3	1:C:338:ALA:H	1.61	0.66
1:A:144:LEU:HB2	1:A:357:ILE:HG12	1.77	0.65
1:B:399:LYS:HG2	1:B:402:LYS:HZ1	1.61	0.65
1:D:108:ILE:HD13	1:D:109:LYS:N	2.12	0.65
1:B:142:ARG:CG	1:B:382:ILE:HD11	2.25	0.65
1:A:20:THR:HG22	1:A:21:GLU:HG3	1.78	0.65
1:C:203:THR:O	1:C:207:THR:HG22	1.95	0.65
1:C:112:ASP:HA	1:C:286:LEU:HG	1.79	0.65
1:D:211:THR:HG23	2:D:419:HOH:O	1.96	0.64
1:B:324:VAL:HG22	1:B:331:GLN:OE1	1.98	0.64
1:A:259:GLU:HG3	2:A:438:HOH:O	1.97	0.64
1:C:217:LEU:HD13	1:C:224:LEU:HD22	1.79	0.64
1:A:217:LEU:HD23	1:A:227:LYS:HD3	1.79	0.64
1:C:391:ILE:H	1:C:391:ILE:CD1	2.02	0.64
1:A:306:TYR:HB2	1:A:344:MET:CE	2.27	0.64
1:C:48:VAL:O	1:C:49:LYS:HB3	1.97	0.63
1:A:111:ILE:CD1	1:A:283:SER:HB3	2.29	0.63
1:D:19:LEU:HD23	1:D:108:ILE:HG12	1.80	0.63
1:D:17:TYR:CD2	1:D:108:ILE:HD11	2.33	0.63
1:A:39:VAL:HG13	1:A:53:MET:SD	2.39	0.63
1:B:315:ASP:O	1:B:319:ILE:HG13	1.99	0.63
1:B:395:ALA:O	1:B:402:LYS:HD3	1.99	0.63
1:B:188:PRO:HG2	1:B:191:THR:OG1	1.99	0.62
1:D:47:LEU:HA	1:D:50:GLN:CB	2.29	0.62
1:B:152:VAL:HG22	1:B:153:ILE:N	2.15	0.62
1:D:207:THR:HG23	1:D:209:HIS:N	2.12	0.61
1:A:20:THR:HG1	1:A:279:PHE:HD2	1.47	0.61
1:D:225:LYS:HE2	1:D:257:ASP:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:HE2	1:A:282:PHE:O	2.00	0.61
1:D:64:GLU:HG2	1:D:65:GLU:N	2.16	0.61
1:D:61:ILE:CD1	1:D:81:ALA:HB2	2.28	0.61
1:A:142:ARG:HG2	1:A:382:ILE:HD11	1.82	0.61
1:D:216:ASN:HA	1:D:240:LEU:HB3	1.83	0.61
1:B:19:LEU:HD22	1:B:108:ILE:HG12	1.80	0.61
1:C:181:PHE:HZ	1:C:187:ALA:HB3	1.66	0.61
1:A:111:ILE:HD13	1:A:283:SER:HB3	1.83	0.61
1:D:145:LEU:HD23	1:D:146:MET:N	2.16	0.61
1:D:19:LEU:HD11	1:D:78:ILE:HD12	1.83	0.61
1:D:74:LYS:HB3	1:D:75:GLN:NE2	2.15	0.60
1:C:51:GLU:HA	1:C:51:GLU:OE2	2.00	0.60
1:C:155:ARG:NH2	1:C:155:ARG:HB3	2.17	0.60
1:A:322:GLU:CD	1:A:325:ARG:HH12	2.04	0.60
1:D:152:VAL:HG11	1:D:181:PHE:CD1	2.36	0.60
1:D:20:THR:HG1	1:D:74:LYS:N	1.98	0.60
1:B:399:LYS:HG2	1:B:402:LYS:NZ	2.16	0.60
1:A:381:ILE:HD11	1:A:391:ILE:HD13	1.83	0.60
1:D:181:PHE:CZ	1:D:192:ARG:HD3	2.37	0.60
1:C:155:ARG:HH21	1:C:155:ARG:HB3	1.66	0.60
1:B:47:LEU:HA	1:B:50:GLN:HB2	1.84	0.60
1:A:252:GLN:O	1:A:256:GLU:HG3	2.02	0.60
1:C:341:HIS:HD2	1:C:343:GLY:H	1.50	0.60
1:B:43:THR:CG2	1:B:43:THR:O	2.50	0.60
1:B:396:GLU:HA	1:B:402:LYS:HD2	1.84	0.60
1:A:28:LYS:O	1:A:32:GLN:HG3	2.02	0.59
1:A:37:LEU:HD11	2:A:490:HOH:O	2.03	0.59
1:D:75:GLN:O	1:D:75:GLN:HG2	2.02	0.59
1:C:278:PRO:HG2	1:C:279:PHE:CD1	2.37	0.59
1:B:241:PHE:HD2	1:B:243:VAL:HG22	1.67	0.59
1:C:200:LEU:HD22	1:C:211:THR:OG1	2.03	0.59
1:B:112:ASP:HA	1:B:286:LEU:HG	1.84	0.59
1:A:181:PHE:CZ	1:A:192:ARG:HD3	2.37	0.59
1:D:165:ARG:NH2	1:D:202:GLU:OE1	2.35	0.59
1:B:243:VAL:HG21	1:B:251:MET:SD	2.43	0.59
1:A:309:VAL:HG22	1:A:338:ALA:CB	2.33	0.59
1:A:181:PHE:CE1	1:A:192:ARG:HD3	2.38	0.58
1:D:28:LYS:O	1:D:32:GLN:HG3	2.04	0.58
1:D:305:PRO:HG2	1:D:306:TYR:CE1	2.39	0.58
1:C:367:HIS:CE1	1:C:369:ASN:HB2	2.39	0.58
1:B:165:ARG:HA	1:B:199:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:PHE:HE1	1:D:108:ILE:HD12	1.69	0.57
1:C:383:ASP:O	1:C:387:GLU:HG2	2.04	0.57
1:B:14:LEU:HD22	1:B:61:ILE:CD1	2.34	0.57
1:D:137:LEU:HD21	1:D:212:LEU:HG	1.86	0.57
1:B:20:THR:HG23	1:B:73:GLU:HG3	1.86	0.57
1:C:78:ILE:HG22	1:C:80:ILE:CD1	2.34	0.57
1:D:364:VAL:HG22	1:D:374:GLY:HA3	1.87	0.57
1:D:103:SER:OG	1:D:104:LEU:HD12	2.05	0.57
1:D:48:VAL:O	1:D:52:GLN:HG2	2.05	0.57
1:A:216:ASN:HA	1:A:240:LEU:HB3	1.87	0.57
1:C:21:GLU:N	1:C:22:PRO:HD3	2.19	0.57
1:B:153:ILE:HA	1:B:181:PHE:CD1	2.40	0.57
1:B:46:PRO:HG2	1:B:47:LEU:H	1.70	0.56
1:B:286:LEU:HD22	1:B:291:LEU:HG	1.87	0.56
1:D:104:LEU:HD12	1:D:104:LEU:N	2.20	0.56
1:B:252:GLN:O	1:B:256:GLU:HG3	2.03	0.56
1:D:244:PHE:HE2	1:D:287:LEU:HD22	1.70	0.56
1:D:244:PHE:CE2	1:D:287:LEU:HD22	2.39	0.56
1:B:389:GLN:OE1	1:B:394:LYS:HD3	2.05	0.56
1:D:13:LEU:HD12	1:D:87:PHE:CZ	2.40	0.56
1:D:74:LYS:HE2	1:D:75:GLN:HB3	1.88	0.56
1:B:311:LEU:HD21	1:B:315:ASP:CB	2.33	0.56
1:A:20:THR:O	1:A:74:LYS:O	2.23	0.56
1:A:364:VAL:HG13	1:A:371:ALA:HA	1.88	0.56
1:C:153:ILE:HD12	1:C:180:ILE:HG13	1.88	0.56
1:D:118:ALA:HA	1:D:121:ARG:NH1	2.21	0.56
1:C:162:GLU:O	1:C:166:GLN:HG2	2.06	0.56
1:C:153:ILE:HD12	1:C:180:ILE:CD1	2.35	0.56
1:D:107:LYS:HD2	1:D:280:TYR:OH	2.04	0.56
1:D:384:ALA:HB2	1:D:394:LYS:HG2	1.88	0.55
1:C:360:ALA:O	1:C:364:VAL:HG23	2.06	0.55
1:D:179:GLU:HG2	1:D:267:HIS:NE2	2.21	0.55
1:C:56:HIS:HD2	1:C:86:ASN:ND2	2.03	0.55
1:B:42:TRP:C	1:B:44:ASP:H	2.07	0.55
1:C:345:VAL:N	1:C:346:PRO:HD2	2.20	0.55
1:D:347:LEU:HD21	1:D:413:ALA:HB3	1.87	0.55
1:D:49:LYS:HA	1:D:52:GLN:CG	2.36	0.55
1:A:157:LEU:HD22	1:A:161:LYS:HG3	1.89	0.55
1:A:189:PHE:CG	1:A:227:LYS:HE2	2.42	0.55
1:B:43:THR:O	1:B:43:THR:HG22	2.06	0.55
1:A:242:ASN:OD1	1:A:267:HIS:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLU:O	1:B:121:ARG:HG3	2.07	0.55
1:B:94:LEU:HD13	1:B:95:LEU:N	2.22	0.55
1:A:335:VAL:HG22	1:A:357:ILE:HB	1.89	0.54
1:D:309:VAL:O	1:D:338:ALA:HB3	2.08	0.54
1:A:193:ILE:HG12	1:A:215:VAL:HG21	1.89	0.54
1:A:94:LEU:HD13	1:A:94:LEU:C	2.28	0.54
1:D:47:LEU:HD12	1:D:48:VAL:N	2.21	0.54
1:A:322:GLU:OE1	1:A:325:ARG:NH1	2.40	0.54
1:D:391:ILE:HD13	1:D:411:ALA:CB	2.37	0.54
1:A:38:THR:CG2	1:A:39:VAL:HG23	2.32	0.54
1:B:172:VAL:HG11	1:B:175:ILE:HD13	1.89	0.54
1:C:201:LYS:HG2	1:C:205:GLU:OE2	2.06	0.54
1:B:153:ILE:HA	1:B:181:PHE:HD1	1.73	0.54
1:C:17:TYR:CE1	1:C:80:ILE:HD13	2.43	0.54
1:C:395:ALA:HB1	1:C:402:LYS:HG3	1.89	0.54
1:B:20:THR:CG2	1:B:73:GLU:HG3	2.38	0.54
1:A:309:VAL:HG22	1:A:338:ALA:HB1	1.90	0.53
1:A:20:THR:HG22	1:A:21:GLU:CG	2.38	0.53
1:A:18:LEU:HD21	1:A:75:GLN:HB3	1.90	0.53
1:B:13:LEU:HD21	1:B:94:LEU:CD2	2.28	0.53
1:C:22:PRO:HB2	1:C:26:THR:HG22	1.90	0.53
1:B:135:LYS:HD2	2:B:430:HOH:O	2.08	0.53
1:B:153:ILE:HD11	1:B:178:ASP:CG	2.28	0.53
1:B:320:HIS:HE1	1:B:355:ASP:O	1.92	0.53
1:A:47:LEU:HB2	2:A:456:HOH:O	2.07	0.53
1:C:37:LEU:HD21	1:C:102:LEU:HG	1.89	0.53
1:B:395:ALA:HB1	1:B:402:LYS:HG3	1.89	0.53
1:C:124:PRO:HB3	1:C:256:GLU:HG2	1.90	0.53
1:B:19:LEU:CD1	1:B:78:ILE:HD12	2.39	0.53
1:D:46:PRO:O	1:D:50:GLN:HB2	2.08	0.53
1:D:49:LYS:HA	1:D:52:GLN:HG2	1.91	0.53
1:D:148:ILE:HD12	1:D:361:GLY:HA2	1.91	0.53
1:B:143:PRO:HD2	1:B:382:ILE:HD13	1.90	0.52
1:B:284:HIS:HB3	1:B:319:ILE:HD11	1.90	0.52
1:B:165:ARG:CA	1:B:199:ILE:HD11	2.38	0.52
1:C:148:ILE:O	1:C:365:HIS:HE1	1.92	0.52
1:A:56:HIS:CB	1:A:86:ASN:HD21	2.23	0.52
1:A:124:PRO:HB3	1:A:256:GLU:HG2	1.90	0.52
1:C:19:LEU:HD11	1:C:78:ILE:HD12	1.91	0.52
1:B:157:LEU:HD13	1:B:195:GLU:HG3	1.92	0.52
1:B:274:PHE:N	1:B:274:PHE:CD2	2.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LYS:O	1:D:85:ILE:HD11	2.10	0.52
1:A:42:TRP:HH2	1:A:54:GLN:HG2	1.75	0.52
1:B:47:LEU:HG	1:B:47:LEU:O	2.10	0.52
1:A:137:LEU:HD21	1:A:212:LEU:HG	1.91	0.52
1:A:142:ARG:HG2	1:A:143:PRO:HD2	1.91	0.52
1:D:150:LYS:HB3	1:D:365:HIS:CG	2.44	0.52
1:A:30:ALA:HB2	1:A:78:ILE:HD13	1.92	0.52
1:D:252:GLN:O	1:D:256:GLU:HG3	2.10	0.52
1:A:145:LEU:HD12	1:A:379:ARG:HG2	1.91	0.52
1:B:172:VAL:HG11	1:B:175:ILE:CD1	2.40	0.52
1:C:123:LEU:HD13	1:C:294:TYR:HB3	1.91	0.51
1:C:197:LYS:HG3	1:C:198:GLN:N	2.24	0.51
1:A:189:PHE:CD1	1:A:227:LYS:HE2	2.46	0.51
1:C:78:ILE:HG22	1:C:80:ILE:HD11	1.91	0.51
1:B:39:VAL:HG21	1:B:42:TRP:CE3	2.46	0.51
1:B:148:ILE:CD1	1:B:149:PHE:H	2.18	0.51
1:C:389:GLN:NE2	1:C:394:LYS:HG2	2.25	0.51
1:A:303:PRO:HD2	1:A:311:LEU:HD22	1.93	0.51
1:A:148:ILE:HD12	1:A:361:GLY:HA2	1.92	0.51
1:D:20:THR:HB	1:D:107:LYS:HB3	1.93	0.50
1:C:340:ILE:HB	1:C:360:ALA:HB2	1.94	0.50
1:A:142:ARG:HG3	1:A:382:ILE:HD11	1.92	0.50
1:C:48:VAL:O	1:C:49:LYS:CB	2.59	0.50
1:B:146:MET:CE	1:B:174:LEU:HD11	2.21	0.50
1:C:168:ALA:HA	1:C:211:THR:HG21	1.93	0.50
1:B:241:PHE:CD2	1:B:243:VAL:HG22	2.46	0.50
1:B:399:LYS:HA	1:B:402:LYS:CE	2.42	0.50
1:A:27:GLU:OE2	1:A:63:VAL:HB	2.12	0.50
1:C:278:PRO:HG2	1:C:279:PHE:CE1	2.47	0.49
1:C:80:ILE:HD12	1:C:80:ILE:N	2.26	0.49
1:A:35:THR:HG22	1:A:57:LYS:HZ3	1.76	0.49
1:B:362:GLY:C	1:B:364:VAL:H	2.15	0.49
1:A:165:ARG:HG2	1:A:199:ILE:HG23	1.94	0.49
1:A:321:GLU:HG2	1:A:325:ARG:NH2	2.28	0.49
1:C:19:LEU:N	1:C:19:LEU:HD23	2.27	0.49
1:B:345:VAL:HB	1:B:346:PRO:HD3	1.95	0.49
1:B:337:SER:HB3	1:B:359:ASN:ND2	2.27	0.49
1:A:152:VAL:HG11	1:A:181:PHE:CG	2.47	0.49
1:B:199:ILE:C	1:B:199:ILE:HD13	2.32	0.49
1:D:315:ASP:O	1:D:319:ILE:HG13	2.12	0.49
1:C:257:ASP:HB3	1:C:260:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLY:O	1:B:133:ILE:HG22	2.13	0.49
1:C:217:LEU:HD11	1:C:224:LEU:HD22	1.93	0.49
1:C:65:GLU:O	1:C:66:ARG:C	2.51	0.49
1:D:389:GLN:NE2	1:D:394:LYS:HD3	2.28	0.49
1:A:150:LYS:HB2	1:A:365:HIS:CG	2.47	0.49
1:B:153:ILE:HD11	1:B:178:ASP:HB2	1.94	0.49
1:B:153:ILE:HG12	1:B:180:ILE:HG13	1.95	0.49
1:C:51:GLU:O	1:C:51:GLU:HG3	2.13	0.49
1:A:281:GLY:HA2	1:B:273:ALA:HB1	1.94	0.49
1:A:157:LEU:O	1:A:161:LYS:HG3	2.13	0.49
1:A:148:ILE:HG22	1:A:149:PHE:N	2.26	0.49
1:D:129:GLY:O	1:D:133:ILE:HG12	2.13	0.49
1:C:206:GLN:HG2	1:C:206:GLN:O	2.12	0.49
1:D:13:LEU:HD11	1:D:94:LEU:HG	1.96	0.48
1:B:131:TYR:CD2	1:D:47:LEU:HD13	2.48	0.48
1:A:265:MET:HG3	1:A:299:PHE:HB2	1.95	0.48
1:D:302:PHE:O	1:D:336:PRO:HA	2.13	0.48
1:B:206:GLN:HG3	1:B:207:THR:HG23	1.95	0.48
1:B:153:ILE:HG22	1:B:153:ILE:O	2.13	0.48
1:B:389:GLN:HE22	1:B:397:GLN:HE22	1.61	0.48
1:A:237:ASP:O	1:A:263:PRO:HD2	2.12	0.48
1:C:49:LYS:O	1:C:51:GLU:N	2.46	0.48
1:D:118:ALA:HA	1:D:121:ARG:CZ	2.43	0.48
1:B:309:VAL:HB	1:B:338:ALA:HB1	1.94	0.48
1:C:146:MET:HG2	1:C:147:SER:N	2.28	0.48
1:C:315:ASP:O	1:C:319:ILE:HG13	2.13	0.48
1:B:42:TRP:CD1	1:B:50:GLN:HG2	2.48	0.48
1:D:391:ILE:HD13	1:D:411:ALA:HB1	1.96	0.48
1:B:148:ILE:HD12	1:B:149:PHE:N	2.21	0.48
1:A:21:GLU:HB2	1:A:22:PRO:CD	2.41	0.48
1:C:73:GLU:N	1:C:73:GLU:OE1	2.47	0.48
1:D:244:PHE:CD1	1:D:271:SER:HB3	2.49	0.48
1:C:147:SER:OG	1:C:167:GLN:NE2	2.46	0.48
1:C:18:LEU:C	1:C:19:LEU:HD23	2.33	0.48
1:B:35:THR:HG22	1:B:57:LYS:NZ	2.29	0.48
1:A:162:GLU:OE1	1:A:162:GLU:HA	2.13	0.48
1:B:384:ALA:HB2	1:B:394:LYS:HG2	1.95	0.48
1:B:217:LEU:HD23	1:B:227:LYS:HZ2	1.79	0.48
1:C:181:PHE:CZ	1:C:187:ALA:HB3	2.48	0.48
1:D:112:ASP:HA	1:D:286:LEU:HG	1.96	0.47
1:A:382:ILE:HD13	1:A:383:ASP:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ILE:HG22	1:B:361:GLY:HA2	1.96	0.47
1:B:14:LEU:HD22	1:B:61:ILE:HD11	1.96	0.47
1:C:144:LEU:HB2	1:C:357:ILE:HG12	1.95	0.47
1:D:164:LEU:HD13	1:D:196:GLY:HA2	1.96	0.47
1:C:78:ILE:CG2	1:C:80:ILE:HD11	2.45	0.47
1:A:62:LYS:HD3	1:A:64:GLU:OE1	2.14	0.47
1:B:181:PHE:HE2	1:B:192:ARG:HD3	1.78	0.47
1:B:142:ARG:HG2	1:B:382:ILE:CD1	2.33	0.47
1:D:179:GLU:H	1:D:179:GLU:HG3	1.40	0.47
1:D:148:ILE:HG12	1:D:176:LYS:CG	2.45	0.47
1:B:157:LEU:O	1:B:161:LYS:HG3	2.14	0.47
1:C:157:LEU:HD21	1:C:192:ARG:HB3	1.97	0.47
1:B:312:PRO:HB2	1:B:315:ASP:OD2	2.15	0.47
1:A:29:LYS:HE2	1:A:108:ILE:HD11	1.97	0.47
1:D:19:LEU:CD1	1:D:78:ILE:HD12	2.44	0.47
1:B:360:ALA:O	1:B:361:GLY:C	2.52	0.47
1:D:354:ILE:HD12	1:D:354:ILE:C	2.35	0.47
1:D:376:ARG:HD2	2:D:434:HOH:O	2.14	0.47
1:B:28:LYS:O	1:B:32:GLN:HG3	2.15	0.46
1:A:65:GLU:HA	1:A:76:ALA:HA	1.97	0.46
1:A:39:VAL:O	1:A:39:VAL:HG12	2.16	0.46
1:C:207:THR:HG23	1:C:209:HIS:N	2.15	0.46
1:C:137:LEU:HD21	1:C:212:LEU:HG	1.96	0.46
1:D:173:ASP:HB2	1:D:174:LEU:HD23	1.95	0.46
1:D:102:LEU:O	1:D:108:ILE:HG21	2.15	0.46
1:D:64:GLU:HG2	1:D:65:GLU:H	1.81	0.46
1:C:26:THR:HG23	1:C:65:GLU:OE1	2.16	0.46
1:D:148:ILE:HG22	1:D:149:PHE:N	2.31	0.46
1:D:191:THR:O	1:D:195:GLU:HG2	2.15	0.46
1:A:244:PHE:CD1	1:A:271:SER:HB3	2.51	0.46
1:B:399:LYS:HA	1:B:402:LYS:HE2	1.98	0.46
1:C:301:LEU:HD13	1:C:335:VAL:CG1	2.45	0.46
1:D:164:LEU:HD23	1:D:175:ILE:HG21	1.97	0.46
1:A:20:THR:O	1:A:21:GLU:HG2	2.16	0.46
1:A:37:LEU:HD13	1:A:37:LEU:O	2.16	0.46
1:A:281:GLY:HA2	1:B:273:ALA:CB	2.46	0.46
1:B:338:ALA:HB3	2:B:479:HOH:O	2.14	0.46
1:B:218:THR:HB	2:B:474:HOH:O	2.16	0.46
1:B:144:LEU:HB2	1:B:357:ILE:HG12	1.98	0.46
1:B:146:MET:HE2	1:B:174:LEU:CD1	2.22	0.46
1:A:33:ILE:O	1:A:37:LEU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:VAL:HG13	1:B:153:ILE:N	2.31	0.46
1:B:140:PHE:O	1:D:52:GLN:HB3	2.16	0.46
1:C:136:LEU:O	1:C:210:LYS:HE3	2.15	0.46
1:A:166:GLN:HB3	1:A:371:ALA:HB3	1.97	0.46
1:A:179:GLU:HG2	1:A:267:HIS:NE2	2.30	0.46
1:C:134:ARG:HD3	1:C:140:PHE:HA	1.97	0.46
1:B:382:ILE:O	1:B:382:ILE:HD12	2.15	0.46
1:A:111:ILE:HD12	1:A:283:SER:HB3	1.98	0.46
1:B:217:LEU:HD23	1:B:227:LYS:NZ	2.30	0.46
1:B:260:ILE:O	1:B:260:ILE:HG22	2.16	0.45
1:B:152:VAL:HG23	1:B:155:ARG:CB	2.46	0.45
1:D:173:ASP:O	1:D:211:THR:HA	2.16	0.45
1:C:323:CYS:HB3	1:C:332:THR:O	2.17	0.45
1:C:207:THR:HG23	1:C:209:HIS:HB3	1.99	0.45
1:B:244:PHE:CD1	1:B:271:SER:HB3	2.51	0.45
1:D:12:GLU:OE1	1:D:59:ARG:NH2	2.49	0.45
1:C:19:LEU:CD2	1:C:108:ILE:HG13	2.47	0.45
1:B:13:LEU:CD2	1:B:94:LEU:HD23	2.33	0.45
1:B:389:GLN:NE2	1:B:397:GLN:HE22	2.15	0.45
1:D:18:LEU:HB2	1:D:111:ILE:CD1	2.47	0.45
1:C:78:ILE:HG22	1:C:80:ILE:HD12	1.99	0.45
1:A:179:GLU:HG2	1:A:267:HIS:CE1	2.52	0.45
1:D:392:ASP:O	1:D:396:GLU:HG2	2.17	0.45
1:B:153:ILE:HD11	1:B:178:ASP:CB	2.46	0.44
1:C:94:LEU:HD11	1:C:113:LEU:HD13	1.99	0.44
1:B:199:ILE:O	1:B:199:ILE:HD13	2.17	0.44
1:D:283:SER:OG	1:D:286:LEU:HB2	2.16	0.44
1:B:45:LEU:H	1:B:46:PRO:HA	1.82	0.44
1:B:148:ILE:O	1:B:365:HIS:NE2	2.49	0.44
1:B:46:PRO:C	1:B:50:GLN:NE2	2.71	0.44
1:B:148:ILE:CG1	1:B:149:PHE:N	2.80	0.44
1:B:395:ALA:O	1:B:402:LYS:CD	2.66	0.44
1:B:152:VAL:HA	1:B:155:ARG:CB	2.47	0.44
1:A:13:LEU:HD13	1:A:13:LEU:C	2.38	0.44
1:A:315:ASP:O	1:A:319:ILE:HG13	2.18	0.44
1:B:322:GLU:CD	1:B:325:ARG:HH12	2.21	0.44
1:B:399:LYS:HA	1:B:402:LYS:HZ3	1.81	0.44
1:B:399:LYS:HA	1:B:402:LYS:NZ	2.32	0.44
1:C:149:PHE:CZ	1:C:160:ILE:HG23	2.52	0.44
1:B:42:TRP:CE3	1:B:53:MET:HE3	2.53	0.44
1:C:28:LYS:HE2	1:C:32:GLN:HE22	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLY:HA2	1:A:40:GLY:CA	2.47	0.44
1:A:152:VAL:HG11	1:A:181:PHE:CD2	2.52	0.44
1:D:108:ILE:HD13	1:D:108:ILE:C	2.38	0.44
1:B:21:GLU:N	1:B:22:PRO:CD	2.81	0.44
1:A:134:ARG:NH2	1:A:354:ILE:HD12	2.32	0.44
1:A:148:ILE:HG12	1:A:176:LYS:HG2	1.99	0.44
1:D:342:PRO:O	1:D:381:ILE:HD13	2.18	0.44
1:B:391:ILE:HD12	1:B:391:ILE:N	2.32	0.44
1:D:66:ARG:O	1:D:67:GLU:C	2.56	0.43
1:C:155:ARG:HH21	1:C:155:ARG:CB	2.30	0.43
1:D:150:LYS:HG3	1:D:151:GLY:N	2.33	0.43
1:B:148:ILE:HG13	1:B:149:PHE:N	2.33	0.43
1:A:147:SER:CB	1:A:172:VAL:HG11	2.44	0.43
1:D:150:LYS:HB3	1:D:365:HIS:CB	2.47	0.43
1:C:179:GLU:HB2	1:C:242:ASN:OD1	2.18	0.43
1:D:18:LEU:HD21	1:D:74:LYS:N	2.33	0.43
1:C:399:LYS:HA	1:C:402:LYS:HB2	2.00	0.43
1:C:19:LEU:HD22	1:C:108:ILE:HG13	1.99	0.43
1:D:389:GLN:HE22	1:D:394:LYS:HD3	1.83	0.43
1:C:302:PHE:O	1:C:337:SER:HB2	2.18	0.43
1:D:207:THR:CG2	1:D:209:HIS:HB3	2.48	0.43
1:A:381:ILE:O	1:A:385:VAL:HG23	2.19	0.43
1:D:331:GLN:HG2	2:D:456:HOH:O	2.18	0.43
1:B:168:ALA:HB1	1:B:211:THR:HG21	2.00	0.43
1:A:35:THR:HG22	1:A:57:LYS:NZ	2.34	0.43
1:D:327:ASP:C	1:D:329:PHE:H	2.22	0.43
1:A:323:CYS:HB3	1:A:332:THR:O	2.18	0.43
1:C:207:THR:CG2	1:C:209:HIS:HB3	2.48	0.43
1:A:109:LYS:HE3	1:A:280:TYR:O	2.18	0.43
1:A:305:PRO:HG3	1:A:316:ALA:CB	2.48	0.43
1:D:186:LEU:C	1:D:188:PRO:HD3	2.38	0.43
1:B:46:PRO:O	1:B:50:GLN:HG3	2.18	0.43
1:D:149:PHE:HB3	1:D:163:GLN:OE1	2.18	0.43
1:A:317:LEU:HD21	1:A:351:ASP:HB3	2.00	0.43
1:A:19:LEU:HD11	1:A:78:ILE:HD12	2.01	0.43
1:C:301:LEU:HA	1:C:335:VAL:HB	2.00	0.43
1:B:182:PHE:CD2	1:B:218:THR:HG21	2.53	0.43
1:A:145:LEU:HD13	1:A:172:VAL:HG12	2.01	0.43
1:C:382:ILE:O	1:C:385:VAL:HG22	2.19	0.42
1:C:17:TYR:HE1	1:C:80:ILE:HD13	1.83	0.42
1:C:153:ILE:HD12	1:C:180:ILE:CG1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:HIS:CG	1:A:268:PRO:HD2	2.54	0.42
1:C:301:LEU:HD13	1:C:335:VAL:HG11	2.00	0.42
1:D:109:LYS:O	1:D:111:ILE:HD13	2.19	0.42
1:B:113:LEU:HG	1:B:286:LEU:HD11	2.01	0.42
1:C:349:MET:SD	1:C:385:VAL:CG2	3.03	0.42
1:D:301:LEU:HD12	1:D:301:LEU:N	2.35	0.42
1:B:42:TRP:C	1:B:44:ASP:N	2.73	0.42
1:A:109:LYS:HE2	1:A:282:PHE:C	2.39	0.42
1:C:201:LYS:HE2	1:C:205:GLU:OE2	2.20	0.42
1:D:157:LEU:HD22	1:D:161:LYS:HG3	2.01	0.42
1:D:207:THR:HG23	1:D:209:HIS:HB3	2.01	0.42
1:B:243:VAL:CG2	1:B:251:MET:SD	3.07	0.42
1:D:13:LEU:HD11	1:D:94:LEU:CG	2.50	0.42
1:D:320:HIS:HE1	1:D:355:ASP:O	2.02	0.42
1:C:52:GLN:HE21	1:C:55:LYS:HD3	1.85	0.42
1:B:322:GLU:OE1	1:B:325:ARG:NH1	2.52	0.42
1:D:324:VAL:HA	1:D:331:GLN:HG3	2.01	0.42
1:B:156:ASP:OD2	1:B:158:SER:HB2	2.19	0.42
1:A:126:PRO:HG3	1:A:297:ALA:O	2.20	0.42
1:C:354:ILE:H	1:C:354:ILE:HD13	1.84	0.42
1:B:293:ARG:HG3	1:B:332:THR:OG1	2.20	0.42
1:D:99:PHE:CE1	1:D:108:ILE:HD12	2.52	0.42
1:B:13:LEU:HD12	1:B:13:LEU:C	2.39	0.42
1:C:48:VAL:O	1:C:48:VAL:CG2	2.68	0.42
1:A:148:ILE:O	1:A:365:HIS:HE1	2.03	0.42
1:A:198:GLN:O	1:A:202:GLU:HG3	2.20	0.42
1:D:19:LEU:O	1:D:76:ALA:HB3	2.20	0.42
1:A:382:ILE:CD1	1:A:382:ILE:C	2.83	0.42
1:D:109:LYS:NZ	1:D:277:SER:O	2.47	0.42
1:D:199:ILE:O	1:D:203:THR:HG23	2.20	0.42
1:B:94:LEU:C	1:B:94:LEU:HD13	2.40	0.42
1:C:339:GLY:O	1:C:344:MET:HE3	2.19	0.42
1:D:267:HIS:CG	1:D:268:PRO:HD2	2.55	0.42
1:D:322:GLU:CD	1:D:325:ARG:NH1	2.74	0.42
1:D:65:GLU:O	1:D:66:ARG:CB	2.68	0.41
1:D:146:MET:CE	1:D:335:VAL:HG11	2.50	0.41
1:D:335:VAL:HG22	1:D:357:ILE:HB	2.01	0.41
1:B:46:PRO:HG2	1:B:47:LEU:N	2.35	0.41
1:A:56:HIS:CG	1:A:86:ASN:HD21	2.38	0.41
1:A:18:LEU:CD2	1:A:75:GLN:HB3	2.51	0.41
1:A:32:GLN:O	1:A:36:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:GLU:HA	1:D:205:GLU:HB2	2.02	0.41
1:B:135:LYS:C	1:B:135:LYS:HD3	2.40	0.41
1:D:17:TYR:HB3	1:D:108:ILE:HD11	2.03	0.41
1:D:107:LYS:HG3	1:D:279:PHE:HB3	2.02	0.41
1:D:225:LYS:O	1:D:229:ARG:HG3	2.20	0.41
1:B:19:LEU:CD2	1:B:108:ILE:HG23	2.50	0.41
1:A:54:GLN:OE1	1:A:57:LYS:HD2	2.20	0.41
1:B:129:GLY:O	1:B:133:ILE:CG2	2.69	0.41
1:D:322:GLU:OE2	1:D:325:ARG:NH1	2.53	0.41
1:D:269:ALA:O	1:D:270:VAL:HB	2.21	0.41
1:D:116:SER:O	1:D:120:LYS:HG3	2.20	0.41
1:D:265:MET:HG3	1:D:299:PHE:HB2	2.02	0.41
1:C:56:HIS:CD2	1:C:86:ASN:ND2	2.86	0.41
1:A:150:LYS:N	1:A:163:GLN:OE1	2.54	0.41
1:C:257:ASP:HA	1:C:258:PRO:HD2	1.87	0.41
1:B:49:LYS:C	1:B:51:GLU:N	2.74	0.41
1:B:148:ILE:HD11	1:B:178:ASP:OD1	2.21	0.41
1:B:362:GLY:C	1:B:364:VAL:N	2.74	0.41
1:D:293:ARG:HG3	1:D:332:THR:OG1	2.20	0.41
1:A:393:GLU:O	1:A:397:GLN:HG3	2.21	0.40
1:C:38:THR:OG1	1:C:39:VAL:N	2.54	0.40
1:B:201:LYS:O	1:B:205:GLU:HG3	2.21	0.40
1:D:108:ILE:HG23	1:D:108:ILE:O	2.20	0.40
1:D:20:THR:HB	1:D:107:LYS:CB	2.52	0.40
1:B:153:ILE:HG13	1:B:181:PHE:HD1	1.86	0.40
1:C:66:ARG:HA	1:C:66:ARG:HD2	1.91	0.40
1:C:337:SER:HA	1:C:359:ASN:HB3	2.03	0.40
1:D:284:HIS:HB3	1:D:319:ILE:HD11	2.04	0.40
1:D:318:ALA:O	1:D:322:GLU:HG2	2.21	0.40
1:C:239:LEU:HG	1:C:262:VAL:HG11	2.03	0.40
1:B:56:HIS:HD2	1:B:86:ASN:ND2	2.19	0.40
1:B:186:LEU:HD12	1:B:186:LEU:N	2.37	0.40
1:B:174:LEU:CD1	1:B:265:MET:HE1	2.52	0.40
1:A:53:MET:CE	1:B:152:VAL:O	2.69	0.40
1:A:21:GLU:O	1:A:22:PRO:C	2.60	0.40
1:A:244:PHE:CZ	1:A:287:LEU:HD13	2.57	0.40
1:C:244:PHE:CZ	1:C:287:LEU:HD13	2.56	0.40
1:C:265:MET:HA	1:C:299:PHE:HB2	2.02	0.40
1:A:43:THR:CG2	1:A:43:THR:O	2.69	0.40
1:B:265:MET:HG3	1:B:299:PHE:HB2	2.04	0.40
1:D:160:ILE:HD13	1:D:181:PHE:HZ	1.87	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	389/425 (92%)	368 (95%)	17 (4%)	4 (1%)	19	21
1	B	392/425 (92%)	363 (93%)	23 (6%)	6 (2%)	13	12
1	C	379/425 (89%)	358 (94%)	20 (5%)	1 (0%)	46	57
1	D	382/425 (90%)	359 (94%)	20 (5%)	3 (1%)	24	27
All	All	1542/1700 (91%)	1448 (94%)	80 (5%)	14 (1%)	21	24

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	VAL
1	A	338	ALA
1	B	46	PRO
1	B	270	VAL
1	C	270	VAL
1	D	66	ARG
1	D	270	VAL
1	A	21	GLU
1	B	43	THR
1	B	152	VAL
1	D	76	ALA
1	B	361	GLY
1	A	124	PRO
1	B	339	GLY

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	314/338 (93%)	294 (94%)	20 (6%)	22	28
1	B	310/338 (92%)	282 (91%)	28 (9%)	12	14
1	C	300/338 (89%)	278 (93%)	22 (7%)	17	22
1	D	301/338 (89%)	273 (91%)	28 (9%)	11	13
All	All	1225/1352 (91%)	1127 (92%)	98 (8%)	15	18

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	37	LEU
1	A	38	THR
1	A	53	MET
1	A	119	PHE
1	A	145	LEU
1	A	157	LEU
1	A	179	GLU
1	A	181	PHE
1	A	217	LEU
1	A	243	VAL
1	A	254	LEU
1	A	286	LEU
1	A	287	LEU
1	A	288	LEU
1	A	311	LEU
1	A	333	PHE
1	A	354	ILE
1	A	364	VAL
1	A	382	ILE
1	B	18	LEU
1	B	29	LYS
1	B	42	TRP
1	B	45	LEU
1	B	49	LYS
1	B	66	ARG
1	B	73	GLU
1	B	74	LYS

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Mol	Chain	Res	Type
1	B	94	LEU
1	B	119	PHE
1	B	127	LYS
1	B	133	ILE
1	B	145	LEU
1	B	148	ILE
1	B	199	ILE
1	B	200	LEU
1	B	211	THR
1	B	217	LEU
1	B	254	LEU
1	B	274	PHE
1	B	286	LEU
1	B	287	LEU
1	B	324	VAL
1	B	333	PHE
1	B	337	SER
1	B	364	VAL
1	B	376	ARG
1	B	382	ILE
1	C	18	LEU
1	C	50	GLN
1	C	136	LEU
1	C	145	LEU
1	C	153	ILE
1	C	155	ARG
1	C	159	ASP
1	C	174	LEU
1	C	184	THR
1	C	197	LYS
1	C	198	GLN
1	C	254	LEU
1	C	286	LEU
1	C	287	LEU
1	C	288	LEU
1	C	333	PHE
1	C	337	SER
1	C	354	ILE
1	C	369	ASN
1	C	387	GLU
1	C	406	ASP
1	C	408	TRP

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Mol	Chain	Res	Type
1	D	18	LEU
1	D	47	LEU
1	D	55	LYS
1	D	75	GLN
1	D	94	LEU
1	D	101	LYS
1	D	107	LYS
1	D	108	ILE
1	D	119	PHE
1	D	127	LYS
1	D	141	GLU
1	D	157	LEU
1	D	174	LEU
1	D	179	GLU
1	D	181	PHE
1	D	186	LEU
1	D	205	GLU
1	D	211	THR
1	D	217	LEU
1	D	254	LEU
1	D	286	LEU
1	D	287	LEU
1	D	288	LEU
1	D	311	LEU
1	D	333	PHE
1	D	337	SER
1	D	364	VAL
1	D	372	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	50	GLN
1	A	52	GLN
1	A	56	HIS
1	A	86	ASN
1	A	89	GLN
1	A	167	GLN
1	A	198	GLN
1	A	320	HIS
1	A	365	HIS

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Mol	Chain	Res	Type
1	A	389	GLN
1	B	50	GLN
1	B	54	GLN
1	B	56	HIS
1	B	75	GLN
1	B	86	ASN
1	B	166	GLN
1	B	167	GLN
1	B	198	GLN
1	B	320	HIS
1	B	397	GLN
1	C	32	GLN
1	C	50	GLN
1	C	52	GLN
1	C	56	HIS
1	C	86	ASN
1	C	89	GLN
1	C	166	GLN
1	C	167	GLN
1	C	284	HIS
1	C	331	GLN
1	C	341	HIS
1	C	365	HIS
1	C	389	GLN
1	D	56	HIS
1	D	75	GLN
1	D	86	ASN
1	D	89	GLN
1	D	167	GLN
1	D	320	HIS
1	D	341	HIS
1	D	365	HIS
1	D	389	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

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	395/425 (92%)	-0.07	10 (2%)	61	70	10, 20, 51, 66	0
1	B	396/425 (93%)	0.23	23 (5%)	26	35	11, 24, 55, 69	0
1	C	385/425 (90%)	0.26	31 (8%)	15	21	12, 26, 57, 79	0
1	D	388/425 (91%)	-0.01	13 (3%)	49	58	11, 21, 47, 76	0
All	All	1564/1700 (92%)	0.10	77 (4%)	33	42	10, 23, 54, 79	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	36	GLY	10.0
1	D	46	PRO	9.7
1	B	46	PRO	5.7
1	C	23	GLY	5.2
1	C	151	GLY	5.1
1	B	48	VAL	5.0
1	C	50	GLN	4.8
1	A	42	TRP	4.6
1	C	406	ASP	4.3
1	B	184	THR	4.3
1	A	70	ALA	4.2
1	C	51	GLU	4.2
1	C	152	VAL	4.1
1	C	405	LEU	4.0
1	A	39	VAL	4.0
1	B	411	ALA	4.0
1	C	395	ALA	4.0
1	C	391	ILE	4.0
1	D	74	LYS	3.9
1	B	45	LEU	3.9
1	B	396	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	71	ALA	3.8
1	C	24	ALA	3.8
1	C	66	ARG	3.8
1	A	22	PRO	3.7
1	C	308	SER	3.6
1	C	49	LYS	3.6
1	B	47	LEU	3.6
1	C	399	LYS	3.5
1	C	65	GLU	3.4
1	C	52	GLN	3.4
1	B	410	LYS	3.4
1	B	408	TRP	3.3
1	C	388	ALA	3.3
1	C	309	VAL	3.3
1	B	404	ALA	3.1
1	D	47	LEU	3.1
1	C	53	MET	3.0
1	B	153	ILE	3.0
1	B	72	SER	3.0
1	D	205	GLU	2.9
1	D	66	ARG	2.9
1	B	363	GLY	2.8
1	B	399	LYS	2.8
1	B	308	SER	2.8
1	C	35	THR	2.8
1	D	24	ALA	2.7
1	C	393	GLU	2.6
1	A	410	LYS	2.6
1	D	413	ALA	2.6
1	B	391	ILE	2.6
1	B	409	GLY	2.5
1	C	387	GLU	2.5
1	D	206	GLN	2.5
1	B	152	VAL	2.5
1	C	390	PRO	2.5
1	B	185	GLY	2.4
1	D	67	GLU	2.4
1	A	72	SER	2.4
1	C	402	LYS	2.4
1	B	364	VAL	2.3
1	C	385	VAL	2.3
1	D	75	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	408	TRP	2.3
1	C	386	LEU	2.3
1	A	43	THR	2.2
1	B	44	ASP	2.2
1	B	405	LEU	2.2
1	B	395	ALA	2.2
1	D	156	ASP	2.1
1	D	28	LYS	2.1
1	C	368	PRO	2.1
1	C	31	GLU	2.1
1	C	64	GLU	2.1
1	A	308	SER	2.1
1	A	53	MET	2.0
1	C	396	GLU	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.