Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 10:47 PM EDT

PDB ID	:	4EGV
Title	:	Crystal structure of a monomeric SCP2-thiolase like protein type 1 (STLP1) from Mycobacterium smegmatis
Authors	:	Janardan, N.; Harijan, R.K.; Wierenga, R.K.; Murthy, M.R.N.
Deposited on	:	2012-04-01
Resolution	:	2.71 Å(reported)

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

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

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

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

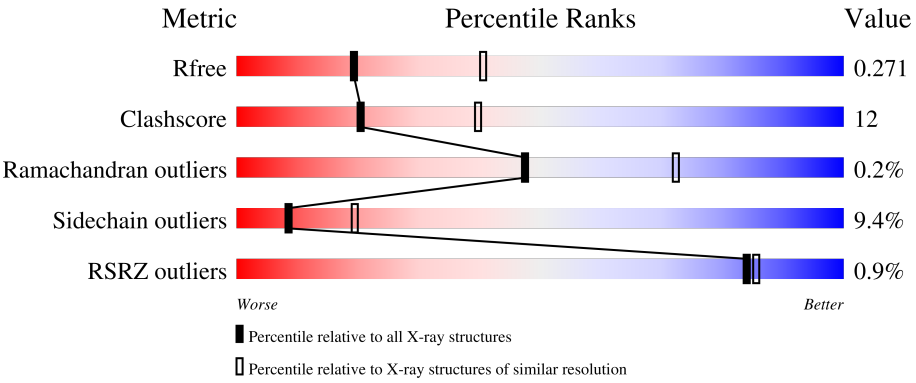
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.71 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	520	% 69% 16% • 14%
1	B	520	% 68% 16% • 13%
1	C	520	% 67% 18% • 13%
1	D	520	% 65% 17% • 14%
1	E	520	% 67% 16% • 14%

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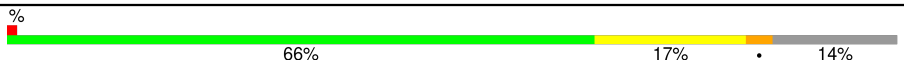
Mol	Chain	Length	Quality of chain
1	F	520	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20206 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	Se	0	0	0
			3327	2086	579	650	3	9			
1	B	452	Total	C	N	O	S	Se	0	3	0
			3376	2115	588	661	3	9			
1	C	453	Total	C	N	O	S	Se	0	0	0
			3373	2116	588	656	3	10			
1	D	445	Total	C	N	O	S	Se	0	0	0
			3299	2066	576	645	3	9			
1	E	447	Total	C	N	O	S	Se	0	2	0
			3336	2090	585	648	3	10			
1	F	449	Total	C	N	O	S	Se	0	0	0
			3335	2090	581	652	3	9			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MSE	-	expression tag	UNP A0R3M0
A	-11	ARG	-	expression tag	UNP A0R3M0
A	-10	GLY	-	expression tag	UNP A0R3M0
A	-9	SER	-	expression tag	UNP A0R3M0
A	-8	HIS	-	expression tag	UNP A0R3M0
A	-7	HIS	-	expression tag	UNP A0R3M0
A	-6	HIS	-	expression tag	UNP A0R3M0
A	-5	HIS	-	expression tag	UNP A0R3M0
A	-4	HIS	-	expression tag	UNP A0R3M0
A	-3	HIS	-	expression tag	UNP A0R3M0
A	-2	MSE	-	expression tag	UNP A0R3M0
A	-1	ALA	-	expression tag	UNP A0R3M0
A	0	SER	-	expression tag	UNP A0R3M0
B	-12	MSE	-	expression tag	UNP A0R3M0
B	-11	ARG	-	expression tag	UNP A0R3M0
B	-10	GLY	-	expression tag	UNP A0R3M0
B	-9	SER	-	expression tag	UNP A0R3M0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP A0R3M0
B	-7	HIS	-	expression tag	UNP A0R3M0
B	-6	HIS	-	expression tag	UNP A0R3M0
B	-5	HIS	-	expression tag	UNP A0R3M0
B	-4	HIS	-	expression tag	UNP A0R3M0
B	-3	HIS	-	expression tag	UNP A0R3M0
B	-2	MSE	-	expression tag	UNP A0R3M0
B	-1	ALA	-	expression tag	UNP A0R3M0
B	0	SER	-	expression tag	UNP A0R3M0
C	-12	MSE	-	expression tag	UNP A0R3M0
C	-11	ARG	-	expression tag	UNP A0R3M0
C	-10	GLY	-	expression tag	UNP A0R3M0
C	-9	SER	-	expression tag	UNP A0R3M0
C	-8	HIS	-	expression tag	UNP A0R3M0
C	-7	HIS	-	expression tag	UNP A0R3M0
C	-6	HIS	-	expression tag	UNP A0R3M0
C	-5	HIS	-	expression tag	UNP A0R3M0
C	-4	HIS	-	expression tag	UNP A0R3M0
C	-3	HIS	-	expression tag	UNP A0R3M0
C	-2	MSE	-	expression tag	UNP A0R3M0
C	-1	ALA	-	expression tag	UNP A0R3M0
C	0	SER	-	expression tag	UNP A0R3M0
D	-12	MSE	-	expression tag	UNP A0R3M0
D	-11	ARG	-	expression tag	UNP A0R3M0
D	-10	GLY	-	expression tag	UNP A0R3M0
D	-9	SER	-	expression tag	UNP A0R3M0
D	-8	HIS	-	expression tag	UNP A0R3M0
D	-7	HIS	-	expression tag	UNP A0R3M0
D	-6	HIS	-	expression tag	UNP A0R3M0
D	-5	HIS	-	expression tag	UNP A0R3M0
D	-4	HIS	-	expression tag	UNP A0R3M0
D	-3	HIS	-	expression tag	UNP A0R3M0
D	-2	MSE	-	expression tag	UNP A0R3M0
D	-1	ALA	-	expression tag	UNP A0R3M0
D	0	SER	-	expression tag	UNP A0R3M0
E	-12	MSE	-	expression tag	UNP A0R3M0
E	-11	ARG	-	expression tag	UNP A0R3M0
E	-10	GLY	-	expression tag	UNP A0R3M0
E	-9	SER	-	expression tag	UNP A0R3M0
E	-8	HIS	-	expression tag	UNP A0R3M0
E	-7	HIS	-	expression tag	UNP A0R3M0
E	-6	HIS	-	expression tag	UNP A0R3M0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP A0R3M0
E	-4	HIS	-	expression tag	UNP A0R3M0
E	-3	HIS	-	expression tag	UNP A0R3M0
E	-2	MSE	-	expression tag	UNP A0R3M0
E	-1	ALA	-	expression tag	UNP A0R3M0
E	0	SER	-	expression tag	UNP A0R3M0
F	-12	MSE	-	expression tag	UNP A0R3M0
F	-11	ARG	-	expression tag	UNP A0R3M0
F	-10	GLY	-	expression tag	UNP A0R3M0
F	-9	SER	-	expression tag	UNP A0R3M0
F	-8	HIS	-	expression tag	UNP A0R3M0
F	-7	HIS	-	expression tag	UNP A0R3M0
F	-6	HIS	-	expression tag	UNP A0R3M0
F	-5	HIS	-	expression tag	UNP A0R3M0
F	-4	HIS	-	expression tag	UNP A0R3M0
F	-3	HIS	-	expression tag	UNP A0R3M0
F	-2	MSE	-	expression tag	UNP A0R3M0
F	-1	ALA	-	expression tag	UNP A0R3M0
F	0	SER	-	expression tag	UNP A0R3M0

- Molecule 2 is water.

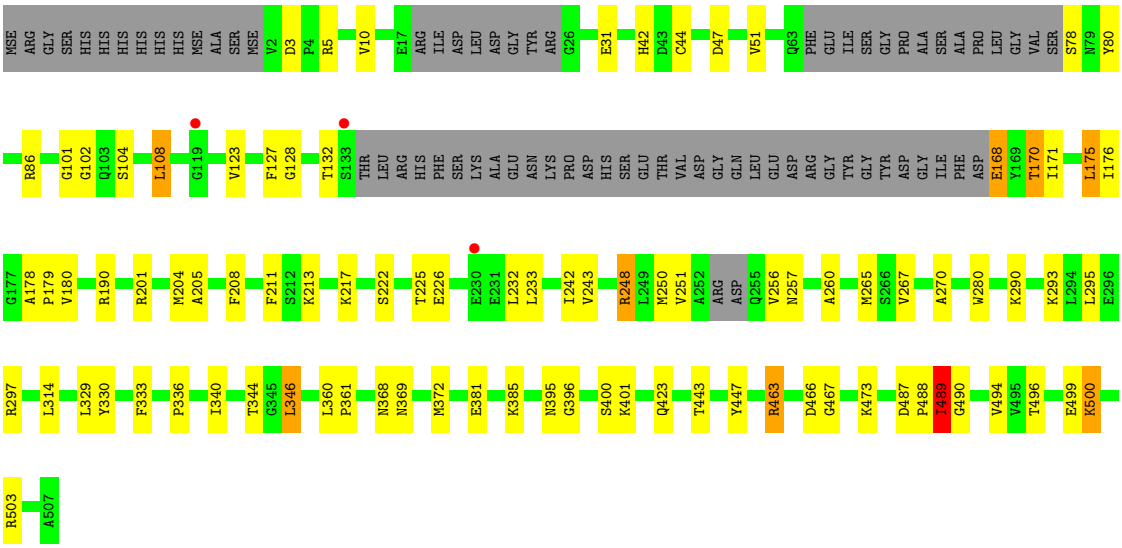
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	36	Total O 36 36	0	0
2	B	29	Total O 29 29	0	0
2	C	37	Total O 37 37	0	0
2	D	18	Total O 18 18	0	0
2	E	25	Total O 25 25	0	0
2	F	15	Total O 15 15	0	0

3 Residue-property plots (i)

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

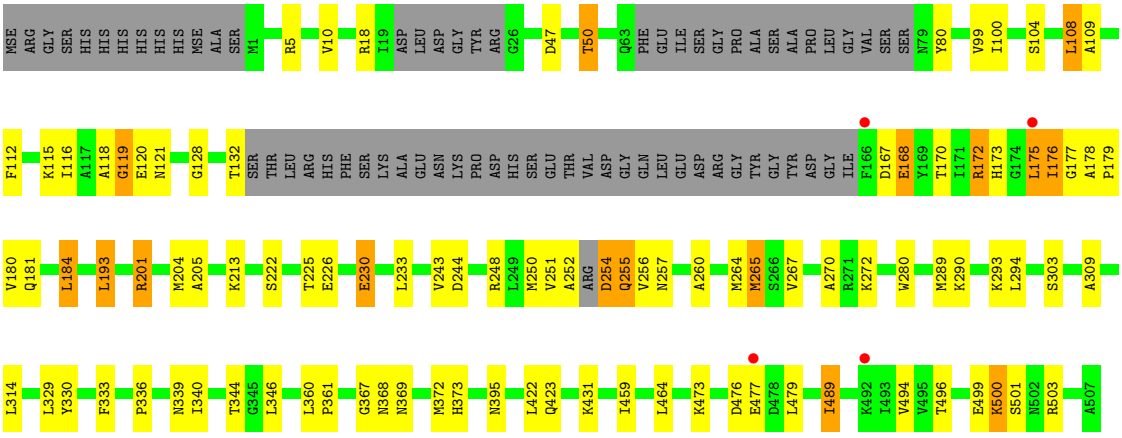
• Molecule 1: Acetyl-CoA acetyltransferase

Chain A:



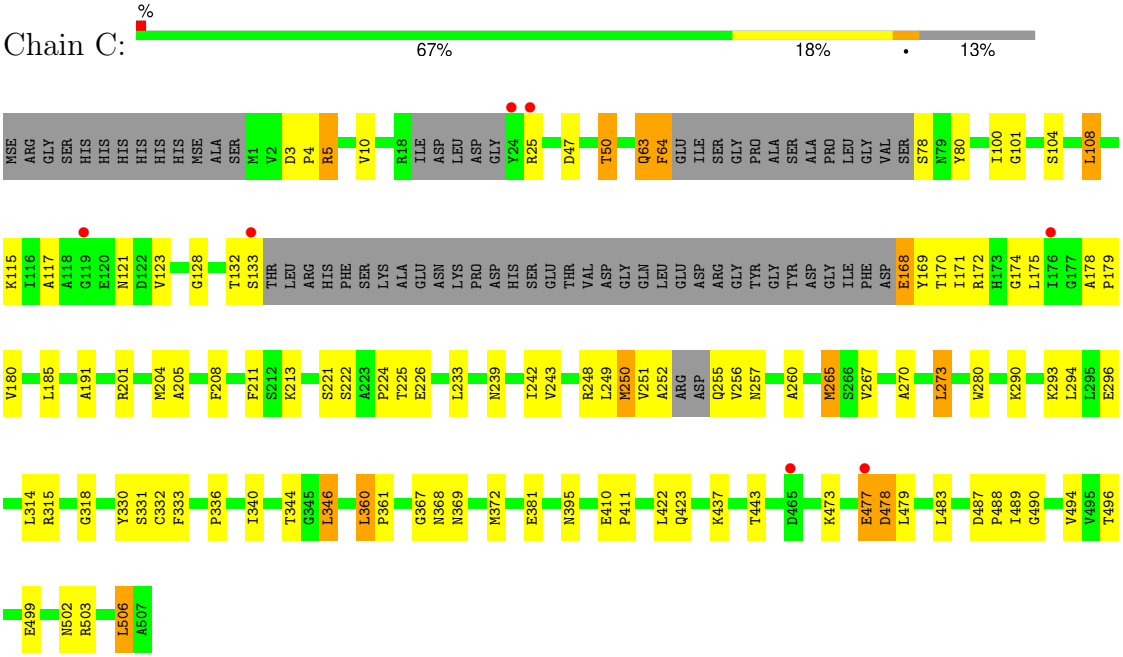
• Molecule 1: Acetyl-CoA acetyltransferase

Chain B:



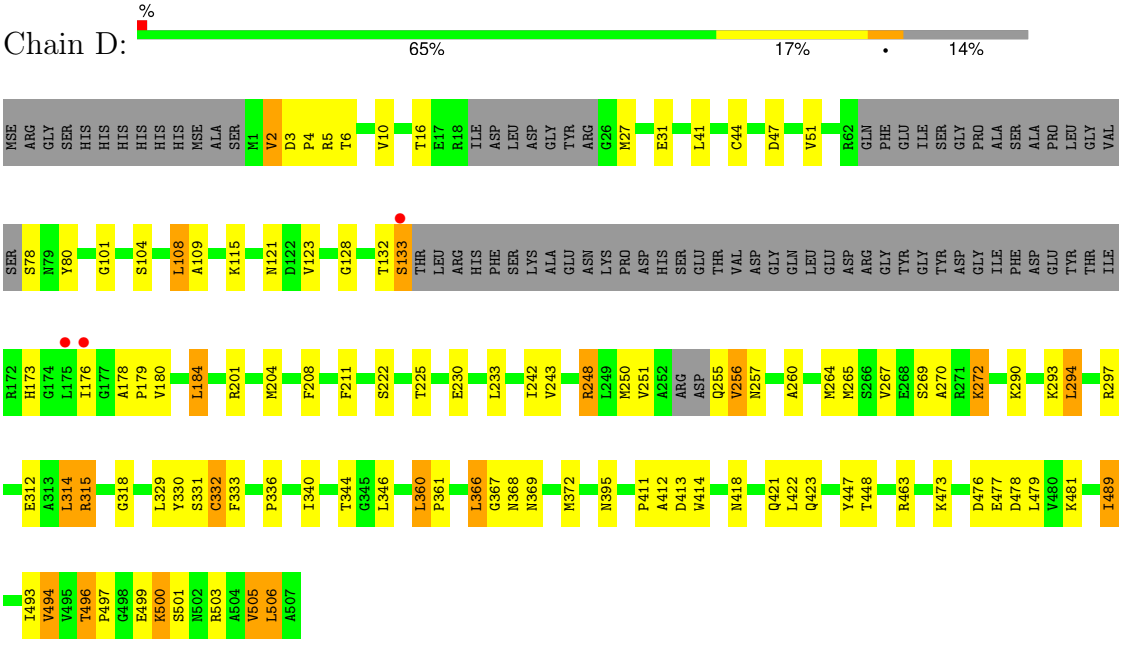
• Molecule 1: Acetyl-CoA acetyltransferase

Chain C:



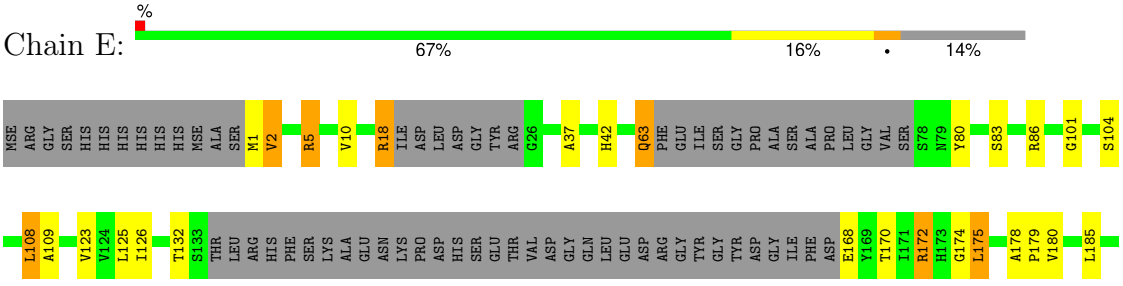
• Molecule 1: Acetyl-CoA acetyltransferase

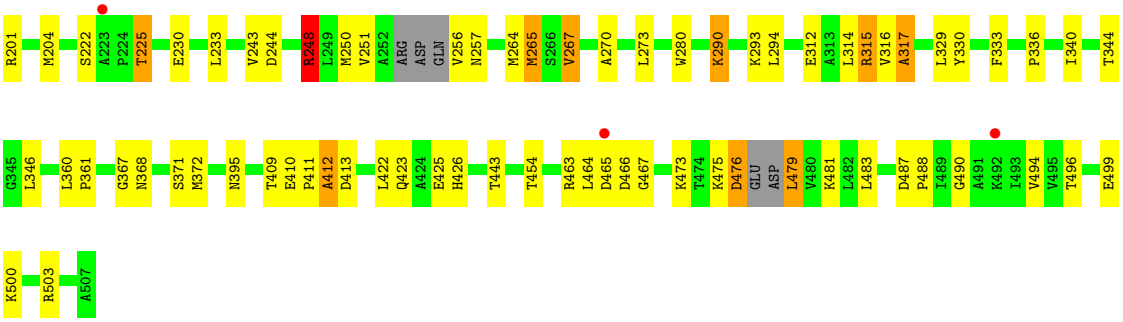
Chain D:



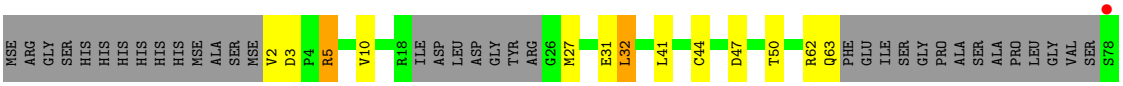
• Molecule 1: Acetyl-CoA acetyltransferase

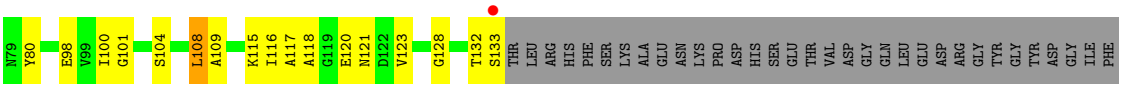
Chain E:

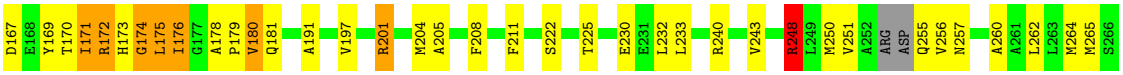


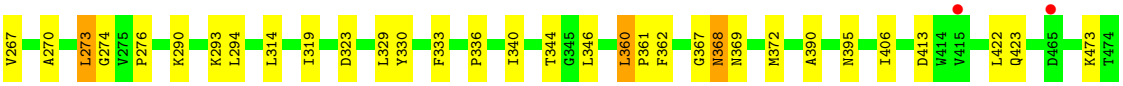


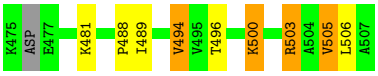
• Molecule 1: Acetyl-CoA acetyltransferase











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	96.31Å 102.00Å 102.42Å 116.46° 101.28° 97.44°	Depositor
Resolution (Å)	47.95 – 2.71 47.95 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.95-2.71) 96.9 (47.95-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.261 0.244 , 0.271	Depositor DCC
R_{free} test set	4398 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	20206	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.99	2/3377 (0.1%)	0.88	5/4572 (0.1%)
1	B	0.93	1/3435 (0.0%)	0.88	6/4649 (0.1%)
1	C	0.92	2/3424 (0.1%)	0.86	3/4634 (0.1%)
1	D	0.92	1/3348 (0.0%)	0.84	4/4532 (0.1%)
1	E	0.91	0/3388	0.87	5/4582 (0.1%)
1	F	0.92	1/3384 (0.0%)	0.88	7/4580 (0.2%)
All	All	0.93	7/20356 (0.0%)	0.87	30/27549 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	477	GLU	CG-CD	5.93	1.60	1.51
1	A	44	CYS	CB-SG	-5.59	1.72	1.81
1	A	31	GLU	CG-CD	5.42	1.60	1.51
1	D	332	CYS	CB-SG	5.38	1.91	1.82
1	F	294	LEU	C-O	-5.26	1.13	1.23
1	B	294	LEU	C-O	-5.15	1.13	1.23
1	C	381	GLU	CG-CD	5.08	1.59	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	ASP	CB-CG-OD2	6.00	123.70	118.30
1	F	32	LEU	CB-CG-CD1	5.97	121.15	111.00
1	F	174	GLY	N-CA-C	-5.95	98.23	113.10
1	C	487	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	466	ASP	CB-CG-OD1	5.86	123.58	118.30
1	F	201	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	86	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	201	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	86	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	201	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	201	ARG	CB-CG-CD	5.70	126.43	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	478	ASP	CB-CG-OD1	5.65	123.39	118.30
1	F	201	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	E	479	LEU	CB-CG-CD2	5.56	120.46	111.00
1	F	32	LEU	CA-CB-CG	5.54	128.03	115.30
1	E	317	ALA	N-CA-C	-5.51	96.12	111.00
1	F	201	ARG	CB-CG-CD	5.42	125.70	111.60
1	F	248	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	173	HIS	N-CA-C	-5.42	96.38	111.00
1	C	174	GLY	N-CA-C	-5.41	99.58	113.10
1	D	256	VAL	CB-CA-C	-5.35	101.24	111.40
1	A	297	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	B	184	LEU	CA-CB-CG	5.21	127.27	115.30
1	C	502	ASN	N-CA-C	-5.20	96.95	111.00
1	D	366	LEU	CB-CG-CD1	5.19	119.82	111.00
1	E	479	LEU	CB-CG-CD1	5.12	119.70	111.00
1	B	193	LEU	CB-CG-CD1	5.11	119.69	111.00
1	E	248	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	E	5	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	172	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3327	0	3278	77	0
1	B	3376	0	3320	82	0
1	C	3373	0	3329	84	0
1	D	3299	0	3252	89	0
1	E	3336	0	3296	93	0
1	F	3335	0	3283	85	0
2	A	36	0	0	3	0
2	B	29	0	0	2	0
2	C	37	0	0	3	0
2	D	18	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	25	0	0	3	0
2	F	15	0	0	1	0
All	All	20206	0	19758	495	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 12.

All (495) 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:176:ILE:HD13	1:B:176:ILE:C	1.51	1.25
1:F:176:ILE:HD12	1:F:176:ILE:O	1.34	1.22
1:A:489:ILE:HD12	1:A:489:ILE:N	1.57	1.13
1:A:489:ILE:H	1:A:489:ILE:CD1	1.50	1.12
1:A:175:LEU:N	1:A:175:LEU:HD23	1.58	1.10
1:A:168:GLU:N	1:A:171:ILE:HD12	1.64	1.10
1:B:175:LEU:HD21	1:B:459:ILE:HG21	1.33	1.10
1:A:487:ASP:OD1	1:A:489:ILE:HD13	1.54	1.07
1:E:174:GLY:O	1:E:175:LEU:HD12	1.61	0.99
1:F:176:ILE:HD12	1:F:176:ILE:C	1.78	0.99
1:A:175:LEU:HD23	1:A:175:LEU:H	1.29	0.97
1:D:132:THR:O	1:D:133:SER:HB2	1.62	0.95
1:E:175:LEU:HD13	1:E:175:LEU:N	1.78	0.95
1:E:175:LEU:N	1:E:175:LEU:CD1	2.30	0.94
1:B:176:ILE:HD13	1:B:176:ILE:O	1.66	0.94
1:E:174:GLY:C	1:E:175:LEU:CD1	2.37	0.93
1:B:176:ILE:HD13	1:B:177:GLY:N	1.84	0.93
1:E:2:VAL:HG22	1:E:413:ASP:OD1	1.70	0.93
1:A:175:LEU:N	1:A:175:LEU:CD2	2.30	0.92
1:B:176:ILE:C	1:B:176:ILE:CD1	2.29	0.91
1:E:18:ARG:NH2	1:F:240:ARG:HE	1.69	0.89
1:E:174:GLY:C	1:E:175:LEU:HD13	1.92	0.88
1:E:18:ARG:HH12	1:F:240:ARG:HH21	1.17	0.88
1:B:175:LEU:CD2	1:B:459:ILE:HG21	2.05	0.87
1:E:83:SER:HA	1:E:86[B]:ARG:HD3	1.57	0.86
1:E:42:HIS:HB2	1:F:503:ARG:NH1	1.89	0.86
1:C:239:ASN:ND2	1:C:249:LEU:H	1.73	0.86
1:F:369:ASN:HD21	1:F:372:MSE:CE	1.90	0.85
1:A:489:ILE:HD12	1:A:489:ILE:H	0.72	0.85
1:E:475:LYS:O	1:E:476:ASP:HB2	1.74	0.84
1:D:41:LEU:O	1:D:44:CYS:SG	2.35	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:HIS:HB2	1:F:503:ARG:HH11	1.43	0.84
1:C:47:ASP:OD2	1:C:50:THR:HG22	1.77	0.84
1:F:27:MSE:HE2	1:F:31:GLU:HB3	1.60	0.83
1:C:251:VAL:O	1:C:252:ALA:HB2	1.76	0.83
1:E:344:THR:HG23	1:E:346:LEU:H	1.44	0.82
1:A:265:MSE:CE	1:A:270:ALA:HB2	2.10	0.82
1:F:494:VAL:HG12	1:F:505:VAL:HG23	1.62	0.82
1:B:344:THR:HG23	1:B:346:LEU:H	1.45	0.82
1:A:369:ASN:HD21	1:A:372:MSE:HE2	1.44	0.81
1:D:312:GLU:HG3	1:D:312:GLU:O	1.81	0.81
1:C:47:ASP:OD2	1:C:50:THR:CG2	2.29	0.81
1:E:174:GLY:O	1:E:175:LEU:CD1	2.30	0.80
1:D:250:MSE:O	1:D:251:VAL:HG12	1.80	0.80
1:A:265:MSE:HE3	1:A:270:ALA:HB2	1.62	0.80
1:A:487:ASP:OD1	1:A:489:ILE:CD1	2.29	0.80
1:D:10:VAL:HG11	1:D:265:MSE:HE2	1.62	0.80
1:B:47:ASP:OD2	1:B:50:THR:CG2	2.30	0.79
1:D:250:MSE:O	1:D:251:VAL:CG1	2.29	0.79
1:B:175:LEU:HD21	1:B:459:ILE:CG2	2.11	0.79
1:E:10:VAL:HG11	1:E:265:MSE:CE	2.12	0.79
1:C:251:VAL:O	1:C:252:ALA:CB	2.30	0.79
1:B:175:LEU:HA	1:B:180:VAL:CG1	2.12	0.79
1:D:360:LEU:HD21	1:D:367:GLY:HA2	1.64	0.79
1:E:63:GLN:OE1	1:E:63:GLN:HA	1.82	0.79
1:B:175:LEU:HA	1:B:180:VAL:HG11	1.63	0.79
1:A:168:GLU:HG2	1:A:170:THR:HG23	1.65	0.78
1:E:10:VAL:HG11	1:E:265:MSE:HE2	1.64	0.78
1:E:443:THR:HG23	1:E:490:GLY:O	1.84	0.78
1:A:128:GLY:N	1:A:372:MSE:HE1	1.98	0.78
1:C:344:THR:HG23	1:C:346:LEU:H	1.48	0.77
1:C:360:LEU:HD21	1:C:367:GLY:HA2	1.65	0.77
1:D:421:GLN:HG2	2:D:606:HOH:O	1.84	0.77
1:D:344:THR:HG23	1:D:346:LEU:H	1.48	0.76
1:D:369:ASN:HD21	1:D:372:MSE:CE	1.98	0.75
1:D:489:ILE:O	1:D:489:ILE:HG22	1.84	0.75
1:F:128:GLY:N	1:F:372:MSE:HE1	2.02	0.75
1:D:250:MSE:C	1:D:251:VAL:HG13	2.07	0.75
1:E:18:ARG:NH1	1:F:240:ARG:HH21	1.84	0.75
1:E:312:GLU:O	1:E:312:GLU:HG3	1.84	0.75
1:F:369:ASN:HD21	1:F:372:MSE:HE2	1.50	0.75
1:D:476:ASP:OD2	1:D:505:VAL:HG23	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:GLY:C	1:E:175:LEU:HD12	2.04	0.74
1:C:369:ASN:HD21	1:C:372:MSE:HE2	1.52	0.74
1:F:132:THR:HG23	1:F:257:ASN:ND2	2.03	0.73
1:D:489:ILE:O	1:D:489:ILE:CG2	2.36	0.73
1:F:176:ILE:C	1:F:176:ILE:CD1	2.52	0.73
1:D:265:MSE:HE3	1:D:270:ALA:HB2	1.71	0.73
1:A:10:VAL:HG11	1:A:265:MSE:HE2	1.70	0.73
1:E:315:ARG:CG	1:E:315:ARG:O	2.36	0.72
1:C:168:GLU:HA	1:C:171:ILE:HD12	1.71	0.72
1:D:476:ASP:OD2	1:D:505:VAL:CG2	2.39	0.71
1:E:312:GLU:O	1:E:316:VAL:HG23	1.90	0.71
1:C:10:VAL:HG11	1:C:265:MSE:HE2	1.71	0.71
1:E:411:PRO:O	1:E:412:ALA:HB2	1.90	0.71
1:F:265:MSE:HE3	1:F:270:ALA:HB2	1.73	0.71
1:B:369:ASN:HD21	1:B:372:MSE:HE2	1.56	0.71
1:C:10:VAL:HG11	1:C:265:MSE:CE	2.19	0.71
1:D:2:VAL:HG22	1:D:413:ASP:OD1	1.90	0.71
1:D:184:LEU:CD1	1:D:447:TYR:C	2.59	0.71
1:A:168:GLU:N	1:A:171:ILE:CD1	2.52	0.70
1:F:170:THR:O	1:F:175:LEU:HB2	1.91	0.70
1:B:10:VAL:HG11	1:B:265:MSE:HE2	1.74	0.70
1:F:369:ASN:ND2	1:F:372:MSE:HE2	2.06	0.70
1:A:190:ARG:HH22	1:A:489:ILE:HD11	1.57	0.69
1:B:10:VAL:HG11	1:B:265:MSE:CE	2.22	0.69
1:C:265:MSE:HE3	1:C:270:ALA:HB2	1.74	0.69
1:A:369:ASN:ND2	1:A:372:MSE:HE2	2.06	0.69
1:E:265:MSE:HE3	1:E:270:ALA:HB2	1.75	0.69
1:A:344:THR:HG23	1:A:346:LEU:H	1.58	0.69
1:A:369:ASN:HD21	1:A:372:MSE:CE	2.06	0.69
1:D:315:ARG:O	1:D:318:GLY:N	2.26	0.69
1:E:475:LYS:O	1:E:476:ASP:CB	2.41	0.68
1:B:118:ALA:O	1:B:119:GLY:C	2.30	0.68
1:B:360:LEU:O	1:B:361:PRO:C	2.28	0.68
1:D:250:MSE:C	1:D:251:VAL:CG1	2.61	0.68
1:F:344:THR:HG23	1:F:346:LEU:H	1.57	0.68
1:F:10:VAL:HG11	1:F:265:MSE:CE	2.24	0.68
1:C:340:ILE:O	1:C:344:THR:HG22	1.93	0.68
1:D:265:MSE:CE	1:D:270:ALA:HB2	2.23	0.68
1:D:369:ASN:HD21	1:D:372:MSE:HE2	1.57	0.68
1:A:489:ILE:N	1:A:489:ILE:CD1	2.29	0.67
1:C:369:ASN:ND2	1:C:372:MSE:HE2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:ARG:O	1:E:315:ARG:HG3	1.92	0.67
1:B:132:THR:HG23	1:B:257:ASN:ND2	2.10	0.67
1:B:265:MSE:HE3	1:B:270:ALA:HB2	1.76	0.67
1:E:360:LEU:O	1:E:361:PRO:C	2.29	0.67
1:A:340:ILE:O	1:A:344:THR:HG22	1.95	0.66
1:C:101:GLY:H	1:C:368:ASN:HD21	1.44	0.66
1:D:10:VAL:HG11	1:D:265:MSE:CE	2.26	0.66
1:D:494:VAL:HG12	1:D:505:VAL:HG12	1.77	0.66
1:A:360:LEU:O	1:A:361:PRO:C	2.33	0.66
1:F:369:ASN:OD1	1:F:372:MSE:HE2	1.96	0.66
1:A:290:LYS:H	1:A:423:GLN:HE22	1.44	0.66
1:D:132:THR:HG23	1:D:257:ASN:ND2	2.10	0.66
1:F:132:THR:O	1:F:133:SER:HB2	1.96	0.66
1:F:360:LEU:O	1:F:361:PRO:C	2.29	0.66
1:D:496:THR:HG22	1:D:497:PRO:HD2	1.78	0.66
1:B:112:PHE:O	1:B:116:ILE:HG12	1.96	0.65
1:A:396:GLY:HA3	1:A:401:LYS:O	1.97	0.65
1:E:126:ILE:HG22	1:E:372:MSE:CE	2.25	0.65
1:E:250:MSE:O	1:E:251:VAL:HG12	1.96	0.65
1:E:409:THR:O	1:E:411:PRO:HD3	1.95	0.65
1:A:168:GLU:N	1:A:168:GLU:OE2	2.30	0.65
1:D:369:ASN:ND2	1:D:372:MSE:HE2	2.12	0.65
1:D:128:GLY:N	1:D:372:MSE:HE1	2.12	0.64
1:C:132:THR:HG23	1:C:257:ASN:ND2	2.11	0.64
1:C:128:GLY:N	1:C:372:MSE:HE1	2.13	0.64
1:F:101:GLY:H	1:F:368:ASN:HD21	1.44	0.64
1:D:222:SER:CB	1:D:256:VAL:HG12	2.28	0.64
1:E:132:THR:HG23	1:E:257:ASN:ND2	2.13	0.64
1:A:222:SER:CB	1:A:256:VAL:HG12	2.28	0.64
1:E:250:MSE:C	1:E:251:VAL:HG13	2.18	0.63
1:C:369:ASN:HD21	1:C:372:MSE:CE	2.11	0.63
1:B:115:LYS:O	1:B:120:GLU:CB	2.46	0.63
1:C:265:MSE:CE	1:C:270:ALA:HB2	2.29	0.63
1:C:333:PHE:O	1:C:336:PRO:HD2	1.99	0.63
1:B:128:GLY:N	1:B:372:MSE:HE1	2.13	0.63
1:F:98:GLU:HG2	1:F:104:SER:HB2	1.80	0.63
1:D:123:VAL:HG22	1:D:265:MSE:HG2	1.81	0.63
1:E:250:MSE:O	1:E:251:VAL:CG1	2.47	0.62
1:E:10:VAL:CG1	1:E:265:MSE:HE2	2.30	0.62
1:A:190:ARG:NH2	1:A:489:ILE:HD11	2.14	0.62
1:B:476:ASP:OD2	1:B:479:LEU:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASP:OD2	1:B:50:THR:HG23	1.99	0.61
1:F:175:LEU:N	1:F:175:LEU:HD23	2.14	0.61
1:A:260:ALA:O	1:A:372:MSE:HE3	2.00	0.61
1:B:369:ASN:HD21	1:B:372:MSE:CE	2.14	0.61
1:B:489:ILE:O	1:B:489:ILE:HG22	1.99	0.61
1:A:42:HIS:NE2	1:C:503:ARG:HD3	2.16	0.61
1:D:369:ASN:OD1	1:D:372:MSE:HE2	2.01	0.61
1:C:260:ALA:O	1:C:372:MSE:HE3	2.00	0.61
1:B:369:ASN:ND2	1:B:372:MSE:HE2	2.15	0.60
1:F:10:VAL:HG11	1:F:265:MSE:HE2	1.84	0.60
1:B:47:ASP:HB3	1:B:50:THR:HG23	1.83	0.60
1:F:171:ILE:HA	1:F:174:GLY:O	2.01	0.60
1:A:10:VAL:HG11	1:A:265:MSE:CE	2.30	0.60
1:E:101:GLY:H	1:E:368:ASN:HD21	1.47	0.60
1:B:176:ILE:CD1	1:B:177:GLY:N	2.62	0.60
1:C:222:SER:CB	1:C:256:VAL:HG12	2.31	0.60
1:B:290:LYS:H	1:B:423:GLN:HE22	1.50	0.59
1:D:290:LYS:H	1:D:423:GLN:HE22	1.49	0.59
1:D:101:GLY:H	1:D:368:ASN:HD21	1.49	0.59
1:A:385:LYS:HE3	2:A:631:HOH:O	2.01	0.59
1:F:260:ALA:HB3	1:F:372:MSE:HE3	1.85	0.59
1:A:101:GLY:H	1:A:368:ASN:HD21	1.51	0.58
1:D:2:VAL:HG13	1:D:3:ASP:N	2.19	0.58
1:D:269:SER:HA	1:D:272:LYS:HE2	1.85	0.58
1:E:250:MSE:C	1:E:251:VAL:CG1	2.70	0.58
1:A:222:SER:HB3	1:A:256:VAL:HG12	1.85	0.58
1:F:265:MSE:CE	1:F:270:ALA:HB2	2.32	0.58
1:C:483:LEU:HD23	1:C:488:PRO:HG3	1.84	0.58
1:D:290:LYS:N	1:D:423:GLN:HE22	2.01	0.58
1:E:265:MSE:CE	1:E:270:ALA:HB2	2.34	0.58
1:B:222:SER:CB	1:B:256:VAL:HG12	2.33	0.58
1:B:47:ASP:OD2	1:B:50:THR:HG22	2.03	0.57
1:D:184:LEU:HD12	1:D:447:TYR:O	2.03	0.57
1:A:47:ASP:O	1:A:51:VAL:HG23	2.03	0.57
1:F:132:THR:HG23	1:F:257:ASN:HD21	1.69	0.57
1:B:132:THR:HG23	1:B:257:ASN:HD21	1.67	0.57
1:B:104:SER:O	1:B:108:LEU:HB2	2.04	0.57
1:D:421:GLN:NE2	2:D:611:HOH:O	2.37	0.57
1:E:185:LEU:HD11	1:E:294:LEU:HD11	1.85	0.57
1:B:176:ILE:O	1:B:176:ILE:CD1	2.46	0.57
1:C:222:SER:HB3	1:C:256:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LYS:N	1:A:423:GLN:HE22	2.01	0.57
1:C:369:ASN:OD1	1:C:372:MSE:HE2	2.04	0.57
1:C:239:ASN:HD21	1:C:249:LEU:H	1.51	0.57
1:A:396:GLY:O	1:A:400:SER:N	2.36	0.56
1:A:265:MSE:CE	1:A:270:ALA:CB	2.82	0.56
1:C:175:LEU:N	1:C:175:LEU:HD23	2.21	0.56
1:E:315:ARG:C	1:E:317:ALA:O	2.43	0.56
1:E:222:SER:CB	1:E:256:VAL:HG12	2.35	0.56
1:C:10:VAL:CG1	1:C:265:MSE:HE2	2.34	0.56
1:D:330:TYR:CD2	1:D:395:ASN:HB3	2.40	0.56
1:E:426:HIS:HB2	2:E:608:HOH:O	2.06	0.56
1:E:222:SER:HB3	1:E:256:VAL:HG12	1.88	0.56
1:F:172:ARG:HD2	1:F:500:LYS:O	2.06	0.56
1:E:185:LEU:HD11	1:E:294:LEU:CD1	2.36	0.56
1:F:330:TYR:CD2	1:F:395:ASN:HB3	2.41	0.56
1:D:132:THR:HG23	1:D:257:ASN:HD21	1.71	0.56
1:E:225:THR:HA	2:E:614:HOH:O	2.06	0.56
1:E:463:ARG:NH1	1:E:467:GLY:O	2.39	0.56
1:F:10:VAL:HG11	1:F:265:MSE:HE1	1.87	0.56
1:E:2:VAL:CG2	1:E:413:ASP:OD1	2.50	0.55
1:E:290:LYS:N	1:E:423:GLN:HE22	2.04	0.55
1:E:330:TYR:CD2	1:E:395:ASN:HB3	2.41	0.55
1:D:248:ARG:O	1:D:251:VAL:O	2.24	0.55
1:D:260:ALA:HB3	1:D:372:MSE:HE3	1.88	0.55
1:C:201:ARG:HA	1:C:204:MSE:HE2	1.89	0.55
1:E:290:LYS:H	1:E:423:GLN:HE22	1.53	0.55
1:D:340:ILE:O	1:D:344:THR:HG22	2.05	0.55
1:E:10:VAL:HG11	1:E:265:MSE:HE1	1.88	0.55
1:F:360:LEU:HD21	1:F:367:GLY:HA2	1.89	0.55
1:B:115:LYS:O	1:B:118:ALA:O	2.24	0.55
1:D:294:LEU:HA	1:D:297:ARG:NE	2.22	0.55
1:D:27:MSE:HG2	1:D:31:GLU:CB	2.37	0.54
1:F:222:SER:HB3	1:F:256:VAL:HG12	1.88	0.54
1:E:126:ILE:HG22	1:E:372:MSE:HE1	1.89	0.54
1:E:248:ARG:O	1:E:251:VAL:O	2.26	0.54
1:F:178:ALA:N	1:F:179:PRO:CD	2.70	0.54
1:F:369:ASN:CG	1:F:372:MSE:HE2	2.27	0.54
1:C:123:VAL:HG22	1:C:265:MSE:HG2	1.88	0.54
1:C:290:LYS:H	1:C:423:GLN:HE22	1.56	0.54
1:A:217:LYS:HE2	1:F:230:GLU:OE2	2.08	0.54
1:D:47:ASP:O	1:D:51:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:THR:HG23	1:E:257:ASN:HD21	1.70	0.54
1:A:123:VAL:HG22	1:A:265:MSE:HG2	1.90	0.54
1:F:222:SER:CB	1:F:256:VAL:HG12	2.38	0.54
1:E:340:ILE:O	1:E:344:THR:HG22	2.08	0.54
1:B:340:ILE:O	1:B:344:THR:HG22	2.07	0.54
1:C:175:LEU:HD22	1:C:180:VAL:HG13	1.89	0.54
1:B:222:SER:HB3	1:B:256:VAL:HG12	1.89	0.53
1:C:178:ALA:N	1:C:179:PRO:CD	2.72	0.53
1:D:250:MSE:O	1:D:251:VAL:HG13	2.07	0.53
1:B:290:LYS:N	1:B:423:GLN:HE22	2.05	0.53
1:D:184:LEU:HD12	1:D:447:TYR:C	2.28	0.53
1:F:47:ASP:OD2	1:F:50:THR:OG1	2.24	0.53
1:A:443:THR:CG2	1:A:490:GLY:HA2	2.38	0.53
1:E:316:VAL:C	1:E:317:ALA:O	2.40	0.53
1:B:260:ALA:O	1:B:372:MSE:HE3	2.09	0.53
1:D:500:LYS:O	1:D:501:SER:HB3	2.07	0.53
1:B:115:LYS:HB3	1:B:121:ASN:HD22	1.74	0.53
1:C:344:THR:HG23	1:C:346:LEU:HB2	1.89	0.53
1:F:248:ARG:O	1:F:251:VAL:O	2.27	0.53
1:D:10:VAL:CG1	1:D:265:MSE:HE2	2.37	0.53
1:D:184:LEU:HD13	1:D:448:THR:HB	1.90	0.53
1:D:222:SER:HB3	1:D:256:VAL:HG12	1.91	0.53
1:E:123:VAL:HG22	1:E:265:MSE:HG2	1.91	0.53
1:D:332:CYS:HA	1:D:360:LEU:HB3	1.91	0.52
1:D:184:LEU:HD11	1:D:447:TYR:C	2.30	0.52
1:B:252:ALA:O	1:B:254:ASP:N	2.42	0.52
1:F:340:ILE:O	1:F:344:THR:HG22	2.09	0.52
1:B:112:PHE:O	1:B:116:ILE:CG1	2.58	0.52
1:D:333:PHE:O	1:D:336:PRO:HD2	2.09	0.52
1:E:126:ILE:HG22	1:E:372:MSE:HE2	1.92	0.52
1:A:265:MSE:HE1	1:A:270:ALA:CB	2.40	0.52
1:F:10:VAL:CG1	1:F:265:MSE:HE2	2.39	0.52
1:C:63:GLN:HG2	2:C:634:HOH:O	2.10	0.52
1:E:42:HIS:CB	1:F:503:ARG:HH11	2.18	0.52
1:D:27:MSE:HG2	1:D:31:GLU:HB3	1.92	0.52
1:F:3:ASP:HB3	1:F:413:ASP:OD1	2.10	0.52
1:F:104:SER:O	1:F:108:LEU:HB2	2.09	0.52
1:C:340:ILE:O	1:C:344:THR:CG2	2.58	0.51
1:C:344:THR:CG2	1:C:346:LEU:HB2	2.40	0.51
1:B:489:ILE:O	1:B:489:ILE:CG2	2.55	0.51
1:A:42:HIS:CD2	1:C:503:ARG:HD3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:THR:O	1:C:133:SER:HB2	2.11	0.51
1:A:132:THR:HG23	1:A:257:ASN:ND2	2.26	0.51
1:B:360:LEU:HD11	1:B:367:GLY:HA2	1.93	0.51
1:A:265:MSE:HE1	1:A:270:ALA:HB2	1.92	0.51
1:C:208:PHE:CE2	1:C:361:PRO:HG2	2.46	0.51
1:C:478:ASP:OD2	1:C:478:ASP:N	2.40	0.51
1:A:330:TYR:CD2	1:A:395:ASN:HB3	2.47	0.51
1:C:132:THR:HG23	1:C:257:ASN:HD21	1.76	0.51
1:D:411:PRO:O	1:D:412:ALA:HB2	2.11	0.50
1:A:232:LEU:HD22	1:A:250:MSE:HE3	1.93	0.50
1:D:3:ASP:OD2	1:D:4:PRO:N	2.45	0.50
1:D:479:LEU:HD13	1:D:506:LEU:HD13	1.92	0.50
1:E:104:SER:O	1:E:108:LEU:HB2	2.11	0.50
1:C:267:VAL:HG22	1:C:280:TRP:CZ3	2.47	0.50
1:C:104:SER:O	1:C:108:LEU:HB2	2.12	0.50
1:E:42:HIS:CD2	1:F:503:ARG:CZ	2.94	0.50
1:F:290:LYS:H	1:F:423:GLN:HE22	1.58	0.50
1:B:230:GLU:HB2	2:B:622:HOH:O	2.10	0.50
1:B:265:MSE:CE	1:B:270:ALA:HB2	2.40	0.50
1:C:290:LYS:N	1:C:423:GLN:HE22	2.10	0.50
1:C:437:LYS:HD2	2:C:621:HOH:O	2.11	0.50
1:A:333:PHE:O	1:A:336:PRO:HD2	2.12	0.50
1:F:290:LYS:N	1:F:423:GLN:HE22	2.10	0.50
1:A:102:GLY:HA3	1:A:395:ASN:O	2.12	0.50
1:D:184:LEU:CD1	1:D:447:TYR:O	2.60	0.50
1:F:333:PHE:O	1:F:336:PRO:HD2	2.12	0.50
1:E:18:ARG:CZ	1:F:240:ARG:HE	2.23	0.49
1:A:208:PHE:O	1:A:211:PHE:HB2	2.13	0.49
1:A:205:ALA:HA	1:A:250:MSE:HE1	1.93	0.49
1:B:333:PHE:O	1:B:336:PRO:HD2	2.12	0.49
1:F:169:TYR:O	1:F:169:TYR:CG	2.66	0.49
1:F:5:ARG:O	1:F:117:ALA:HA	2.12	0.49
1:C:169:TYR:HD2	1:C:172:ARG:NH2	2.10	0.49
1:C:369:ASN:CG	1:C:372:MSE:HE2	2.33	0.49
1:B:173:HIS:HB3	1:B:175:LEU:HD11	1.94	0.49
1:C:332:CYS:HA	1:C:360:LEU:HB3	1.94	0.49
1:B:167:ASP:HB3	1:B:170:THR:HB	1.95	0.49
1:B:180:VAL:HA	1:B:243:VAL:HG11	1.95	0.49
1:D:3:ASP:OD2	1:D:4:PRO:HD2	2.13	0.49
1:E:180:VAL:HA	1:E:243:VAL:HG11	1.95	0.48
1:B:10:VAL:CG1	1:B:265:MSE:HE2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:CG1	1:A:265:MSE:HE2	2.42	0.48
1:F:41:LEU:O	1:F:44:CYS:SG	2.68	0.48
1:C:47:ASP:HB3	1:C:50:THR:HG23	1.94	0.48
1:E:109:ALA:HA	1:E:264:MSE:HE1	1.95	0.48
1:D:312:GLU:OE2	1:D:418:ASN:N	2.31	0.48
1:A:488:PRO:O	1:A:489:ILE:C	2.52	0.48
1:D:242:ILE:HD11	1:D:248:ARG:HG3	1.95	0.48
1:F:274:GLY:O	1:F:276:PRO:HD3	2.13	0.48
1:C:222:SER:HB3	1:C:256:VAL:CG1	2.44	0.48
1:D:208:PHE:CE2	1:D:361:PRO:HG2	2.49	0.48
1:E:126:ILE:CG2	1:E:372:MSE:CE	2.91	0.48
1:A:344:THR:HG23	1:A:346:LEU:HB2	1.95	0.48
1:E:333:PHE:O	1:E:336:PRO:HD2	2.14	0.48
1:C:178:ALA:HB3	1:C:179:PRO:HD3	1.96	0.48
1:D:208:PHE:O	1:D:211:PHE:HB2	2.13	0.48
1:D:369:ASN:CG	1:D:372:MSE:HE2	2.33	0.47
1:A:340:ILE:O	1:A:344:THR:CG2	2.63	0.47
1:B:168:GLU:O	1:B:172:ARG:HG2	2.13	0.47
1:D:115:LYS:HB3	1:D:121:ASN:HD22	1.78	0.47
1:A:104:SER:O	1:A:108:LEU:HB2	2.14	0.47
1:C:479:LEU:HD13	1:C:506:LEU:HD13	1.95	0.47
1:E:126:ILE:CG2	1:E:372:MSE:HE2	2.44	0.47
1:E:270:ALA:O	1:E:273:LEU:O	2.33	0.47
1:F:369:ASN:ND2	1:F:372:MSE:CE	2.66	0.47
1:A:385:LYS:CE	2:A:631:HOH:O	2.59	0.47
1:C:205:ALA:HA	1:C:250:MSE:HE1	1.96	0.47
1:A:222:SER:HB3	1:A:256:VAL:CG1	2.45	0.47
1:B:10:VAL:HG11	1:B:265:MSE:HE1	1.97	0.47
1:C:242:ILE:HD11	1:C:248:ARG:HG3	1.95	0.47
1:A:265:MSE:HE3	1:A:270:ALA:CB	2.40	0.47
1:C:180:VAL:HA	1:C:243:VAL:HG11	1.97	0.47
1:D:104:SER:O	1:D:108:LEU:HB2	2.15	0.47
1:F:260:ALA:O	1:F:372:MSE:HE3	2.15	0.47
1:E:42:HIS:CB	1:F:503:ARG:NH1	2.72	0.47
1:E:464:LEU:O	1:E:465:ASP:C	2.53	0.47
1:A:180:VAL:HA	1:A:243:VAL:HG11	1.96	0.47
1:B:369:ASN:OD1	1:B:372:MSE:HE2	2.15	0.47
1:C:175:LEU:HD23	1:C:175:LEU:H	1.79	0.47
1:D:180:VAL:HA	1:D:243:VAL:HG11	1.96	0.47
1:D:294:LEU:HA	1:D:297:ARG:CD	2.45	0.47
1:C:296:GLU:HG2	2:C:637:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:SER:O	1:D:361:PRO:HD3	2.15	0.46
1:D:178:ALA:N	1:D:179:PRO:CD	2.78	0.46
1:D:201:ARG:HA	1:D:204:MSE:HE2	1.97	0.46
1:E:42:HIS:CD2	1:F:503:ARG:NE	2.83	0.46
1:E:312:GLU:O	1:E:312:GLU:CG	2.61	0.46
1:F:205:ALA:HA	1:F:250:MSE:HE1	1.97	0.46
1:B:176:ILE:HD13	1:B:177:GLY:CA	2.45	0.46
1:B:265:MSE:HE2	1:B:265:MSE:HB2	1.74	0.46
1:C:63:GLN:O	1:C:64:PHE:HD2	1.99	0.46
1:F:180:VAL:HA	1:F:243:VAL:HG11	1.97	0.46
1:C:443:THR:CG2	1:C:490:GLY:HA2	2.46	0.46
1:D:6:THR:HG21	1:D:412:ALA:O	2.16	0.46
1:D:265:MSE:HE2	1:D:265:MSE:HB2	1.78	0.46
1:E:464:LEU:HA	1:E:464:LEU:HD23	1.60	0.46
1:B:118:ALA:O	1:B:119:GLY:O	2.34	0.46
1:E:201:ARG:HA	1:E:204:MSE:HE2	1.97	0.46
1:A:42:HIS:CD2	1:C:503:ARG:NH1	2.83	0.46
1:E:360:LEU:HD23	1:E:360:LEU:HA	1.44	0.46
1:F:208:PHE:O	1:F:211:PHE:HB2	2.16	0.46
1:E:172:ARG:NH1	1:E:499:GLU:HA	2.30	0.45
1:B:330:TYR:CD2	1:B:395:ASN:HB3	2.52	0.45
1:C:47:ASP:OD2	1:C:50:THR:HG23	2.14	0.45
1:C:115:LYS:HB3	1:C:121:ASN:HD22	1.80	0.45
1:F:197:VAL:HB	2:F:606:HOH:O	2.16	0.45
1:B:178:ALA:N	1:B:179:PRO:CD	2.79	0.45
1:B:255:GLN:HA	1:B:255:GLN:HE21	1.82	0.45
1:C:208:PHE:HE2	1:C:361:PRO:HG2	1.81	0.45
1:E:411:PRO:O	1:E:412:ALA:CB	2.55	0.45
1:B:172:ARG:HD2	1:B:500:LYS:O	2.16	0.45
1:D:3:ASP:OD2	1:D:4:PRO:CD	2.65	0.45
1:E:175:LEU:HD12	1:E:175:LEU:HA	1.48	0.45
1:C:10:VAL:HG11	1:C:265:MSE:HE1	1.96	0.45
1:D:222:SER:HB3	1:D:256:VAL:CG1	2.46	0.45
1:F:201:ARG:HA	1:F:204:MSE:HE2	1.99	0.45
1:B:360:LEU:HD23	1:B:360:LEU:HA	1.65	0.45
1:C:410:GLU:HA	1:C:411:PRO:HD3	1.60	0.45
1:E:425:GLU:HG3	2:E:601:HOH:O	2.17	0.45
1:C:169:TYR:HD2	1:C:172:ARG:HH21	1.63	0.45
1:F:62:ARG:HB2	1:F:98:GLU:O	2.17	0.45
1:A:178:ALA:HB3	1:A:179:PRO:HD3	1.99	0.44
1:E:487:ASP:HA	1:E:488:PRO:HD2	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ALA:HA	1:B:250:MSE:HE1	2.00	0.44
1:B:251:VAL:O	1:B:251:VAL:HG23	2.17	0.44
1:A:369:ASN:OD1	1:A:372:MSE:HE2	2.18	0.44
1:F:169:TYR:CE1	1:F:173:HIS:HE1	2.35	0.44
1:B:431:LYS:HG2	2:B:621:HOH:O	2.16	0.44
1:D:265:MSE:CE	1:D:270:ALA:CB	2.95	0.44
1:D:314:LEU:HD12	1:D:314:LEU:HA	1.74	0.44
1:A:201:ARG:HA	1:A:204:MSE:HE2	1.98	0.44
1:C:213:LYS:HA	1:C:226:GLU:HG3	2.00	0.44
1:C:443:THR:HG23	1:C:490:GLY:O	2.18	0.44
1:D:269:SER:HA	1:D:272:LYS:CG	2.47	0.44
1:F:488:PRO:O	1:F:489:ILE:C	2.53	0.44
1:A:127:PHE:C	1:A:372:MSE:HE1	2.38	0.44
1:A:463:ARG:HA	1:A:463:ARG:HD3	1.79	0.44
1:C:330:TYR:CD2	1:C:395:ASN:HB3	2.52	0.44
1:A:265:MSE:HE2	1:A:265:MSE:HB2	1.86	0.44
1:C:315:ARG:O	1:C:318:GLY:N	2.50	0.44
1:F:109:ALA:HA	1:F:264:MSE:HE1	1.99	0.43
1:A:213:LYS:HA	1:A:226:GLU:HG3	1.99	0.43
1:C:265:MSE:HE2	1:C:265:MSE:HB2	1.81	0.43
1:F:222:SER:HB3	1:F:256:VAL:CG1	2.49	0.43
1:B:289:MSE:HG2	1:B:309:ALA:HB2	2.01	0.43
1:B:280:TRP:CD1	1:B:280:TRP:N	2.85	0.43
1:D:476:ASP:CG	1:D:505:VAL:HG23	2.38	0.43
1:F:390:ALA:O	1:F:406:ILE:HA	2.18	0.43
1:A:369:ASN:CG	1:A:372:MSE:HE2	2.39	0.43
1:C:5:ARG:O	1:C:117:ALA:HA	2.19	0.43
1:D:413:ASP:O	1:D:414:TRP:C	2.53	0.43
1:F:175:LEU:HA	1:F:175:LEU:HD22	1.62	0.43
1:A:447:TYR:CE2	1:A:488:PRO:HG2	2.53	0.43
1:B:47:ASP:CB	1:B:50:THR:HG23	2.48	0.43
1:B:222:SER:HB3	1:B:256:VAL:CG1	2.49	0.43
1:A:344:THR:CG2	1:A:346:LEU:HB2	2.49	0.42
1:C:191:ALA:HB2	1:C:489:ILE:HD12	2.00	0.42
1:E:443:THR:CG2	1:E:490:GLY:HA2	2.49	0.42
1:D:178:ALA:HB3	1:D:179:PRO:HD3	2.00	0.42
1:F:232:LEU:HD22	1:F:250:MSE:HE3	2.01	0.42
1:F:319:ILE:HB	1:F:323:ASP:HB2	2.01	0.42
1:B:109:ALA:HA	1:B:264:MSE:HE1	2.02	0.42
1:B:175:LEU:HA	1:B:180:VAL:HG13	1.99	0.42
1:C:270:ALA:O	1:C:273:LEU:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:LYS:HD3	1:B:500:LYS:HA	1.65	0.42
1:E:168:GLU:O	1:E:172:ARG:HG3	2.19	0.42
1:E:360:LEU:O	1:E:361:PRO:O	2.37	0.42
1:C:3:ASP:OD2	1:C:4:PRO:N	2.52	0.42
1:D:496:THR:CG2	1:D:497:PRO:HD2	2.48	0.42
1:C:185:LEU:HD11	1:C:294:LEU:HD13	2.01	0.42
1:C:221:SER:HB2	1:C:224:PRO:HG3	2.02	0.42
1:C:280:TRP:CD1	1:C:280:TRP:N	2.86	0.42
1:E:178:ALA:HB3	1:E:179:PRO:HD3	2.02	0.42
1:C:331:SER:O	1:C:361:PRO:HD3	2.20	0.42
1:D:109:ALA:HA	1:D:264:MSE:HE1	2.00	0.42
1:E:360:LEU:HD11	1:E:367:GLY:HA2	2.02	0.42
1:C:208:PHE:O	1:C:211:PHE:HB2	2.19	0.42
1:D:340:ILE:O	1:D:344:THR:CG2	2.67	0.42
1:E:37:ALA:HB1	1:E:125:LEU:HD21	2.02	0.42
1:D:16:THR:HB	1:E:454:THR:HB	2.02	0.42
1:E:280:TRP:CD1	1:E:280:TRP:N	2.85	0.42
1:F:116:ILE:O	1:F:118:ALA:O	2.37	0.42
1:B:303:SER:HB3	1:B:339:ASN:ND2	2.35	0.41
1:E:222:SER:HB3	1:E:256:VAL:CG1	2.49	0.41
1:F:115:LYS:O	1:F:120:GLU:CB	2.68	0.41
1:D:500:LYS:HD3	1:D:500:LYS:HA	1.62	0.41
1:F:191:ALA:HB2	1:F:489:ILE:HD12	2.01	0.41
1:C:3:ASP:OD2	1:C:3:ASP:C	2.59	0.41
1:A:242:ILE:HD11	1:A:248:ARG:HG3	2.03	0.41
1:A:500:LYS:HA	1:A:500:LYS:HD3	1.65	0.41
1:B:289:MSE:CG	1:B:309:ALA:HB2	2.51	0.41
1:E:185:LEU:CD1	1:E:294:LEU:HD11	2.50	0.41
1:F:100:ILE:HG13	1:F:368:ASN:HD21	1.86	0.41
1:F:340:ILE:O	1:F:344:THR:CG2	2.68	0.41
1:F:506:LEU:HA	1:F:506:LEU:HD23	1.78	0.41
1:B:201:ARG:HA	1:B:204:MSE:HE2	2.01	0.41
1:B:260:ALA:HB2	1:B:373:HIS:CE1	2.55	0.41
1:A:280:TRP:N	1:A:280:TRP:CD1	2.84	0.41
1:E:483:LEU:HA	1:E:488:PRO:HG3	2.03	0.41
1:B:213:LYS:HA	1:B:226:GLU:HG3	2.03	0.41
1:B:476:ASP:OD2	1:B:479:LEU:HB2	2.21	0.41
1:E:267:VAL:HG22	1:E:280:TRP:CZ3	2.55	0.41
1:F:115:LYS:HB3	1:F:121:ASN:HD22	1.86	0.41
1:F:255:GLN:HE21	1:F:255:GLN:HB3	1.64	0.41
1:F:265:MSE:HE2	1:F:265:MSE:HB2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:ALA:O	1:F:273:LEU:O	2.39	0.41
1:A:381:GLU:HG2	2:A:633:HOH:O	2.20	0.41
1:B:116:ILE:HD13	1:B:121:ASN:O	2.20	0.41
1:A:463:ARG:NH1	1:A:467:GLY:O	2.53	0.40
1:F:123:VAL:HG22	1:F:265:MSE:HG2	2.02	0.40
1:B:340:ILE:O	1:B:344:THR:CG2	2.68	0.40
1:C:443:THR:HG23	1:C:490:GLY:C	2.41	0.40
1:E:265:MSE:HE2	1:E:265:MSE:HB2	1.77	0.40
1:F:489:ILE:H	1:F:489:ILE:HG12	1.60	0.40
1:D:27:MSE:HG2	1:D:31:GLU:HB2	2.02	0.40
1:A:248:ARG:O	1:A:251:VAL:O	2.38	0.40
1:B:290:LYS:HB2	1:B:290:LYS:HE3	1.88	0.40
1:B:360:LEU:O	1:B:361:PRO:O	2.40	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	438/520 (84%)	417 (95%)	20 (5%)	1 (0%)	47 72
1	B	445/520 (86%)	425 (96%)	19 (4%)	1 (0%)	47 72
1	C	443/520 (85%)	423 (96%)	20 (4%)	0	100 100
1	D	435/520 (84%)	414 (95%)	21 (5%)	0	100 100
1	E	437/520 (84%)	420 (96%)	15 (3%)	2 (0%)	29 53
1	F	437/520 (84%)	420 (96%)	17 (4%)	0	100 100
All	All	2635/3120 (84%)	2519 (96%)	112 (4%)	4 (0%)	47 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	119	GLY
1	E	412	ALA
1	E	466	ASP
1	A	489	ILE

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	343/394 (87%)	318 (93%)	25 (7%)	14 31
1	B	347/394 (88%)	309 (89%)	38 (11%)	6 14
1	C	348/394 (88%)	319 (92%)	29 (8%)	11 25
1	D	340/394 (86%)	304 (89%)	36 (11%)	6 15
1	E	344/394 (87%)	310 (90%)	34 (10%)	8 17
1	F	344/394 (87%)	311 (90%)	33 (10%)	8 19
All	All	2066/2364 (87%)	1871 (91%)	195 (9%)	8 19

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	78	SER
1	A	80	TYR
1	A	108	LEU
1	A	168	GLU
1	A	170	THR
1	A	175	LEU
1	A	176	ILE
1	A	225	THR
1	A	233	LEU
1	A	248	ARG
1	A	267	VAL
1	A	293	LYS
1	A	295	LEU
1	A	314	LEU

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Mol	Chain	Res	Type
1	A	329	LEU
1	A	346	LEU
1	A	463	ARG
1	A	473	LYS
1	A	489	ILE
1	A	494	VAL
1	A	496	THR
1	A	499	GLU
1	A	500	LYS
1	A	503	ARG
1	B	5	ARG
1	B	18	ARG
1	B	50	THR
1	B	80	TYR
1	B	99	VAL
1	B	100	ILE
1	B	108	LEU
1	B	168	GLU
1	B	175	LEU
1	B	176	ILE
1	B	181	GLN
1	B	184	LEU
1	B	193	LEU
1	B	225	THR
1	B	230	GLU
1	B	233	LEU
1	B	244	ASP
1	B	248	ARG
1	B	254	ASP
1	B	255	GLN
1	B	265	MSE
1	B	267	VAL
1	B	272	LYS
1	B	293	LYS
1	B	314	LEU
1	B	329	LEU
1	B	368	ASN
1	B	422	LEU
1	B	464	LEU
1	B	473	LYS
1	B	477	GLU
1	B	489	ILE

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Mol	Chain	Res	Type
1	B	494	VAL
1	B	496	THR
1	B	499	GLU
1	B	500	LYS
1	B	501	SER
1	B	503	ARG
1	C	5	ARG
1	C	25	ARG
1	C	50	THR
1	C	63	GLN
1	C	64	PHE
1	C	78	SER
1	C	80	TYR
1	C	100	ILE
1	C	108	LEU
1	C	168	GLU
1	C	170	THR
1	C	225	THR
1	C	233	LEU
1	C	250	MSE
1	C	255	GLN
1	C	265	MSE
1	C	273	LEU
1	C	293	LYS
1	C	314	LEU
1	C	346	LEU
1	C	360	LEU
1	C	422	LEU
1	C	473	LYS
1	C	477	GLU
1	C	478	ASP
1	C	494	VAL
1	C	496	THR
1	C	499	GLU
1	C	506	LEU
1	D	2	VAL
1	D	5	ARG
1	D	78	SER
1	D	80	TYR
1	D	108	LEU
1	D	133	SER
1	D	176	ILE

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Mol	Chain	Res	Type
1	D	184	LEU
1	D	225	THR
1	D	230	GLU
1	D	233	LEU
1	D	248	ARG
1	D	255	GLN
1	D	267	VAL
1	D	272	LYS
1	D	293	LYS
1	D	294	LEU
1	D	314	LEU
1	D	315	ARG
1	D	329	LEU
1	D	360	LEU
1	D	366	LEU
1	D	422	LEU
1	D	463	ARG
1	D	473	LYS
1	D	477	GLU
1	D	481	LYS
1	D	489	ILE
1	D	493	ILE
1	D	494	VAL
1	D	496	THR
1	D	499	GLU
1	D	500	LYS
1	D	503	ARG
1	D	505	VAL
1	D	506	LEU
1	E	1	MSE
1	E	2	VAL
1	E	5	ARG
1	E	18	ARG
1	E	63	GLN
1	E	80	TYR
1	E	108	LEU
1	E	170	THR
1	E	172	ARG
1	E	175	LEU
1	E	225	THR
1	E	230[A]	GLU
1	E	230[B]	GLU

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Mol	Chain	Res	Type
1	E	233	LEU
1	E	244	ASP
1	E	248	ARG
1	E	265	MSE
1	E	267	VAL
1	E	290	LYS
1	E	293	LYS
1	E	314	LEU
1	E	315	ARG
1	E	329	LEU
1	E	371	SER
1	E	410	GLU
1	E	422	LEU
1	E	473	LYS
1	E	476	ASP
1	E	479	LEU
1	E	481	LYS
1	E	494	VAL
1	E	496	THR
1	E	500	LYS
1	E	503	ARG
1	F	2	VAL
1	F	5	ARG
1	F	32	LEU
1	F	63	GLN
1	F	80	TYR
1	F	108	LEU
1	F	167	ASP
1	F	171	ILE
1	F	172	ARG
1	F	175	LEU
1	F	176	ILE
1	F	180	VAL
1	F	181	GLN
1	F	225	THR
1	F	233	LEU
1	F	248	ARG
1	F	262	LEU
1	F	267	VAL
1	F	273	LEU
1	F	293	LYS
1	F	314	LEU

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Mol	Chain	Res	Type
1	F	329	LEU
1	F	360	LEU
1	F	362	PHE
1	F	368	ASN
1	F	422	LEU
1	F	473	LYS
1	F	481	LYS
1	F	494	VAL
1	F	496	THR
1	F	500	LYS
1	F	503	ARG
1	F	505	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	257	ASN
1	A	368	ASN
1	A	388	GLN
1	A	423	GLN
1	B	42	HIS
1	B	63	GLN
1	B	121	ASN
1	B	255	GLN
1	B	257	ASN
1	B	368	ASN
1	B	388	GLN
1	B	423	GLN
1	C	181	GLN
1	C	239	ASN
1	C	257	ASN
1	C	368	ASN
1	C	388	GLN
1	C	423	GLN
1	D	106	GLN
1	D	121	ASN
1	D	257	ASN
1	D	368	ASN
1	D	388	GLN
1	D	423	GLN
1	E	42	HIS

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Mol	Chain	Res	Type
1	E	106	GLN
1	E	257	ASN
1	E	368	ASN
1	E	423	GLN
1	F	173	HIS
1	F	181	GLN
1	F	255	GLN
1	F	257	ASN
1	F	368	ASN
1	F	369	ASN
1	F	388	GLN
1	F	423	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 monosaccharides 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	439/520 (84%)	0.04	3 (0%)	87	89	23, 46, 64, 69	0
1	B	442/520 (85%)	-0.05	4 (0%)	84	85	25, 46, 64, 69	0
1	C	443/520 (85%)	0.03	7 (1%)	72	74	25, 46, 64, 69	0
1	D	435/520 (83%)	-0.16	3 (0%)	87	89	25, 46, 64, 69	0
1	E	437/520 (84%)	-0.11	3 (0%)	87	89	25, 46, 64, 69	0
1	F	440/520 (84%)	-0.04	4 (0%)	84	85	25, 46, 64, 76	0
All	All	2636/3120 (84%)	-0.05	24 (0%)	84	85	23, 46, 64, 76	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	GLY	6.0
1	C	119	GLY	4.4
1	C	25	ARG	3.9
1	F	133	SER	3.6
1	C	176	ILE	3.4
1	C	133	SER	3.3
1	B	492	LYS	3.3
1	C	477	GLU	2.8
1	D	133	SER	2.7
1	C	24	TYR	2.7
1	A	133	SER	2.7
1	F	78	SER	2.6
1	B	166	PHE	2.6
1	C	465	ASP	2.4
1	A	230	GLU	2.4
1	E	492	LYS	2.4
1	F	465	ASP	2.4
1	D	176	ILE	2.3
1	D	175	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	415	VAL	2.2
1	E	465	ASP	2.2
1	B	477	GLU	2.1
1	E	223	ALA	2.1
1	B	175	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.