Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 01:33 PM JST

PDB ID	:	5HYW
Title	:	The crystal structure of the D3-ASK1 complex
Authors	:	Yao, R.F.; Ming, Z.H.; Yan, L.M.; Rao, Z.H.; Lou, Z.Y.; Xie, D.X.
Deposited on	:	2016-02-02
Resolution	:	3.01 Å(reported)

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

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

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

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

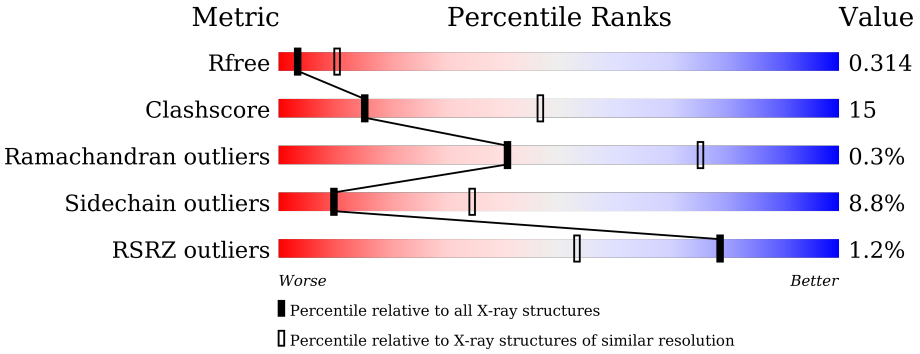
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	740	55% 20% • 22%
1	C	740	.% 57% 17% • • 22%
2	B	169	2% 34% 8% • 56%
2	D	169	2% 34% 5% • 59%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10174 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 F-box/LRR-repeat MAX2 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	580	4510	2885	785	813	27	0	0	0
1	C	575	4478	2866	783	802	27	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	expression tag	UNP Q5VMP0
A	-18	ALA	-	expression tag	UNP Q5VMP0
A	-17	MET	-	expression tag	UNP Q5VMP0
A	-16	GLY	-	expression tag	UNP Q5VMP0
A	-15	SER	-	expression tag	UNP Q5VMP0
A	-14	GLY	-	expression tag	UNP Q5VMP0
A	-13	ILE	-	expression tag	UNP Q5VMP0
A	-12	GLN	-	expression tag	UNP Q5VMP0
A	-11	ARG	-	expression tag	UNP Q5VMP0
A	-10	PRO	-	expression tag	UNP Q5VMP0
A	-9	THR	-	expression tag	UNP Q5VMP0
A	-8	SER	-	expression tag	UNP Q5VMP0
A	-7	THR	-	expression tag	UNP Q5VMP0
A	-6	SER	-	expression tag	UNP Q5VMP0
A	-5	SER	-	expression tag	UNP Q5VMP0
A	-4	LEU	-	expression tag	UNP Q5VMP0
A	-3	VAL	-	expression tag	UNP Q5VMP0
A	-2	ALA	-	expression tag	UNP Q5VMP0
A	-1	ALA	-	expression tag	UNP Q5VMP0
A	0	ALA	-	expression tag	UNP Q5VMP0
C	-19	GLY	-	expression tag	UNP Q5VMP0
C	-18	ALA	-	expression tag	UNP Q5VMP0
C	-17	MET	-	expression tag	UNP Q5VMP0
C	-16	GLY	-	expression tag	UNP Q5VMP0
C	-15	SER	-	expression tag	UNP Q5VMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	GLY	-	expression tag	UNP Q5VMP0
C	-13	ILE	-	expression tag	UNP Q5VMP0
C	-12	GLN	-	expression tag	UNP Q5VMP0
C	-11	ARG	-	expression tag	UNP Q5VMP0
C	-10	PRO	-	expression tag	UNP Q5VMP0
C	-9	THR	-	expression tag	UNP Q5VMP0
C	-8	SER	-	expression tag	UNP Q5VMP0
C	-7	THR	-	expression tag	UNP Q5VMP0
C	-6	SER	-	expression tag	UNP Q5VMP0
C	-5	SER	-	expression tag	UNP Q5VMP0
C	-4	LEU	-	expression tag	UNP Q5VMP0
C	-3	VAL	-	expression tag	UNP Q5VMP0
C	-2	ALA	-	expression tag	UNP Q5VMP0
C	-1	ALA	-	expression tag	UNP Q5VMP0
C	0	ALA	-	expression tag	UNP Q5VMP0

- Molecule 2 is a protein called SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	74	609	385	98	123	3	0	0	0
			Total	C	N	O	S			
2	D	70	577	365	94	115	3	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	expression tag	UNP Q39255
B	-7	ASP	-	expression tag	UNP Q39255
B	-6	TYR	-	expression tag	UNP Q39255
B	-5	LYS	-	expression tag	UNP Q39255
B	-4	ASP	-	expression tag	UNP Q39255
B	-3	ASP	-	expression tag	UNP Q39255
B	-2	ASP	-	expression tag	UNP Q39255
B	-1	ASP	-	expression tag	UNP Q39255
B	0	LYS	-	expression tag	UNP Q39255
D	-8	MET	-	expression tag	UNP Q39255
D	-7	ASP	-	expression tag	UNP Q39255
D	-6	TYR	-	expression tag	UNP Q39255
D	-5	LYS	-	expression tag	UNP Q39255
D	-4	ASP	-	expression tag	UNP Q39255
D	-3	ASP	-	expression tag	UNP Q39255

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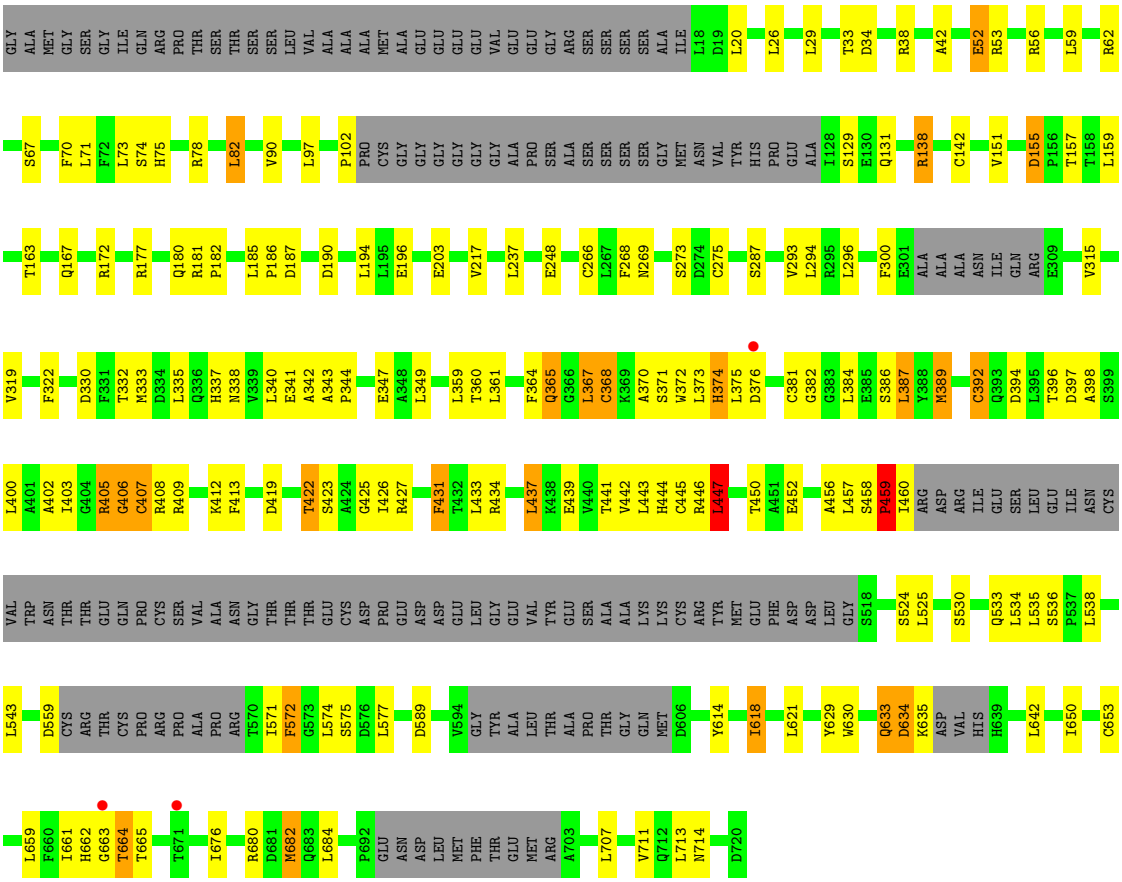
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ASP	-	expression tag	UNP Q39255
D	-1	ASP	-	expression tag	UNP Q39255
D	0	LYS	-	expression tag	UNP Q39255

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.

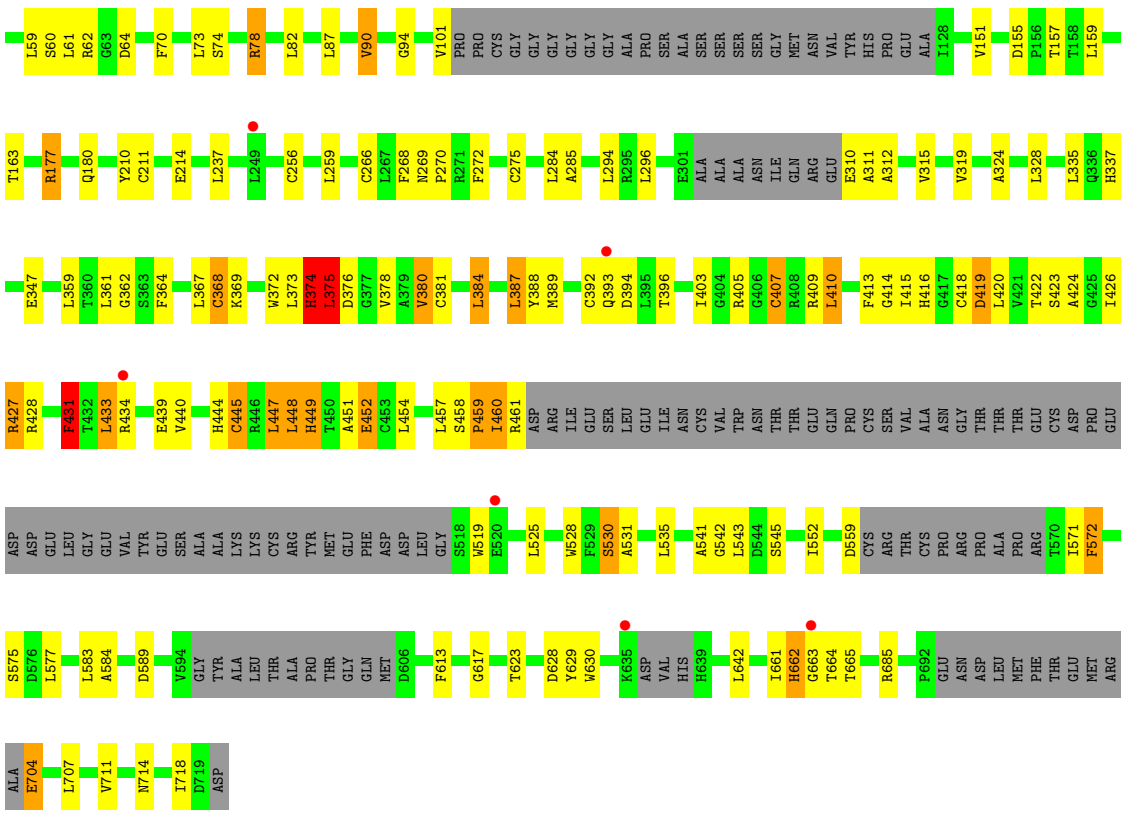
• Molecule 1: F-box/LRR-repeat MAX2 homolog

Chain A: 55% 20% • 22%



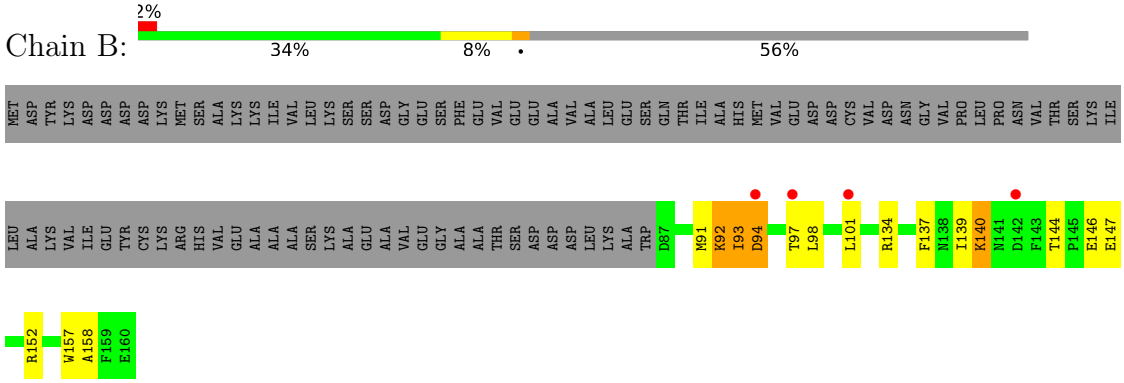
• Molecule 1: F-box/LRR-repeat MAX2 homolog

Chain C: % 57% 17% • • 22%



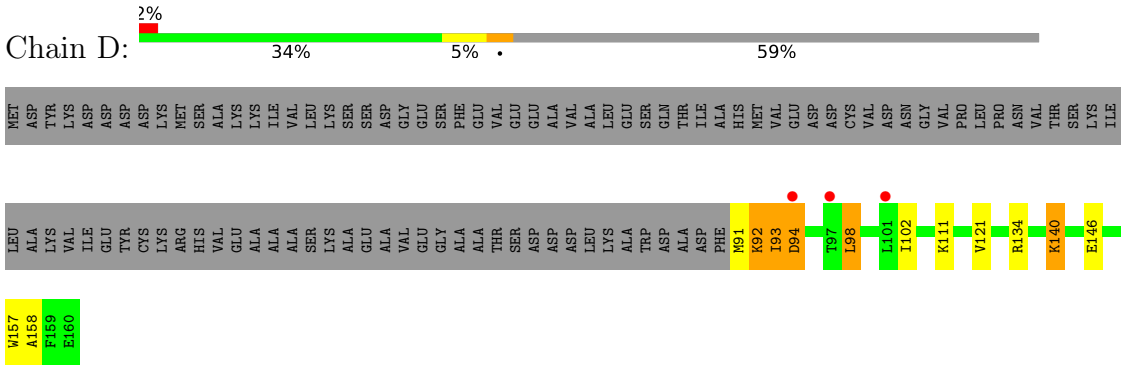
- Molecule 2: SKP1-like protein 1A

Chain B:



- Molecule 2: SKP1-like protein 1A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	79.27Å 79.27Å 327.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.89 – 3.01 37.26 – 3.01	Depositor EDS
% Data completeness (in resolution range)	81.3 (81.89-3.01) 81.3 (37.26-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.235 , 0.312 0.246 , 0.314	Depositor DCC
R_{free} test set	1631 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 24.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10174	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.59	0/4612	0.99	27/6268 (0.4%)
1	C	0.59	1/4580 (0.0%)	1.00	31/6223 (0.5%)
2	B	0.54	0/618	0.76	1/835 (0.1%)
2	D	0.58	0/585	0.81	3/790 (0.4%)
All	All	0.59	1/10395 (0.0%)	0.97	62/14116 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	459	PRO	N-CD	8.86	1.60	1.47

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	405	ARG	CB-CA-C	-11.76	86.89	110.40
1	A	386	SER	N-CA-C	10.67	139.81	111.00
1	A	572	PHE	CB-CA-C	10.61	131.62	110.40
1	C	542	GLY	N-CA-C	10.53	139.44	113.10
1	C	458	SER	C-N-CD	-9.39	99.94	120.60
1	C	374	HIS	N-CA-C	8.51	133.98	111.00
1	A	407	CYS	N-CA-CB	-8.08	96.06	110.60
1	A	406	GLY	N-CA-C	8.00	133.11	113.10
1	C	572	PHE	N-CA-C	-7.98	89.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	634	ASP	N-CA-C	7.61	131.54	111.00
1	A	387	LEU	N-CA-C	7.49	131.22	111.00
1	C	447	LEU	CB-CA-C	-7.41	96.12	110.20
1	C	664	THR	N-CA-CB	-7.32	96.39	110.30
1	A	370	ALA	N-CA-CB	-7.31	99.86	110.10
1	A	407	CYS	N-CA-C	7.31	130.75	111.00
1	C	541	ALA	N-CA-C	-7.30	91.29	111.00
1	A	633	GLN	CB-CA-C	-7.15	96.10	110.40
1	C	32	LEU	CA-CB-CG	7.11	131.65	115.30
1	C	530	SER	CB-CA-C	7.09	123.57	110.10
1	A	405	ARG	N-CA-C	6.99	129.87	111.00
1	C	664	THR	N-CA-C	6.99	129.87	111.00
1	A	662	HIS	CB-CA-C	6.92	124.23	110.40
1	A	102	PRO	N-CA-CB	6.69	111.33	103.30
1	C	662	HIS	CB-CA-C	6.64	123.69	110.40
1	A	373	LEU	N-CA-C	6.60	128.82	111.00
1	A	664	THR	N-CA-CB	-6.57	97.83	110.30
1	C	27	HIS	CB-CA-C	-6.49	97.42	110.40
1	A	187	ASP	N-CA-CB	6.27	121.89	110.60
1	C	374	HIS	CB-CA-C	-6.25	97.91	110.40
1	A	373	LEU	N-CA-CB	-6.24	97.92	110.40
1	A	78	ARG	NE-CZ-NH1	6.17	123.38	120.30
2	D	140	LYS	CB-CA-C	6.16	122.73	110.40
1	C	375	LEU	N-CA-C	-6.16	94.38	111.00
1	A	572	PHE	N-CA-C	-6.13	94.46	111.00
1	C	541	ALA	CB-CA-C	-6.10	100.95	110.10
1	C	459	PRO	N-CA-CB	6.05	110.56	103.30
1	C	571	ILE	CB-CA-C	6.01	123.62	111.60
1	A	186	PRO	N-CA-C	5.99	127.68	112.10
1	C	531	ALA	N-CA-C	5.85	126.79	111.00
1	A	386	SER	CB-CA-C	-5.83	99.02	110.10
1	A	664	THR	N-CA-C	5.68	126.35	111.00
1	C	56	ARG	NE-CZ-NH2	-5.67	117.46	120.30
2	D	134	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	365	GLN	N-CA-C	5.63	126.19	111.00
1	C	78	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	426	ILE	N-CA-C	5.55	125.99	111.00
1	C	427	ARG	N-CA-CB	-5.51	100.67	110.60
1	C	459	PRO	CA-N-CD	-5.47	103.84	111.50
1	A	186	PRO	CB-CA-C	-5.42	98.44	112.00
1	C	531	ALA	CB-CA-C	5.35	118.12	110.10
1	C	431	PHE	CB-CG-CD1	5.32	124.52	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	433	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	177	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	448	LEU	N-CA-CB	5.23	120.87	110.40
2	D	94	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	94	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	375	LEU	CB-CA-C	-5.15	100.42	110.20
1	A	459	PRO	CA-N-CD	-5.12	104.34	111.50
1	A	407	CYS	CB-CA-C	-5.08	100.24	110.40
1	C	447	LEU	N-CA-C	5.07	124.68	111.00
1	C	56	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	C	458	SER	CB-CA-C	5.00	119.60	110.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	PHE	Peptide
1	A	422	THR	Peptide
1	A	447	LEU	Peptide
1	C	364	PHE	Peptide
1	C	460	ILE	Peptide
1	C	94	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	4510	0	4529	144	0
1	C	4478	0	4511	123	0
2	B	609	0	591	18	0
2	D	577	0	569	23	0
All	All	10174	0	10200	303	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 15.

All (303) 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)
2:D:91:MET:C	2:D:92:LYS:HD3	1.24	1.50
2:D:91:MET:O	2:D:92:LYS:HD3	1.28	1.26
1:A:372:TRP:O	1:A:374:HIS:CE1	1.89	1.26
1:C:375:LEU:HD23	1:C:375:LEU:O	1.34	1.25
2:B:92:LYS:O	2:B:93:ILE:HG13	1.35	1.22
2:D:93:ILE:CG2	2:D:94:ASP:H	1.54	1.18
1:C:447:LEU:CD1	1:C:448:LEU:HD22	1.75	1.14
1:C:380:VAL:HG13	1:C:405:ARG:HG3	1.20	1.14
2:D:91:MET:O	2:D:92:LYS:CD	1.97	1.13
2:D:93:ILE:HG22	2:D:94:ASP:N	1.58	1.13
1:A:634:ASP:O	1:A:635:LYS:HG2	1.49	1.12
2:D:93:ILE:HG22	2:D:94:ASP:H	0.98	1.12
2:D:91:MET:C	2:D:92:LYS:CD	2.19	1.11
1:A:405:ARG:O	1:A:405:ARG:HG2	1.38	1.10
1:C:447:LEU:HD11	1:C:448:LEU:HD22	1.32	1.10
1:A:367:LEU:HD23	1:A:375:LEU:HD12	1.13	1.09
1:A:341:GLU:N	1:A:341:GLU:OE1	1.87	1.07
1:A:367:LEU:HD23	1:A:375:LEU:CD1	1.85	1.07
1:A:437:LEU:O	1:A:460:ILE:HD13	1.56	1.06
1:C:380:VAL:CG1	1:C:405:ARG:CD	2.34	1.04
1:A:365:GLN:HA	1:A:389:MET:HE3	1.32	1.04
1:A:371:SER:C	1:A:372:TRP:CE3	2.30	1.04
1:A:405:ARG:O	1:A:405:ARG:CG	2.02	1.04
1:C:380:VAL:HG12	1:C:405:ARG:HD2	1.40	1.01
1:C:362:GLY:O	1:C:387:LEU:O	1.81	0.99
1:C:375:LEU:O	1:C:375:LEU:CD2	2.09	0.99
1:A:372:TRP:O	1:A:374:HIS:ND1	1.97	0.97
1:A:571:ILE:HD12	1:A:572:PHE:O	1.64	0.96
1:A:340:LEU:HB3	1:A:341:GLU:OE1	1.65	0.95
1:A:389:MET:HE2	1:A:389:MET:HA	1.47	0.95
1:C:380:VAL:HG12	1:C:405:ARG:CD	1.96	0.95
1:C:380:VAL:HG13	1:C:405:ARG:CG	1.98	0.94
1:C:380:VAL:CG1	1:C:405:ARG:CG	2.45	0.94
1:C:380:VAL:CG1	1:C:405:ARG:HG3	1.97	0.93
1:A:367:LEU:CD2	1:A:375:LEU:HD12	1.99	0.92
1:A:365:GLN:HA	1:A:389:MET:CE	2.00	0.91
1:C:380:VAL:HG11	1:C:405:ARG:NE	1.86	0.90
1:C:389:MET:HG2	1:C:392:CYS:HB2	1.53	0.90
1:A:367:LEU:CD2	1:A:375:LEU:CD1	2.51	0.89
2:B:92:LYS:O	2:B:93:ILE:CG1	2.22	0.86
1:C:372:TRP:O	1:C:374:HIS:CE1	2.30	0.84
1:A:396:THR:O	1:A:400:LEU:HD12	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:MET:HE2	1:A:389:MET:CA	2.03	0.84
2:B:93:ILE:HG21	2:B:97:THR:HG22	1.60	0.83
1:A:371:SER:HB3	1:A:372:TRP:CZ3	2.12	0.83
1:A:396:THR:O	1:A:400:LEU:CD1	2.27	0.82
1:C:447:LEU:HD12	1:C:448:LEU:HD22	1.62	0.82
1:A:634:ASP:O	1:A:635:LYS:CG	2.28	0.82
1:C:347:GLU:HG2	1:C:374:HIS:O	1.79	0.82
1:A:371:SER:HB3	1:A:372:TRP:CE3	2.15	0.81
1:C:642:LEU:HD21	1:C:661:ILE:HD12	1.63	0.80
1:C:380:VAL:CG1	1:C:405:ARG:NE	2.45	0.78
1:A:365:GLN:HE21	1:A:389:MET:CE	1.97	0.77
1:A:400:LEU:HD12	1:A:400:LEU:N	2.00	0.76
1:C:29:LEU:O	1:C:38:ARG:NH2	2.19	0.76
1:C:378:VAL:O	1:C:403:ILE:HG22	1.86	0.74
1:C:424:ALA:HB2	1:C:447:LEU:HB2	1.70	0.74
1:C:445:CYS:SG	1:C:461:ARG:NH2	2.61	0.74
1:A:371:SER:C	1:A:372:TRP:HE3	1.91	0.74
2:B:93:ILE:HG21	2:B:97:THR:CG2	2.17	0.74
1:A:365:GLN:NE2	1:A:389:MET:HE2	2.03	0.74
2:B:92:LYS:C	2:B:93:ILE:HG13	2.08	0.74
1:A:163:THR:O	1:A:167:GLN:HG3	1.88	0.73
1:C:311:ALA:HB1	1:C:312:ALA:HA	1.71	0.73
1:A:437:LEU:O	1:A:460:ILE:CD1	2.35	0.73
1:C:394:ASP:HB3	1:C:422:THR:HG21	1.70	0.73
1:C:447:LEU:HD11	1:C:448:LEU:CD2	2.14	0.73
1:A:365:GLN:NE2	1:A:389:MET:CE	2.52	0.72
1:A:661:ILE:HG22	1:A:663:GLY:O	1.89	0.72
1:A:371:SER:CB	1:A:372:TRP:CE3	2.73	0.72
1:C:392:CYS:HB3	1:C:415:ILE:HG23	1.71	0.71
2:D:93:ILE:CG2	2:D:94:ASP:N	2.24	0.70
1:A:365:GLN:CA	1:A:389:MET:HE3	2.16	0.70
1:C:393:GLN:O	1:C:396:THR:OG1	2.07	0.70
1:C:375:LEU:O	1:C:375:LEU:CG	2.38	0.69
1:A:338:ASN:ND2	1:A:365:GLN:OE1	2.26	0.69
2:D:92:LYS:O	2:D:93:ILE:HG13	1.94	0.68
1:A:397:ASP:HA	1:A:400:LEU:HD13	1.76	0.68
2:D:91:MET:CA	2:D:92:LYS:HD3	2.22	0.68
1:C:447:LEU:HD12	1:C:448:LEU:N	2.09	0.68
1:C:427:ARG:H	1:C:428:ARG:NH1	1.92	0.67
1:A:372:TRP:O	1:A:374:HIS:HE1	1.75	0.67
1:C:447:LEU:HD12	1:C:447:LEU:C	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:SER:HB2	1:A:533:GLN:HG3	1.77	0.66
1:A:371:SER:CB	1:A:372:TRP:HE3	2.07	0.66
1:C:661:ILE:HG22	1:C:663:GLY:O	1.96	0.66
2:D:92:LYS:HD3	2:D:92:LYS:N	2.03	0.66
1:C:375:LEU:HD23	1:C:375:LEU:C	2.13	0.65
1:A:405:ARG:O	1:A:405:ARG:CD	2.45	0.65
1:A:382:GLY:HA2	1:A:406:GLY:O	1.97	0.64
1:A:398:ALA:HB2	1:A:422:THR:HG21	1.78	0.64
1:C:387:LEU:HG	1:C:413:PHE:HB3	1.79	0.64
1:A:371:SER:CA	1:A:372:TRP:CE3	2.80	0.64
1:A:287:SER:O	1:C:78:ARG:NH2	2.31	0.64
1:C:380:VAL:CG1	1:C:405:ARG:HD2	2.08	0.64
1:C:444:HIS:HA	1:C:461:ARG:CZ	2.28	0.64
1:C:270:PRO:HG3	1:C:311:ALA:HB3	1.80	0.64
2:B:93:ILE:HG22	2:B:94:ASP:N	2.14	0.63
1:C:389:MET:CG	1:C:392:CYS:HB2	2.26	0.62
1:C:380:VAL:HG12	1:C:405:ARG:CG	2.23	0.62
1:A:159:LEU:HD22	1:A:194:LEU:HD21	1.80	0.62
2:D:91:MET:O	2:D:92:LYS:HD2	1.93	0.62
1:A:71:LEU:O	1:A:138:ARG:NH1	2.33	0.62
1:C:359:LEU:HD11	1:C:361:LEU:HD11	1.81	0.62
1:C:368:CYS:H	1:C:389:MET:HE1	1.65	0.62
1:C:428:ARG:HB2	1:C:431:PHE:CE1	2.35	0.62
1:A:365:GLN:HE21	1:A:389:MET:HE1	1.65	0.61
2:D:92:LYS:C	2:D:93:ILE:HG13	2.20	0.61
1:C:374:HIS:ND1	1:C:374:HIS:N	2.49	0.60
2:D:91:MET:CE	2:D:98:LEU:HD11	2.32	0.60
1:A:340:LEU:CB	1:A:341:GLU:OE1	2.47	0.60
1:C:387:LEU:C	1:C:387:LEU:HD23	2.22	0.60
2:D:91:MET:HE1	2:D:98:LEU:HD21	1.82	0.60
1:A:344:PRO:HA	1:A:347:GLU:OE1	2.02	0.59
2:B:93:ILE:CG2	2:B:97:THR:CG2	2.80	0.59
1:A:574:LEU:HD22	1:A:614:TYR:O	2.01	0.59
2:D:91:MET:HE1	2:D:98:LEU:HD11	1.84	0.59
1:C:387:LEU:HD23	1:C:388:TYR:HB3	1.85	0.58
1:A:530:SER:HB2	1:A:533:GLN:HE21	1.68	0.58
1:A:371:SER:HB3	1:A:372:TRP:HZ3	1.65	0.58
1:A:400:LEU:HD12	1:A:400:LEU:H	1.67	0.58
1:C:387:LEU:HG	1:C:413:PHE:CB	2.34	0.58
1:A:376:ASP:HB3	1:A:402:ALA:HB3	1.86	0.58
2:B:93:ILE:CG2	2:B:97:THR:HB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:HG	1:A:456:ALA:HB3	1.86	0.57
1:A:371:SER:O	1:A:372:TRP:CE3	2.57	0.57
1:A:431:PHE:CE2	1:A:450:THR:HG21	2.40	0.57
1:C:427:ARG:H	1:C:428:ARG:HH11	1.53	0.57
1:A:155:ASP:OD1	1:A:157:THR:OG1	2.20	0.57
2:D:93:ILE:HG23	2:D:94:ASP:H	1.61	0.57
1:A:457:LEU:HB3	1:A:525:LEU:HD12	1.87	0.57
1:C:662:HIS:HA	1:C:685:ARG:O	2.04	0.56
1:A:589:ASP:HA	1:A:630:TRP:HB2	1.87	0.56
1:A:431:PHE:CE1	1:A:434:ARG:CZ	2.88	0.56
1:A:372:TRP:CE3	1:A:372:TRP:N	2.72	0.56
1:A:315:VAL:O	1:A:319:VAL:HG23	2.05	0.56
1:A:322:PHE:CZ	1:A:349:LEU:HD12	2.41	0.56
1:C:369:LYS:O	1:C:374:HIS:CE1	2.60	0.55
1:A:361:LEU:HD13	1:A:367:LEU:HD21	1.88	0.55
1:C:642:LEU:CD2	1:C:661:ILE:HD12	2.35	0.55
1:A:365:GLN:C	1:A:389:MET:HE3	2.28	0.55
1:A:182:PRO:O	1:A:185:LEU:HD12	2.07	0.54
1:C:449:HIS:O	1:C:452:GLU:OE2	2.25	0.54
2:B:93:ILE:CG2	2:B:94:ASP:N	2.71	0.54
1:C:403:ILE:O	1:C:407:CYS:HB2	2.08	0.54
2:B:93:ILE:HG22	2:B:97:THR:HB	1.90	0.54
1:A:266:CYS:HB2	1:A:268:PHE:CE1	2.43	0.53
1:A:629:TYR:HB3	1:A:661:ILE:HD13	1.89	0.53
1:C:444:HIS:ND1	1:C:461:ARG:NH1	2.57	0.53
1:C:704:GLU:N	1:C:707:LEU:HD12	2.22	0.53
1:A:70:PHE:HB2	2:B:157:TRP:CH2	2.44	0.53
1:C:447:LEU:CD1	1:C:447:LEU:C	2.78	0.53
1:C:629:TYR:HB3	1:C:661:ILE:HD13	1.91	0.53
1:A:634:ASP:O	1:A:634:ASP:OD1	2.26	0.52
1:C:535:LEU:HD12	1:C:572:PHE:CE2	2.45	0.52
1:C:294:LEU:HD11	1:C:296:LEU:HD21	1.91	0.52
1:A:365:GLN:O	1:A:389:MET:HE1	2.10	0.52
1:A:413:PHE:HA	1:A:437:LEU:HB2	1.92	0.52
1:C:38:ARG:NH1	1:C:52:GLU:OE1	2.38	0.51
1:A:389:MET:CE	1:A:389:MET:CA	2.85	0.51
1:C:159:LEU:O	1:C:163:THR:HG23	2.11	0.51
1:C:155:ASP:OD2	1:C:157:THR:OG1	2.29	0.51
1:C:434:ARG:HG2	1:C:454:LEU:HD11	1.92	0.51
1:A:389:MET:HG3	1:A:392:CYS:HB2	1.92	0.51
1:A:403:ILE:HG22	1:A:403:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:PRO:O	1:A:460:ILE:HG22	2.11	0.50
1:A:365:GLN:CA	1:A:389:MET:CE	2.82	0.50
1:A:400:LEU:CD1	1:A:400:LEU:N	2.72	0.50
1:C:62:ARG:NH2	1:C:714:ASN:OD1	2.44	0.50
1:A:59:LEU:HD21	2:B:158:ALA:HB2	1.94	0.50
1:A:422:THR:HG23	1:A:425:GLY:HA3	1.94	0.50
1:A:618:ILE:HD12	1:A:653:CYS:SG	2.51	0.49
2:D:92:LYS:O	2:D:93:ILE:CG1	2.59	0.49
1:C:387:LEU:HD23	1:C:388:TYR:CB	2.42	0.49
1:A:409:ARG:HD3	1:A:433:LEU:HD22	1.95	0.49
1:A:361:LEU:HD22	1:A:364:PHE:CD2	2.48	0.49
1:C:21:PRO:HG2	1:C:24:LEU:HD12	1.94	0.49
1:C:457:LEU:HB3	1:C:525:LEU:HD12	1.94	0.49
1:A:664:THR:HA	1:A:684:LEU:HD22	1.95	0.48
1:C:589:ASP:HA	1:C:630:TRP:HB2	1.95	0.48
1:A:396:THR:O	1:A:400:LEU:HD11	2.13	0.48
1:C:451:ALA:O	1:C:452:GLU:C	2.48	0.48
1:C:269:ASN:HD22	1:C:272:PHE:HE2	1.60	0.48
1:A:294:LEU:HD11	1:A:296:LEU:HD21	1.96	0.48
1:A:405:ARG:O	1:A:405:ARG:HD2	2.14	0.48
1:C:642:LEU:HB2	1:C:665:THR:HG23	1.95	0.48
1:A:372:TRP:HE3	1:A:372:TRP:N	2.09	0.48
1:A:381:CYS:O	1:A:406:GLY:C	2.51	0.48
1:A:431:PHE:CD2	1:A:450:THR:HG21	2.48	0.48
1:A:405:ARG:HD2	1:A:405:ARG:C	2.33	0.48
1:A:431:PHE:CD1	1:A:431:PHE:C	2.85	0.48
1:C:552:ILE:HG22	1:C:583:LEU:HD11	1.96	0.48
1:C:211:CYS:O	1:C:237:LEU:HD13	2.14	0.47
1:C:311:ALA:HB1	1:C:312:ALA:CA	2.40	0.47
1:A:367:LEU:HD22	1:A:375:LEU:CD1	2.41	0.47
1:A:577:LEU:HB2	1:A:621:LEU:HD21	1.96	0.47
1:C:584:ALA:HA	1:C:623:THR:O	2.15	0.47
1:C:447:LEU:HD12	1:C:448:LEU:CA	2.45	0.47
1:C:642:LEU:HD21	1:C:661:ILE:CD1	2.40	0.47
1:A:38:ARG:HD3	1:A:56:ARG:HG3	1.97	0.47
1:A:42:ALA:HB2	1:A:52:GLU:HG2	1.96	0.47
1:A:172:ARG:HG3	1:A:203:GLU:HB2	1.95	0.47
1:A:408:ARG:HA	1:A:431:PHE:HA	1.97	0.47
1:A:538:LEU:HD11	1:A:543:LEU:HD12	1.97	0.47
1:C:389:MET:HG2	1:C:389:MET:O	2.15	0.47
1:A:389:MET:SD	1:A:389:MET:C	2.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ILE:H	1:A:427:ARG:HH21	1.63	0.47
2:B:91:MET:CE	2:B:98:LEU:HD13	2.44	0.47
1:A:293:VAL:HG13	1:A:330:ASP:HB3	1.97	0.46
1:A:365:GLN:HE22	1:A:389:MET:HA	1.79	0.46
1:C:375:LEU:CD2	1:C:375:LEU:C	2.80	0.46
1:A:680:ARG:O	1:A:713:LEU:HD21	2.15	0.46
1:C:70:PHE:HB2	2:D:157:TRP:CH2	2.51	0.46
1:C:388:TYR:CG	1:C:388:TYR:O	2.69	0.46
1:A:459:PRO:C	1:A:460:ILE:CG2	2.84	0.46
1:A:422:THR:O	1:A:422:THR:HG22	2.15	0.45
1:C:388:TYR:O	1:C:388:TYR:CD1	2.69	0.45
1:A:365:GLN:O	1:A:389:MET:CE	2.64	0.45
1:C:59:LEU:HD13	1:C:60:SER:N	2.31	0.45
1:C:416:HIS:CG	1:C:440:VAL:HB	2.51	0.45
1:C:519:TRP:NE1	1:C:543:LEU:HD23	2.32	0.45
1:C:535:LEU:HD22	1:C:577:LEU:HD11	1.98	0.45
1:A:535:LEU:HD22	1:A:577:LEU:HD11	1.99	0.45
1:A:618:ILE:CD1	1:A:650:ILE:HA	2.45	0.45
1:A:442:VAL:O	1:A:443:LEU:HD23	2.16	0.45
1:C:266:CYS:HB2	1:C:268:PHE:CE2	2.51	0.45
1:A:371:SER:CB	1:A:372:TRP:CZ3	2.91	0.45
1:A:634:ASP:O	1:A:635:LYS:CB	2.65	0.45
2:D:91:MET:N	2:D:92:LYS:HE3	2.31	0.45
1:A:269:ASN:OD1	1:A:337:HIS:NE2	2.44	0.44
1:A:389:MET:SD	1:A:392:CYS:N	2.90	0.44
1:A:642:LEU:HD23	1:A:665:THR:CG2	2.47	0.44
1:C:535:LEU:HD12	1:C:572:PHE:CZ	2.53	0.44
1:A:365:GLN:HE21	1:A:365:GLN:CA	2.29	0.44
1:C:34:ASP:C	1:C:34:ASP:OD1	2.55	0.44
1:C:27:HIS:CG	1:C:27:HIS:O	2.70	0.44
1:C:32:LEU:HD12	1:C:32:LEU:O	2.18	0.44
1:C:707:LEU:O	1:C:711:VAL:HG23	2.18	0.44
1:C:444:HIS:HA	1:C:461:ARG:NH2	2.32	0.44
1:C:575:SER:OG	1:C:617:GLY:HA3	2.18	0.44
1:C:420:LEU:HD21	1:C:444:HIS:HD2	1.82	0.44
1:A:707:LEU:O	1:A:711:VAL:HG23	2.17	0.44
1:A:365:GLN:HA	1:A:365:GLN:HE21	1.83	0.43
2:B:139:ILE:HG22	2:B:140:LYS:N	2.33	0.43
1:C:52:GLU:HG3	1:C:53:ARG:HD3	1.99	0.43
1:C:387:LEU:C	1:C:387:LEU:CD2	2.85	0.43
2:B:134:ARG:O	2:B:137:PHE:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:PHE:HB2	1:C:613:PHE:CE2	2.54	0.43
1:C:431:PHE:CD1	1:C:431:PHE:N	2.87	0.43
1:C:59:LEU:HD21	2:D:158:ALA:HB2	2.01	0.43
1:A:457:LEU:HD23	1:A:459:PRO:HG3	2.00	0.43
1:A:59:LEU:HB2	1:A:82:LEU:HD11	2.01	0.43
1:A:439:GLU:OE2	1:A:439:GLU:N	2.52	0.43
1:C:177:ARG:NH1	1:C:210:TYR:O	2.48	0.43
1:C:460:ILE:HG23	1:C:528:TRP:O	2.19	0.43
1:C:559:ASP:N	1:C:559:ASP:OD1	2.51	0.43
1:A:217:VAL:HG21	1:A:248:GLU:HG2	2.01	0.43
1:A:359:LEU:HD11	1:A:361:LEU:HD11	2.00	0.43
1:C:42:ALA:HB2	1:C:52:GLU:HG2	2.01	0.43
1:A:397:ASP:HA	1:A:400:LEU:CD1	2.46	0.42
1:A:653:CYS:O	1:A:676:ILE:HG23	2.19	0.42
1:C:367:LEU:N	1:C:389:MET:HE3	2.34	0.42
1:A:659:LEU:O	1:A:682:MET:HA	2.20	0.42
1:C:373:LEU:HD22	1:C:376:ASP:HB3	2.01	0.42
1:C:394:ASP:OD1	1:C:419:ASP:N	2.53	0.42
1:C:256:CYS:HB3	1:C:259:LEU:HD13	2.02	0.42
1:A:62:ARG:NH2	1:A:714:ASN:OD1	2.53	0.42
1:A:73:LEU:O	1:A:74:SER:C	2.58	0.42
1:C:87:LEU:O	1:C:90:VAL:HB	2.19	0.42
1:C:388:TYR:H	1:C:414:GLY:H	1.68	0.42
1:A:394:ASP:OD2	1:A:419:ASP:OD1	2.38	0.42
1:A:535:LEU:O	1:A:535:LEU:HD23	2.19	0.42
1:C:375:LEU:O	1:C:375:LEU:HG	2.19	0.42
1:A:340:LEU:C	1:A:341:GLU:OE1	2.54	0.42
1:A:642:LEU:O	1:A:665:THR:HG22	2.20	0.42
1:C:285:ALA:HB1	1:C:324:ALA:HB3	2.01	0.42
1:C:367:LEU:N	1:C:389:MET:CE	2.83	0.42
1:C:384:LEU:O	1:C:410:LEU:HA	2.19	0.42
1:A:181:ARG:HH21	1:A:185:LEU:HB2	1.84	0.41
1:A:342:ALA:O	1:A:343:ALA:C	2.59	0.41
2:D:102:ILE:HD11	2:D:121:VAL:HG21	2.03	0.41
1:C:269:ASN:HA	1:C:337:HIS:CD2	2.55	0.41
1:C:409:ARG:HH11	1:C:433:LEU:HD13	1.84	0.41
2:D:92:LYS:CD	2:D:92:LYS:N	2.72	0.41
1:A:182:PRO:HB2	1:A:185:LEU:CD1	2.51	0.41
1:A:67:SER:O	1:A:71:LEU:HD12	2.20	0.41
1:A:423:SER:HB2	1:A:447:LEU:HD23	2.03	0.41
1:C:315:VAL:O	1:C:319:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:O	1:A:38:ARG:NH2	2.54	0.41
1:A:332:THR:HG23	1:A:360:THR:HB	2.03	0.41
1:A:368:CYS:HB3	1:A:396:THR:HG22	2.03	0.41
1:A:419:ASP:OD1	1:A:419:ASP:C	2.58	0.41
2:B:144:THR:HG22	2:B:147:GLU:CD	2.41	0.41
1:C:416:HIS:CG	1:C:416:HIS:O	2.73	0.41
1:A:397:ASP:CA	1:A:400:LEU:HD13	2.47	0.41
1:C:73:LEU:O	1:C:74:SER:C	2.60	0.41
1:C:270:PRO:CG	1:C:311:ALA:HB3	2.50	0.41
2:B:93:ILE:CG2	2:B:97:THR:CB	2.99	0.40
1:A:365:GLN:C	1:A:389:MET:CE	2.89	0.40
1:A:365:GLN:NE2	1:A:389:MET:HA	2.37	0.40
1:C:59:LEU:HD11	1:C:61:LEU:HD12	2.03	0.40
2:B:140:LYS:O	2:B:140:LYS:CG	2.70	0.40
1:C:431:PHE:N	1:C:431:PHE:HD1	2.19	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	564/740 (76%)	497 (88%)	66 (12%)	1 (0%)	47	81
1	C	559/740 (76%)	496 (89%)	62 (11%)	1 (0%)	47	81
2	B	72/169 (43%)	67 (93%)	4 (6%)	1 (1%)	11	41
2	D	68/169 (40%)	63 (93%)	4 (6%)	1 (2%)	10	40
All	All	1263/1818 (70%)	1123 (89%)	136 (11%)	4 (0%)	41	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	PRO
1	C	459	PRO
2	D	93	ILE
2	B	93	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	488/615 (79%)	438 (90%)	50 (10%)	7 27
1	C	485/615 (79%)	448 (92%)	37 (8%)	13 41
2	B	67/146 (46%)	62 (92%)	5 (8%)	13 42
2	D	64/146 (44%)	59 (92%)	5 (8%)	12 40
All	All	1104/1522 (72%)	1007 (91%)	97 (9%)	10 34

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	26	LEU
1	A	33	THR
1	A	34	ASP
1	A	52	GLU
1	A	53	ARG
1	A	75	HIS
1	A	82	LEU
1	A	90	VAL
1	A	97	LEU
1	A	129	SER
1	A	131	GLN
1	A	138	ARG
1	A	142	CYS
1	A	151	VAL
1	A	155	ASP
1	A	180	GLN
1	A	190	ASP

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Mol	Chain	Res	Type
1	A	196	GLU
1	A	237	LEU
1	A	273	SER
1	A	275	CYS
1	A	333	MET
1	A	335	LEU
1	A	367	LEU
1	A	368	CYS
1	A	374	HIS
1	A	384	LEU
1	A	387	LEU
1	A	389	MET
1	A	392	CYS
1	A	407	CYS
1	A	412	LYS
1	A	431	PHE
1	A	437	LEU
1	A	441	THR
1	A	444	HIS
1	A	445	CYS
1	A	446	ARG
1	A	447	LEU
1	A	452	GLU
1	A	458	SER
1	A	524	SER
1	A	534	LEU
1	A	536	SER
1	A	559	ASP
1	A	575	SER
1	A	618	ILE
1	A	633	GLN
1	A	682	MET
2	B	92	LYS
2	B	101	LEU
2	B	140	LYS
2	B	146	GLU
2	B	152	ARG
1	C	32	LEU
1	C	52	GLU
1	C	64	ASP
1	C	82	LEU
1	C	90	VAL

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Mol	Chain	Res	Type
1	C	101	VAL
1	C	151	VAL
1	C	177	ARG
1	C	180	GLN
1	C	214	GLU
1	C	275	CYS
1	C	284	LEU
1	C	310	GLU
1	C	328	LEU
1	C	335	LEU
1	C	368	CYS
1	C	374	HIS
1	C	375	LEU
1	C	380	VAL
1	C	381	CYS
1	C	384	LEU
1	C	387	LEU
1	C	407	CYS
1	C	410	LEU
1	C	418	CYS
1	C	419	ASP
1	C	423	SER
1	C	431	PHE
1	C	439	GLU
1	C	445	CYS
1	C	449	HIS
1	C	452	GLU
1	C	530	SER
1	C	545	SER
1	C	628	ASP
1	C	704	GLU
1	C	718	ILE
2	D	92	LYS
2	D	98	LEU
2	D	111	LYS
2	D	140	LYS
2	D	146	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	ASN

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Mol	Chain	Res	Type
1	A	365	GLN
1	A	374	HIS
1	A	533	GLN
1	C	75	HIS
2	D	109	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	580/740 (78%)	0.07	3 (0%)	91	75	29, 58, 97, 128	0
1	C	575/740 (77%)	0.08	6 (1%)	82	58	30, 57, 94, 129	0
2	B	74/169 (43%)	0.17	4 (5%)	25	9	34, 74, 97, 115	0
2	D	70/169 (41%)	0.23	3 (4%)	35	13	38, 78, 99, 107	0
All	All	1299/1818 (71%)	0.09	16 (1%)	79	53	29, 59, 97, 129	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ASP	4.6
2	B	142	ASP	4.1
2	D	101	LEU	3.7
2	B	97	THR	3.5
2	D	94	ASP	3.5
1	C	393	GLN	3.1
1	C	663	GLY	2.5
2	B	101	LEU	2.5
1	C	635	LYS	2.5
2	D	97	THR	2.4
1	A	663	GLY	2.4
2	B	94	ASP	2.3
1	C	520	GLU	2.2
1	C	434	ARG	2.2
1	C	249	LEU	2.1
1	A	671	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.