Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:23 PM GMT

PDB ID	:	5CUF
Title	:	X-ray crystal structure of SeMet human Sestrin2
Authors	:	Kim, H.; An, S.; Ro, S.-H.; Lee, J.H.; Cho, U.-S.
Deposited on	:	2015-07-24
Resolution	:	3.50 Å(reported)

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

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

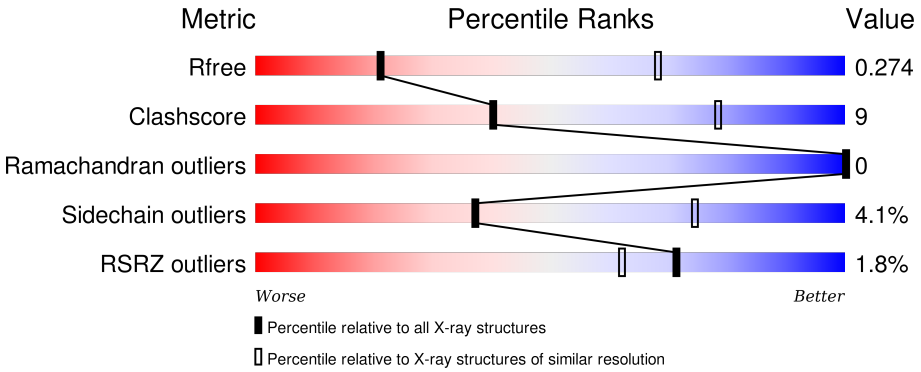
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	483	59% 14% 24%
1	B	483	63% 11% 24%
1	C	483	62% 13% 23%
1	D	483	64% 11% 23%
1	E	483	65% 11% 24%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15032 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 Sestrin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	Se	0	0	0
			3001	1920	521	543	6	11			
1	B	368	Total	C	N	O	S	Se	0	0	0
			3001	1920	521	543	6	11			
1	C	370	Total	C	N	O	S	Se	0	0	0
			3012	1926	523	546	6	11			
1	D	370	Total	C	N	O	S	Se	0	0	0
			3012	1926	523	546	6	11			
1	E	369	Total	C	N	O	S	Se	0	0	0
			3006	1923	522	544	6	11			

There are 15 discrepancies between the modelled and reference sequences:

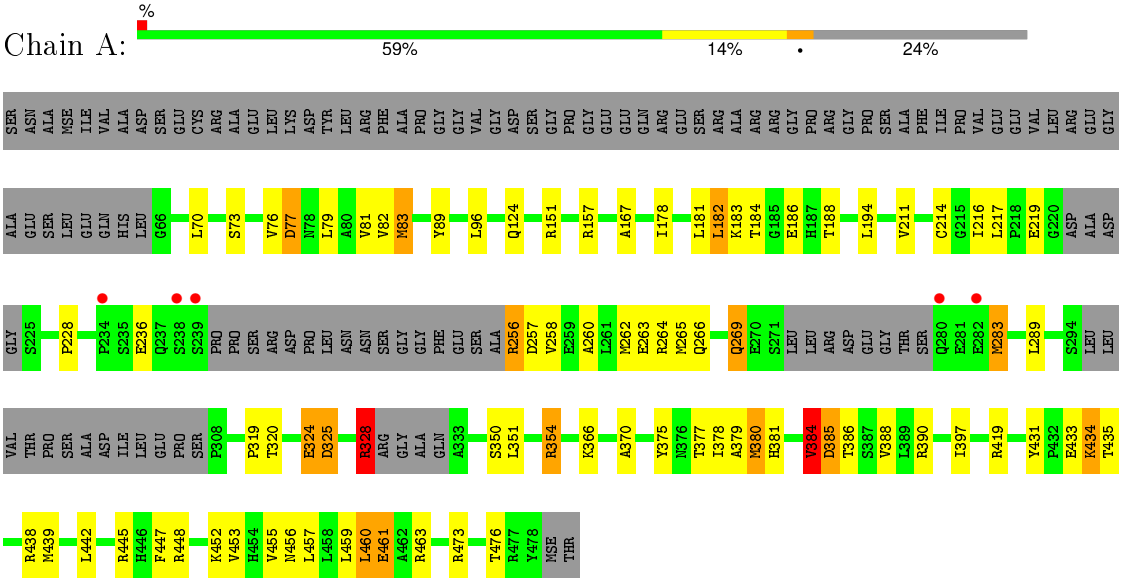
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P58004
A	-1	ASN	-	expression tag	UNP P58004
A	0	ALA	-	expression tag	UNP P58004
B	-2	SER	-	expression tag	UNP P58004
B	-1	ASN	-	expression tag	UNP P58004
B	0	ALA	-	expression tag	UNP P58004
C	-2	SER	-	expression tag	UNP P58004
C	-1	ASN	-	expression tag	UNP P58004
C	0	ALA	-	expression tag	UNP P58004
D	-2	SER	-	expression tag	UNP P58004
D	-1	ASN	-	expression tag	UNP P58004
D	0	ALA	-	expression tag	UNP P58004
E	-2	SER	-	expression tag	UNP P58004
E	-1	ASN	-	expression tag	UNP P58004
E	0	ALA	-	expression tag	UNP P58004

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.

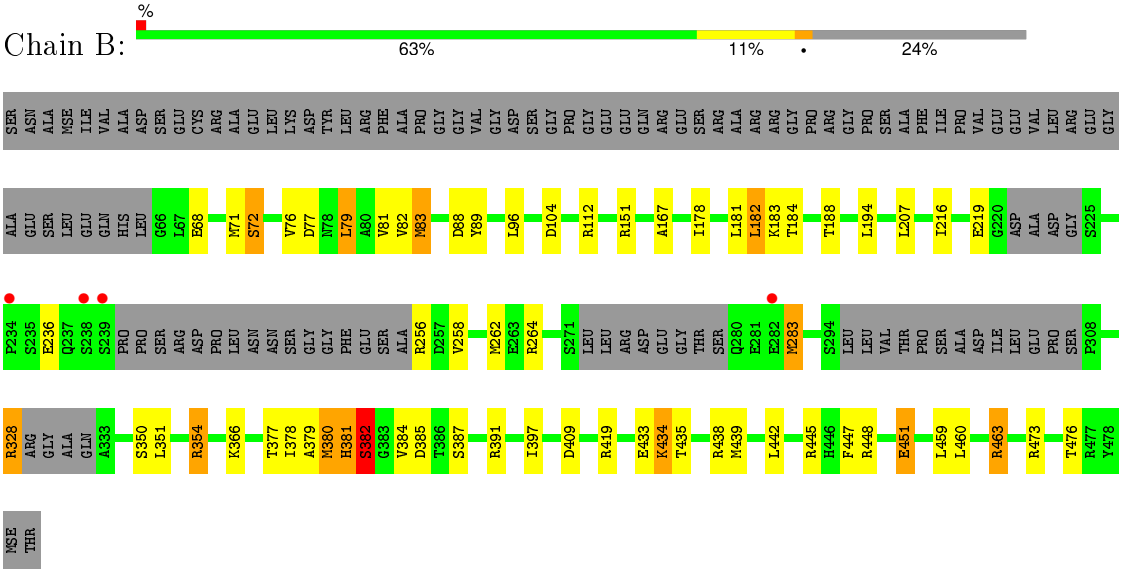
- Molecule 1: Sestrin-2

Chain A:



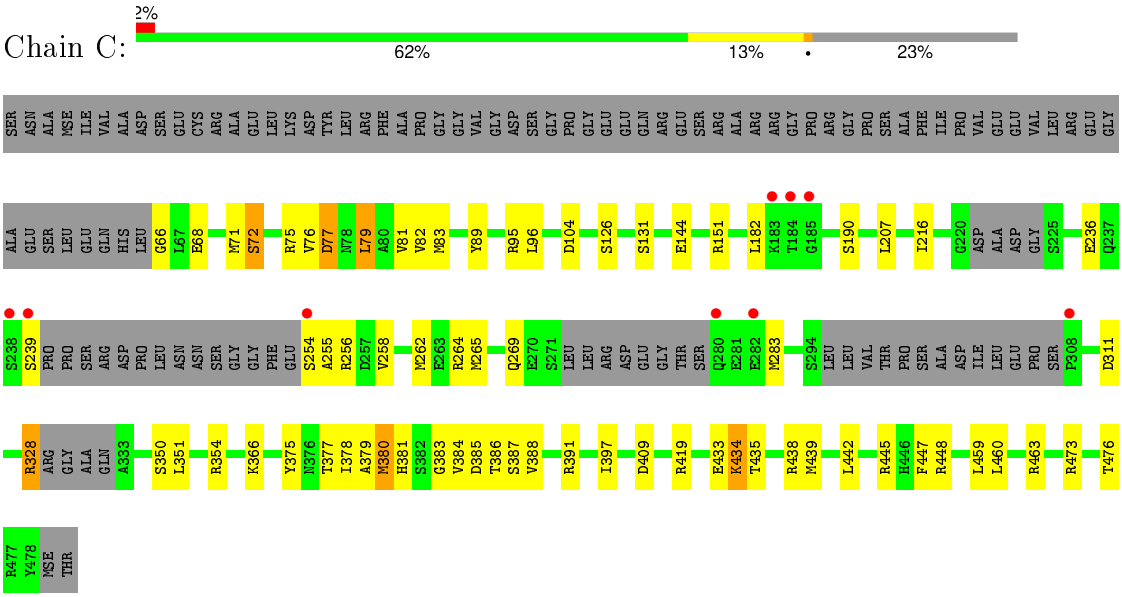
- Molecule 1: Sestrin-2

Chain B:



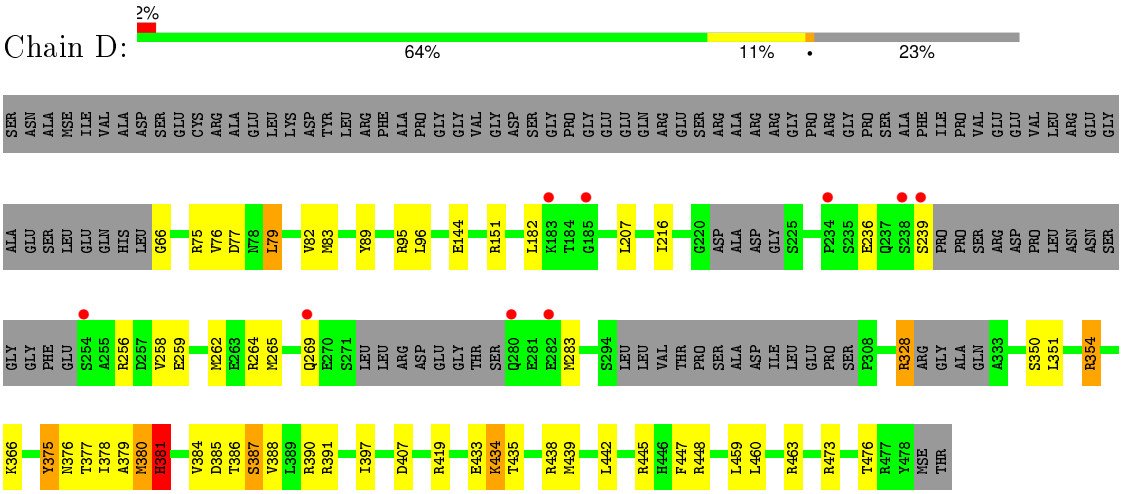
- Molecule 1: Sestrin-2

Chain C:



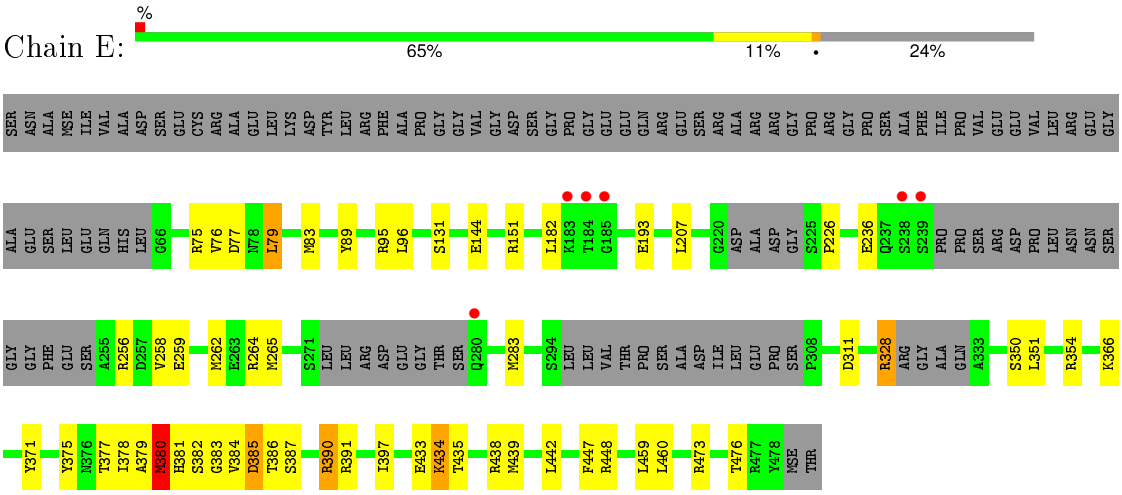
- Molecule 1: Sestrin-2

Chain D:



- Molecule 1: Sestrin-2

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	292.68Å 292.68Å 292.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.12 – 3.50 44.12 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.12-3.50) 100.0 (44.12-3.50)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.235 , 0.272 0.240 , 0.274	Depositor DCC
R_{free} test set	2592 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	94.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.5	EDS
Estimated twinning fraction	0.007 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 52390 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15032	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.25% 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	1.07	5/3070 (0.2%)	1.05	18/4141 (0.4%)
1	B	0.99	4/3070 (0.1%)	0.98	15/4141 (0.4%)
1	C	0.95	3/3081 (0.1%)	0.93	10/4156 (0.2%)
1	D	0.96	1/3081 (0.0%)	0.94	12/4156 (0.3%)
1	E	0.96	4/3075 (0.1%)	0.95	9/4148 (0.2%)
All	All	0.99	17/15377 (0.1%)	0.97	64/20742 (0.3%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	GLU	CD-OE1	7.41	1.33	1.25
1	A	324	GLU	CD-OE2	7.17	1.33	1.25
1	B	387	SER	CB-OG	-6.46	1.33	1.42
1	D	259	GLU	CD-OE2	-6.27	1.18	1.25
1	B	219	GLU	CD-OE1	-6.26	1.18	1.25
1	B	382	SER	CB-OG	-5.82	1.34	1.42
1	E	259	GLU	CD-OE2	-5.81	1.19	1.25
1	B	451	GLU	CD-OE1	-5.77	1.19	1.25
1	A	186	GLU	CG-CD	-5.58	1.43	1.51
1	E	193	GLU	CD-OE2	-5.56	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	383	GLY	N-CA	5.53	1.54	1.46
1	E	131	SER	CB-OG	-5.47	1.35	1.42
1	C	126	SER	CB-OG	-5.42	1.35	1.42
1	C	190	SER	CB-OG	-5.22	1.35	1.42
1	C	383	GLY	N-CA	5.21	1.53	1.46
1	A	325	ASP	CB-CG	5.18	1.62	1.51
1	A	219	GLU	CD-OE1	-5.09	1.20	1.25

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	390	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	A	385	ASP	CB-CG-OD1	9.88	127.19	118.30
1	E	390	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	A	325	ASP	CB-CG-OD2	9.04	126.44	118.30
1	A	77	ASP	CB-CG-OD2	-8.64	110.53	118.30
1	D	448	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	E	473	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	B	391	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	D	473	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	C	448	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	D	381	HIS	N-CA-C	-7.50	90.74	111.00
1	A	354	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	448	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	C	473	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	354	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	151	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	E	448	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	256	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	390	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	E	385	ASP	CB-CG-OD2	6.53	124.17	118.30
1	E	151	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	E	328	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	473	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	448	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	463	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	E	380	MSE	CG-SE-CE	6.11	112.35	98.90
1	B	409	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	409	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	473	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	83	MSE	CG-SE-CE	-5.98	85.75	98.90
1	A	151	ARG	NE-CZ-NH1	5.86	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	445	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	445	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	328	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	83	MSE	CA-CB-CG	-5.79	103.46	113.30
1	A	445	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	384	VAL	CB-CA-C	-5.68	100.61	111.40
1	D	445	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	328	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	463	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	391	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	384	VAL	N-CA-C	5.52	125.91	111.00
1	C	239	SER	N-CA-C	-5.52	96.09	111.00
1	D	239	SER	N-CA-C	-5.49	96.17	111.00
1	A	384	VAL	N-CA-C	5.48	125.80	111.00
1	A	328	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	381	HIS	N-CA-C	-5.43	96.33	111.00
1	D	463	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	328	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	391	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	88	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	157	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	283	MSE	CG-SE-CE	5.18	110.29	98.90
1	B	283	MSE	CG-SE-CE	5.17	110.27	98.90
1	E	391	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	D	407	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	324	GLU	OE1-CD-OE2	5.10	129.42	123.30
1	B	112	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	375	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	C	77	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	D	354	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	151	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	D	151	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	324	GLU	CG-CD-OE2	-5.00	108.29	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	GLU	Peptide
1	B	236	GLU	Peptide
1	C	236	GLU	Peptide
1	D	236	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	E	236	GLU	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	3001	0	2917	81	0
1	B	3001	0	2917	54	0
1	C	3012	0	2927	60	0
1	D	3012	0	2927	42	0
1	E	3006	0	2922	38	0
All	All	15032	0	14610	259	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 9.

All (259) 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:E:262:MSE:HE1	1:E:381:HIS:CE1	1.36	1.58
1:C:254:SER:HB3	1:C:380:MSE:CE	1.51	1.41
1:C:378:ILE:HD11	1:C:386:THR:CG2	1.60	1.31
1:E:262:MSE:HE1	1:E:381:HIS:ND1	1.49	1.24
1:E:262:MSE:CE	1:E:381:HIS:CE1	2.27	1.17
1:C:380:MSE:O	1:C:380:MSE:HG2	1.45	1.15
1:A:378:ILE:HD11	1:A:386:THR:HG21	1.17	1.15
1:D:380:MSE:O	1:D:380:MSE:HG2	1.33	1.14
1:A:378:ILE:HD11	1:A:386:THR:CG2	1.81	1.10
1:E:380:MSE:HG2	1:E:380:MSE:O	1.49	1.08
1:C:378:ILE:CG1	1:C:384:VAL:HG21	1.83	1.08
1:A:380:MSE:O	1:A:380:MSE:HG2	1.48	1.08
1:B:380:MSE:HE2	1:B:381:HIS:CD2	1.89	1.08
1:A:89:TYR:OH	1:A:461:GLU:OE1	1.71	1.07
1:C:378:ILE:HD11	1:C:386:THR:HG21	1.13	1.07
1:B:178:ILE:O	1:B:182:LEU:HD13	1.54	1.07
1:B:262:MSE:HE1	1:B:381:HIS:CD2	1.91	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ILE:HG12	1:A:384:VAL:HG21	1.31	1.06
1:C:254:SER:CB	1:C:380:MSE:HE3	1.87	1.02
1:C:378:ILE:HG12	1:C:384:VAL:CG2	1.88	1.02
1:C:83:MSE:HE1	1:C:89:TYR:CE2	1.97	1.00
1:C:254:SER:CB	1:C:380:MSE:CE	2.40	0.98
1:C:378:ILE:CD1	1:C:386:THR:HG21	1.92	0.98
1:C:378:ILE:HG12	1:C:384:VAL:HG21	0.98	0.98
1:B:83:MSE:CE	1:B:89:TYR:HE2	1.78	0.97
1:E:262:MSE:CE	1:E:381:HIS:ND1	2.26	0.96
1:B:83:MSE:CE	1:B:89:TYR:CE2	2.50	0.95
1:C:378:ILE:HD11	1:C:386:THR:HG22	1.49	0.93
1:A:262:MSE:HE1	1:A:381:HIS:ND1	1.83	0.92
1:B:184:THR:O	1:B:188:THR:HG21	1.71	0.90
1:C:83:MSE:HE1	1:C:89:TYR:HE2	1.36	0.90
1:C:254:SER:HB3	1:C:380:MSE:HE3	0.91	0.89
1:A:378:ILE:CD1	1:A:386:THR:HG21	2.02	0.89
1:B:184:THR:O	1:B:188:THR:CG2	2.21	0.88
1:A:380:MSE:O	1:A:380:MSE:CG	2.21	0.88
1:A:378:ILE:HG12	1:A:384:VAL:CG2	2.07	0.85
1:B:380:MSE:CE	1:B:381:HIS:CD2	2.59	0.85
1:A:182:LEU:HD23	1:B:354:ARG:HD3	1.59	0.84
1:A:319:PRO:O	1:A:320:THR:OG1	1.92	0.84
1:A:378:ILE:CG1	1:A:384:VAL:HG21	2.07	0.84
1:D:385:ASP:OD1	1:D:387:SER:OG	1.94	0.84
1:A:70:LEU:O	1:A:73:SER:OG	1.94	0.83
1:A:354:ARG:HD3	1:B:182:LEU:HD23	1.59	0.82
1:B:83:MSE:HE2	1:B:89:TYR:CE2	2.14	0.81
1:B:181:LEU:C	1:B:182:LEU:HD12	2.04	0.78
1:A:181:LEU:C	1:A:182:LEU:HD12	2.04	0.78
1:E:380:MSE:CG	1:E:380:MSE:O	2.29	0.78
1:A:178:ILE:O	1:A:182:LEU:HD13	1.85	0.76
1:D:380:MSE:CG	1:D:380:MSE:O	2.21	0.76
1:B:377:THR:HG22	1:B:382:SER:HA	1.67	0.75
1:A:262:MSE:HE1	1:A:381:HIS:CG	2.21	0.75
1:D:79:LEU:O	1:D:79:LEU:HD12	1.87	0.74
1:A:83:MSE:CE	1:A:89:TYR:HE2	2.01	0.73
1:C:79:LEU:HD12	1:C:79:LEU:O	1.89	0.73
1:E:79:LEU:HD21	1:E:207:LEU:HD22	1.70	0.72
1:D:77:ASP:OD1	1:E:75:ARG:NH2	2.20	0.72
1:A:214:CYS:SG	1:A:456:ASN:OD1	2.48	0.72
1:B:380:MSE:O	1:B:380:MSE:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:O	1:B:79:LEU:HD12	1.89	0.71
1:E:79:LEU:O	1:E:79:LEU:HD12	1.91	0.71
1:A:377:THR:O	1:A:378:ILE:HD13	1.91	0.70
1:A:79:LEU:HD12	1:A:211:VAL:CG2	2.22	0.70
1:A:79:LEU:HD12	1:A:211:VAL:HG22	1.74	0.70
1:A:83:MSE:CE	1:A:89:TYR:CE2	2.76	0.69
1:A:83:MSE:HE2	1:A:89:TYR:CE2	2.28	0.69
1:C:77:ASP:OD1	1:D:75:ARG:NH2	2.24	0.69
1:B:79:LEU:HD21	1:B:207:LEU:HD22	1.75	0.69
1:C:68:GLU:O	1:C:72:SER:OG	2.11	0.69
1:D:79:LEU:HD21	1:D:207:LEU:HD22	1.75	0.68
1:E:262:MSE:SE	1:E:381:HIS:ND1	2.76	0.68
1:B:379:ALA:HB1	1:B:447:PHE:HA	1.77	0.67
1:C:377:THR:O	1:C:378:ILE:HD13	1.94	0.67
1:C:79:LEU:HD21	1:C:207:LEU:HD22	1.77	0.67
1:B:83:MSE:HE2	1:B:89:TYR:CD2	2.29	0.66
1:B:262:MSE:CE	1:B:381:HIS:CD2	2.75	0.66
1:C:379:ALA:HB1	1:C:447:PHE:HA	1.77	0.66
1:A:460:LEU:HD12	1:A:461:GLU:N	2.10	0.66
1:B:68:GLU:O	1:B:72:SER:OG	2.12	0.66
1:B:380:MSE:HE2	1:B:381:HIS:HD2	1.58	0.65
1:C:83:MSE:HE1	1:C:89:TYR:CD2	2.31	0.65
1:B:380:MSE:CE	1:B:381:HIS:NE2	2.59	0.65
1:B:262:MSE:HE1	1:B:381:HIS:NE2	2.12	0.65
1:E:380:MSE:HE2	1:E:381:HIS:CD2	2.33	0.64
1:B:184:THR:O	1:B:188:THR:HG23	1.97	0.64
1:C:75:ARG:NH2	1:E:77:ASP:OD1	2.25	0.63
1:A:83:MSE:HE2	1:A:89:TYR:CD2	2.34	0.63
1:B:71:MSE:HE3	1:B:81:VAL:O	1.98	0.62
1:A:452:LYS:O	1:A:455:VAL:HG22	1.98	0.62
1:B:83:MSE:HE1	1:B:89:TYR:HE2	1.63	0.62
1:A:378:ILE:HD11	1:A:386:THR:HG22	1.80	0.62
1:D:376:ASN:ND2	1:D:384:VAL:O	2.31	0.61
1:C:254:SER:HB3	1:C:380:MSE:HE2	1.72	0.61
1:D:379:ALA:HB1	1:D:447:PHE:HA	1.82	0.61
1:D:384:VAL:HG22	1:D:385:ASP:N	2.15	0.61
1:C:71:MSE:HE3	1:C:81:VAL:O	2.01	0.60
1:B:182:LEU:N	1:B:182:LEU:HD12	2.16	0.60
1:D:379:ALA:CB	1:D:447:PHE:HA	2.32	0.60
1:A:459:LEU:C	1:A:459:LEU:HD23	2.22	0.60
1:E:379:ALA:HB1	1:E:447:PHE:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:MSE:HE1	1:A:381:HIS:CE1	2.37	0.59
1:A:257:ASP:OD1	1:A:258:VAL:N	2.36	0.58
1:A:167:ALA:O	1:A:463:ARG:NH2	2.34	0.58
1:B:79:LEU:C	1:B:79:LEU:HD12	2.25	0.57
1:C:378:ILE:CD1	1:C:386:THR:CG2	2.55	0.57
1:E:79:LEU:HD12	1:E:79:LEU:C	2.25	0.57
1:C:380:MSE:O	1:C:380:MSE:CG	2.28	0.57
1:A:89:TYR:CE1	1:A:370:ALA:HB2	2.40	0.56
1:B:379:ALA:CB	1:B:447:PHE:HA	2.35	0.56
1:A:460:LEU:HD12	1:A:460:LEU:C	2.25	0.56
1:D:79:LEU:C	1:D:79:LEU:HD12	2.25	0.56
1:C:79:LEU:HD12	1:C:79:LEU:C	2.25	0.56
1:C:379:ALA:CB	1:C:447:PHE:HA	2.36	0.56
1:B:258:VAL:HG12	1:B:262:MSE:HE2	1.88	0.56
1:B:378:ILE:O	1:B:378:ILE:HG22	2.07	0.55
1:D:378:ILE:O	1:D:378:ILE:HG22	2.06	0.55
1:D:378:ILE:HB	1:D:381:HIS:CB	2.37	0.54
1:E:379:ALA:CB	1:E:447:PHE:HA	2.37	0.54
1:A:183:LYS:O	1:A:183:LYS:HG2	2.07	0.54
1:E:258:VAL:HG12	1:E:262:MSE:HE2	1.90	0.54
1:E:378:ILE:HG22	1:E:378:ILE:O	2.08	0.54
1:B:183:LYS:O	1:B:183:LYS:HG2	2.08	0.54
1:A:350:SER:O	1:A:354:ARG:HG3	2.08	0.53
1:D:378:ILE:HB	1:D:381:HIS:HB2	1.91	0.53
1:A:262:MSE:CE	1:A:381:HIS:ND1	2.65	0.53
1:C:254:SER:CB	1:C:380:MSE:HE2	2.34	0.53
1:C:265:MSE:HE1	1:C:386:THR:HA	1.91	0.52
1:A:269:GLN:NE2	1:A:388:VAL:CG2	2.72	0.52
1:C:269:GLN:HE21	1:C:388:VAL:CG2	2.22	0.52
1:C:255:ALA:N	1:C:380:MSE:HE1	2.24	0.52
1:D:258:VAL:HG12	1:D:262:MSE:HE2	1.92	0.52
1:A:182:LEU:HD12	1:A:182:LEU:N	2.24	0.52
1:C:255:ALA:H	1:C:380:MSE:HE1	1.73	0.51
1:B:350:SER:O	1:B:354:ARG:HG3	2.09	0.51
1:D:144:GLU:HG2	1:E:95:ARG:HH22	1.76	0.51
1:B:377:THR:HB	1:B:381:HIS:O	2.11	0.51
1:A:89:TYR:CZ	1:A:461:GLU:OE1	2.61	0.51
1:A:76:VAL:HG22	1:A:77:ASP:N	2.25	0.51
1:A:262:MSE:O	1:A:266:GLN:HG2	2.09	0.51
1:A:257:ASP:O	1:A:260:ALA:HB3	2.10	0.51
1:C:144:GLU:HG2	1:D:95:ARG:NH2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:HG12	1:C:262:MSE:HE2	1.93	0.51
1:A:459:LEU:HD23	1:A:460:LEU:N	2.26	0.51
1:C:144:GLU:HG2	1:D:95:ARG:HH22	1.74	0.51
1:C:311:ASP:OD2	1:D:66:GLY:O	2.29	0.50
1:A:269:GLN:NE2	1:A:388:VAL:HG21	2.27	0.50
1:A:378:ILE:HG22	1:A:378:ILE:O	2.10	0.50
1:A:354:ARG:CD	1:B:182:LEU:HD23	2.36	0.50
1:E:375:TYR:O	1:E:377:THR:HG23	2.12	0.50
1:C:262:MSE:HE1	1:C:381:HIS:CD2	2.46	0.50
1:A:375:TYR:O	1:A:377:THR:HG23	2.11	0.50
1:E:371:TYR:O	1:E:390:ARG:NH1	2.44	0.50
1:B:380:MSE:HE3	1:B:381:HIS:NE2	2.26	0.50
1:C:254:SER:N	1:C:380:MSE:HE2	2.27	0.49
1:B:83:MSE:CE	1:B:89:TYR:CD2	2.90	0.49
1:D:269:GLN:HE21	1:D:388:VAL:CG2	2.25	0.49
1:C:351:LEU:HD22	1:C:476:THR:HG23	1.94	0.49
1:D:83:MSE:HE3	1:D:89:TYR:CE2	2.48	0.49
1:A:435:THR:HG23	1:A:439:MSE:HE2	1.93	0.49
1:D:435:THR:HG23	1:D:439:MSE:HE2	1.94	0.49
1:C:435:THR:HG23	1:C:439:MSE:HE2	1.94	0.49
1:C:76:VAL:HG22	1:C:77:ASP:N	2.27	0.49
1:E:433:GLU:O	1:E:434:LYS:HG2	2.13	0.49
1:A:263:GLU:HA	1:A:266:GLN:HG3	1.95	0.49
1:A:460:LEU:HD11	1:A:461:GLU:OE1	2.12	0.49
1:D:76:VAL:HG22	1:D:77:ASP:N	2.27	0.48
1:B:182:LEU:N	1:B:182:LEU:CD1	2.76	0.48
1:B:433:GLU:O	1:B:434:LYS:HG2	2.13	0.48
1:B:435:THR:HG23	1:B:439:MSE:HE2	1.94	0.48
1:A:265:MSE:CE	1:A:386:THR:HA	2.44	0.48
1:E:351:LEU:HD22	1:E:476:THR:HG23	1.96	0.48
1:A:265:MSE:HE1	1:A:386:THR:HA	1.95	0.47
1:D:375:TYR:O	1:D:377:THR:HG23	2.15	0.47
1:E:438:ARG:O	1:E:442:LEU:HB2	2.14	0.47
1:D:144:GLU:HG2	1:E:95:ARG:NH2	2.30	0.47
1:E:96:LEU:HD22	1:E:366:LYS:HE2	1.96	0.47
1:B:178:ILE:O	1:B:182:LEU:CD1	2.44	0.47
1:B:181:LEU:HB2	1:B:182:LEU:HD12	1.96	0.47
1:C:82:VAL:HG21	1:C:216:ILE:CD1	2.43	0.47
1:B:351:LEU:HD22	1:B:476:THR:HG23	1.97	0.47
1:A:182:LEU:HD11	1:A:194:LEU:HD22	1.97	0.47
1:A:433:GLU:O	1:A:434:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:CD1	1:A:182:LEU:N	2.78	0.47
1:A:265:MSE:O	1:A:269:GLN:HG2	2.15	0.47
1:E:435:THR:HG23	1:E:439:MSE:HE2	1.96	0.47
1:B:76:VAL:HG22	1:B:77:ASP:N	2.31	0.46
1:C:433:GLU:O	1:C:434:LYS:HG2	2.14	0.46
1:C:378:ILE:O	1:C:378:ILE:HG22	2.14	0.46
1:D:433:GLU:O	1:D:434:LYS:HG2	2.15	0.46
1:A:438:ARG:O	1:A:442:LEU:HB2	2.16	0.46
1:C:66:GLY:O	1:E:311:ASP:OD2	2.33	0.46
1:A:96:LEU:HD22	1:A:366:LYS:HE2	1.96	0.46
1:A:351:LEU:HD22	1:A:476:THR:HG23	1.97	0.46
1:D:351:LEU:HD22	1:D:476:THR:HG23	1.97	0.46
1:A:324:GLU:HB2	1:A:431:TYR:OH	2.16	0.46
1:A:82:VAL:HG21	1:A:216:ILE:CD1	2.45	0.46
1:A:181:LEU:HB2	1:A:182:LEU:HD12	1.97	0.46
1:A:182:LEU:HD23	1:B:354:ARG:CD	2.37	0.46
1:D:96:LEU:HD22	1:D:366:LYS:HE2	1.97	0.46
1:C:96:LEU:HD22	1:C:366:LYS:HE2	1.97	0.46
1:B:379:ALA:HB2	1:B:451:GLU:OE1	2.16	0.46
1:A:263:GLU:O	1:A:266:GLN:HB2	2.15	0.46
1:A:83:MSE:HE1	1:A:89:TYR:HE2	1.76	0.46
1:B:77:ASP:O	1:B:81:VAL:HG23	2.16	0.45
1:E:378:ILE:HD11	1:E:386:THR:HG22	1.96	0.45
1:C:438:ARG:O	1:C:442:LEU:HB2	2.16	0.45
1:D:384:VAL:CG2	1:D:385:ASP:N	2.78	0.45
1:A:77:ASP:O	1:A:81:VAL:HG23	2.16	0.45
1:B:83:MSE:HE3	1:B:89:TYR:CE2	2.47	0.45
1:C:83:MSE:CE	1:C:89:TYR:CD2	3.00	0.45
1:A:181:LEU:CB	1:A:182:LEU:HD12	2.47	0.45
1:D:387:SER:HA	1:D:390:ARG:NH2	2.32	0.45
1:E:83:MSE:HE3	1:E:89:TYR:CE2	2.51	0.45
1:C:265:MSE:CE	1:C:386:THR:HA	2.46	0.45
1:C:77:ASP:O	1:C:81:VAL:HG23	2.16	0.45
1:D:83:MSE:CE	1:D:89:TYR:CE2	3.00	0.45
1:D:438:ARG:O	1:D:442:LEU:HB2	2.17	0.44
1:D:82:VAL:HG21	1:D:216:ILE:CD1	2.48	0.44
1:E:265:MSE:HE1	1:E:386:THR:HA	1.99	0.44
1:B:397:ILE:HD13	1:B:459:LEU:HA	1.99	0.44
1:A:325:ASP:OD2	1:A:328:ARG:CB	2.65	0.44
1:B:438:ARG:O	1:B:442:LEU:HB2	2.17	0.44
1:A:380:MSE:HE2	1:A:381:HIS:ND1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:HD22	1:B:366:LYS:HE2	1.99	0.44
1:D:378:ILE:O	1:D:381:HIS:HB2	2.18	0.44
1:B:82:VAL:HG21	1:B:216:ILE:CD1	2.48	0.44
1:A:181:LEU:HB2	1:A:182:LEU:CD1	2.48	0.43
1:A:379:ALA:HB1	1:A:447:PHE:HA	2.00	0.43
1:C:95:ARG:NH2	1:E:144:GLU:HG2	2.33	0.43
1:C:350:SER:O	1:C:354:ARG:HG3	2.19	0.43
1:A:89:TYR:OH	1:A:461:GLU:CD	2.50	0.43
1:C:397:ILE:HD13	1:C:459:LEU:HA	2.01	0.43
1:C:379:ALA:HB2	1:C:447:PHE:CD2	2.54	0.43
1:D:397:ILE:HD13	1:D:459:LEU:HA	2.00	0.42
1:D:378:ILE:HD11	1:D:386:THR:HG22	2.01	0.42
1:E:384:VAL:HG12	1:E:385:ASP:N	2.34	0.42
1:A:453:VAL:O	1:A:457:LEU:HG	2.20	0.42
1:A:184:THR:N	1:A:188:THR:HG21	2.35	0.42
1:A:325:ASP:OD2	1:A:328:ARG:HB2	2.20	0.42
1:D:350:SER:O	1:D:354:ARG:HG3	2.20	0.42
1:D:265:MSE:HE1	1:D:386:THR:HA	2.00	0.42
1:C:375:TYR:O	1:C:377:THR:HG23	2.19	0.41
1:C:269:GLN:CG	1:C:388:VAL:HG21	2.49	0.41
1:D:83:MSE:HE3	1:D:89:TYR:HE2	1.86	0.41
1:A:379:ALA:CB	1:A:447:PHE:HA	2.50	0.41
1:B:181:LEU:HD13	1:B:194:LEU:HD13	2.01	0.41
1:A:289:LEU:HD22	1:D:376:ASN:ND2	2.36	0.41
1:C:131:SER:HA	1:D:75:ARG:HD2	2.03	0.41
1:E:350:SER:O	1:E:354:ARG:HG3	2.20	0.41
1:C:262:MSE:HE1	1:C:381:HIS:CG	2.55	0.41
1:A:397:ILE:HD13	1:A:459:LEU:HA	2.02	0.41
1:E:83:MSE:CE	1:E:89:TYR:CE2	3.03	0.41
1:C:254:SER:CA	1:C:380:MSE:CE	2.97	0.41
1:E:397:ILE:HD13	1:E:459:LEU:HA	2.03	0.41
1:A:217:LEU:HG	1:A:228:PRO:HD3	2.03	0.41
1:B:167:ALA:O	1:B:463:ARG:NH2	2.52	0.41
1:E:76:VAL:HG22	1:E:77:ASP:N	2.36	0.40
1:E:380:MSE:CE	1:E:381:HIS:CD2	3.02	0.40
1:E:378:ILE:HD11	1:E:386:THR:CG2	2.51	0.40
1:A:319:PRO:C	1:A:320:THR:HG1	2.02	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	356/483 (74%)	337 (95%)	19 (5%)	0	100	100
1	B	356/483 (74%)	335 (94%)	21 (6%)	0	100	100
1	C	358/483 (74%)	337 (94%)	21 (6%)	0	100	100
1	D	358/483 (74%)	337 (94%)	21 (6%)	0	100	100
1	E	357/483 (74%)	334 (94%)	23 (6%)	0	100	100
All	All	1785/2415 (74%)	1680 (94%)	105 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	321/399 (80%)	307 (96%)	14 (4%)	35	73
1	B	321/399 (80%)	307 (96%)	14 (4%)	35	73
1	C	322/399 (81%)	308 (96%)	14 (4%)	35	74
1	D	322/399 (81%)	310 (96%)	12 (4%)	41	76
1	E	321/399 (80%)	309 (96%)	12 (4%)	41	76
All	All	1607/1995 (81%)	1541 (96%)	66 (4%)	37	74

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	182	LEU
1	A	256	ARG
1	A	264	ARG
1	A	269	GLN
1	A	283	MSE
1	A	328	ARG
1	A	380	MSE
1	A	384	VAL
1	A	385	ASP
1	A	419	ARG
1	A	434	LYS
1	A	460	LEU
1	A	461	GLU
1	B	72	SER
1	B	79	LEU
1	B	104	ASP
1	B	182	LEU
1	B	256	ARG
1	B	264	ARG
1	B	283	MSE
1	B	328	ARG
1	B	380	MSE
1	B	382	SER
1	B	385	ASP
1	B	419	ARG
1	B	434	LYS
1	B	460	LEU
1	C	72	SER
1	C	79	LEU
1	C	104	ASP
1	C	182	LEU
1	C	256	ARG
1	C	264	ARG
1	C	283	MSE
1	C	328	ARG
1	C	380	MSE
1	C	385	ASP
1	C	387	SER
1	C	419	ARG
1	C	434	LYS
1	C	460	LEU
1	D	79	LEU

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Mol	Chain	Res	Type
1	D	182	LEU
1	D	256	ARG
1	D	264	ARG
1	D	283	MSE
1	D	328	ARG
1	D	380	MSE
1	D	381	HIS
1	D	387	SER
1	D	419	ARG
1	D	434	LYS
1	D	460	LEU
1	E	79	LEU
1	E	182	LEU
1	E	226	PRO
1	E	256	ARG
1	E	264	ARG
1	E	283	MSE
1	E	328	ARG
1	E	380	MSE
1	E	382	SER
1	E	387	SER
1	E	434	LYS
1	E	460	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	B	381	HIS
1	C	269	GLN
1	D	269	GLN

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

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	357/483 (73%)	-0.06	5 (1%)	78	68	78, 98, 126, 183	0
1	B	357/483 (73%)	-0.00	4 (1%)	82	73	74, 97, 126, 177	0
1	C	359/483 (74%)	0.09	9 (2%)	61	50	85, 108, 130, 178	0
1	D	359/483 (74%)	0.06	9 (2%)	61	50	83, 106, 129, 199	0
1	E	358/483 (74%)	0.07	6 (1%)	73	64	86, 107, 128, 202	0
All	All	1790/2415 (74%)	0.03	33 (1%)	71	62	74, 104, 128, 202	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	239	SER	4.9
1	E	238	SER	4.6
1	D	254	SER	4.2
1	D	185	GLY	4.0
1	D	238	SER	3.8
1	B	239	SER	3.8
1	A	239	SER	3.8
1	E	185	GLY	3.5
1	C	239	SER	3.5
1	C	185	GLY	3.3
1	C	238	SER	3.3
1	B	238	SER	3.3
1	A	282	GLU	3.2
1	D	239	SER	3.1
1	C	183	LYS	3.0
1	D	183	LYS	2.9
1	B	234	PRO	2.7
1	D	269	GLN	2.7
1	C	282	GLU	2.6
1	A	238	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	183	LYS	2.6
1	A	234	PRO	2.5
1	E	280	GLN	2.5
1	C	280	GLN	2.5
1	C	308	PRO	2.4
1	D	280	GLN	2.3
1	C	184	THR	2.3
1	A	280	GLN	2.2
1	D	234	PRO	2.2
1	B	282	GLU	2.1
1	E	184	THR	2.1
1	C	254	SER	2.1
1	D	282	GLU	2.1

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.