Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:39 PM GMT

PDB ID	:	1GN4
Title	:	H145E MUTANT OF MYCOBACTERIUM TUBERCULOSIS IRON-SUPEROXIDE DISMUTASE.
Authors	:	Bunting, K.A.; Cooper, J.B.; Badasso, M.O.; Tickle, I.J.; Newton, M.; Wood, S.P.; Zhang, Y.; Young, D.B.
Deposited on	:	2001-10-02
Resolution	:	2.50 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:

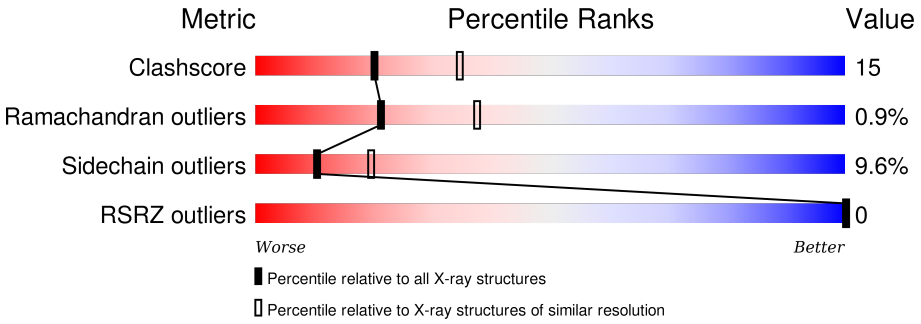
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	207	40% 43% 12%
1	B	207	32% 52% 9%
1	C	207	38% 41% 16%
1	D	207	40% 43% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6560 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 SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1567	1011	267	288	1			
1	B	198	Total	C	N	O	S	0	0	0
			1567	1011	267	288	1			
1	C	198	Total	C	N	O	S	0	0	0
			1567	1011	267	288	1			
1	D	198	Total	C	N	O	S	0	0	0
			1567	1011	267	288	1			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is water.

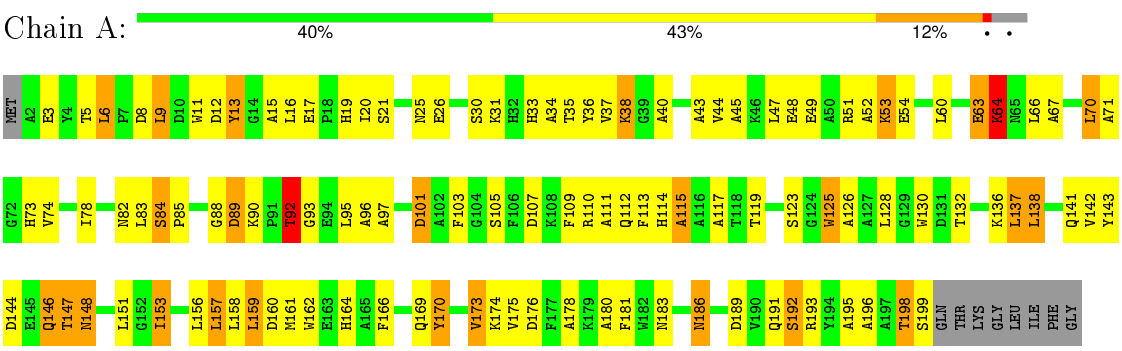
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		
3	B	81	Total	O	0	0
			81	81		
3	C	69	Total	O	0	0
			69	69		
3	D	68	Total	O	0	0
			68	68		

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.

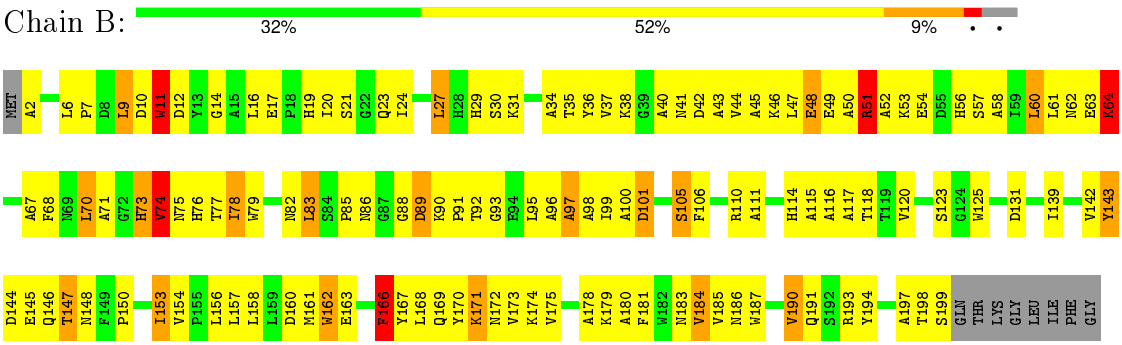
- Molecule 1: SUPEROXIDE DISMUTASE

Chain A:



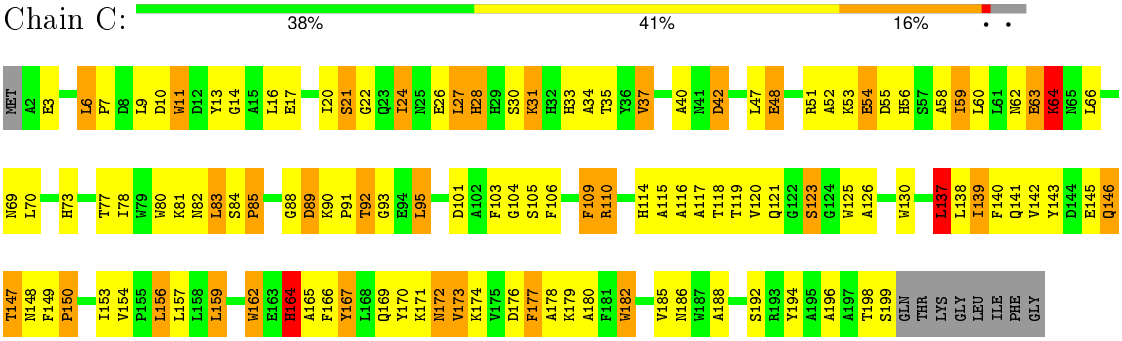
- Molecule 1: SUPEROXIDE DISMUTASE

Chain B:



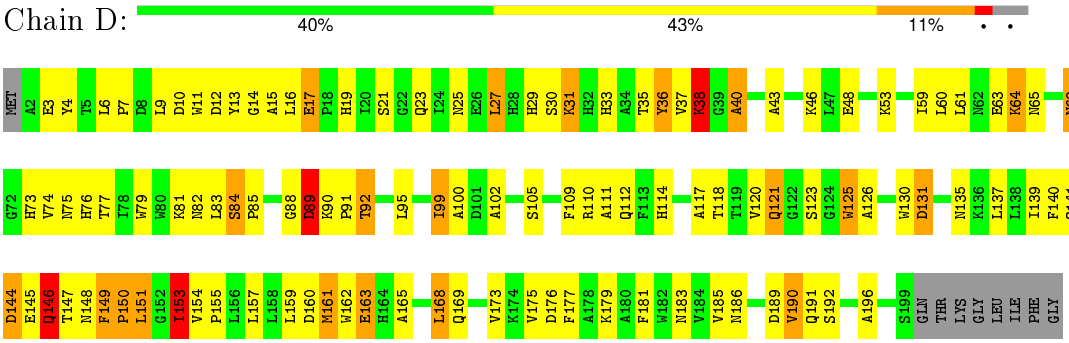
- Molecule 1: SUPEROXIDE DISMUTASE

Chain C:



- Molecule 1: SUPEROXIDE DISMUTASE

Chain D:


40%
43%
11%
MET A2 E3 Y4 T5 L6 P7 D8 L9 D10 W11 D12 Y13 G14 A15 L16 E17 P18 H19 I20 S21 G22 Q23 I24 N25 E26 L27 H28 H29 S30 K31 H32 H33 A34 T35 Y36 V37 K38 G39 A40 A43 K46 L47 E48 K53 I59 L60 L61 N62 E63 K64 N65 N69 L70 A71
G72 H73 V74 N75 H76 T77 I78 W79 W80 K81 N82 L83 S84 P85 G88 D89 K90 P91 T92 L95 I99 A100 D101 A102 S105 F109 R110 A111 Q112 F113 H114 A117 T118 T119 V120 Q121 G122 S123 G124 W125 A126 W130 D131 N135 K136 L137 L138 I139 F140 Q141 V142 Y143
D144 E145 Q146 T147 N148 F149 P150 L151 G152 I153 Y154 P155 L156 L157 L158 L159 D160 M161 W162 E163 H164 A165 L168 Q169 V173 K174 V175 D176 F177 A178 K179 A180 F181 W182 N183 V184 V185 N186 D189 V190 Q191 S192 A196 S199 GLN THR LYS GLY LEU ILE PHE GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.66Å 102.86Å 73.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 12.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-2.50) 95.0 (12.54-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.50Å)	Xtriage
Refinement program	CCP4	Depositor
R, R_{free}	0.172 , 0.225 0.153 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 86.5	EDS
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 27288 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6560	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.75	44/1615 (2.7%)	2.24	87/2203 (3.9%)
1	B	1.76	53/1615 (3.3%)	2.24	95/2203 (4.3%)
1	C	1.75	50/1615 (3.1%)	2.25	98/2203 (4.4%)
1	D	1.62	39/1615 (2.4%)	2.19	84/2203 (3.8%)
All	All	1.72	186/6460 (2.9%)	2.23	364/8812 (4.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	0
1	D	1	0
All	All	3	0

All (186) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	117	ALA	CA-CB	10.24	1.74	1.52
1	C	177	PHE	N-CA	10.22	1.66	1.46
1	A	175	VAL	N-CA	9.98	1.66	1.46
1	C	150	PRO	CA-CB	9.91	1.73	1.53
1	A	114	HIS	N-CA	9.87	1.66	1.46
1	A	30	SER	CA-CB	9.82	1.67	1.52
1	C	55	ASP	N-CA	9.46	1.65	1.46
1	D	141	GLN	N-CA	9.09	1.64	1.46
1	B	76	HIS	N-CA	8.87	1.64	1.46
1	C	172	ASN	N-CA	8.63	1.63	1.46
1	C	40	ALA	N-CA	8.55	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	ALA	N-CA	8.28	1.62	1.46
1	B	63	GLU	N-CA	8.20	1.62	1.46
1	B	47	LEU	N-CA	8.15	1.62	1.46
1	B	46	LYS	N-CA	7.96	1.62	1.46
1	A	157	LEU	N-CA	7.78	1.61	1.46
1	C	83	LEU	N-CA	7.78	1.61	1.46
1	D	121	GLN	N-CA	7.74	1.61	1.46
1	B	67	ALA	N-CA	7.68	1.61	1.46
1	D	169	GLN	N-CA	7.68	1.61	1.46
1	B	46	LYS	CA-CB	7.66	1.70	1.53
1	A	37	VAL	N-CA	7.63	1.61	1.46
1	A	126	ALA	N-CA	7.62	1.61	1.46
1	B	40	ALA	CA-CB	7.54	1.68	1.52
1	C	186	ASN	N-CA	7.50	1.61	1.46
1	C	154	VAL	N-CA	7.43	1.61	1.46
1	B	12	ASP	N-CA	7.42	1.61	1.46
1	B	79	TRP	N-CA	7.39	1.61	1.46
1	B	44	VAL	N-CA	7.37	1.61	1.46
1	C	198	THR	CB-OG1	7.36	1.57	1.43
1	D	61	LEU	N-CA	7.29	1.60	1.46
1	C	194	TYR	N-CA	7.22	1.60	1.46
1	D	83	LEU	N-CA	7.21	1.60	1.46
1	D	177	PHE	N-CA	7.19	1.60	1.46
1	C	70	LEU	N-CA	7.13	1.60	1.46
1	A	63	GLU	N-CA	7.10	1.60	1.46
1	C	165	ALA	N-CA	7.09	1.60	1.46
1	D	111	ALA	N-CA	7.04	1.60	1.46
1	A	192	SER	CA-CB	7.02	1.63	1.52
1	B	40	ALA	N-CA	6.99	1.60	1.46
1	C	157	LEU	N-CA	6.98	1.60	1.46
1	C	21	SER	CA-CB	6.94	1.63	1.52
1	A	105	SER	CA-CB	6.94	1.63	1.52
1	B	68	PHE	N-CA	6.91	1.60	1.46
1	C	101	ASP	CA-CB	6.88	1.69	1.53
1	B	78	ILE	N-CA	6.88	1.60	1.46
1	A	97	ALA	N-CA	6.82	1.59	1.46
1	B	169	GLN	N-CA	6.82	1.59	1.46
1	D	79	TRP	N-CA	6.81	1.59	1.46
1	B	70	LEU	N-CA	6.78	1.59	1.46
1	A	180	ALA	CA-CB	6.76	1.66	1.52
1	B	27	LEU	N-CA	6.74	1.59	1.46
1	A	109	PHE	N-CA	6.68	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	35	THR	N-CA	6.67	1.59	1.46
1	A	92	THR	CA-CB	6.57	1.70	1.53
1	C	114	HIS	N-CA	6.56	1.59	1.46
1	B	41	ASN	N-CA	6.52	1.59	1.46
1	B	145	GLU	N-CA	6.48	1.59	1.46
1	A	38	LYS	N-CA	6.45	1.59	1.46
1	B	50	ALA	N-CA	6.44	1.59	1.46
1	B	74	VAL	N-CA	6.44	1.59	1.46
1	B	142	VAL	N-CA	6.44	1.59	1.46
1	A	193	ARG	N-CA	6.40	1.59	1.46
1	D	35	THR	N-CA	6.38	1.59	1.46
1	A	115	ALA	N-CA	6.37	1.59	1.46
1	C	63	GLU	N-CA	6.35	1.59	1.46
1	C	73	HIS	N-CA	6.35	1.59	1.46
1	C	120	VAL	CA-CB	6.35	1.68	1.54
1	B	38	LYS	N-CA	6.33	1.59	1.46
1	B	178	ALA	CA-CB	6.33	1.65	1.52
1	D	4	TYR	CA-CB	6.31	1.67	1.53
1	A	161	MET	CA-CB	-6.27	1.40	1.53
1	C	180	ALA	N-CA	6.25	1.58	1.46
1	D	131	ASP	CA-CB	6.24	1.67	1.53
1	A	196	ALA	CA-CB	6.24	1.65	1.52
1	D	37	VAL	CA-CB	6.23	1.67	1.54
1	D	46	LYS	N-CA	6.22	1.58	1.46
1	A	195	ALA	N-CA	6.20	1.58	1.46
1	D	36	TYR	N-CA	6.20	1.58	1.46
1	A	35	THR	CB-OG1	6.19	1.55	1.43
1	B	64	LYS	N-CA	6.19	1.58	1.46
1	D	143	TYR	N-CA	6.17	1.58	1.46
1	C	48	GLU	N-CA	6.17	1.58	1.46
1	D	192	SER	CA-CB	6.15	1.62	1.52
1	A	40	ALA	CA-CB	6.12	1.65	1.52
1	A	178	ALA	CA-CB	6.10	1.65	1.52
1	C	149	PHE	N-CA	6.07	1.58	1.46
1	D	159	LEU	N-CA	6.06	1.58	1.46
1	B	162	TRP	N-CA	6.02	1.58	1.46
1	C	126	ALA	N-CA	6.02	1.58	1.46
1	B	115	ALA	N-CA	5.99	1.58	1.46
1	B	190	VAL	N-CA	5.96	1.58	1.46
1	A	52	ALA	CA-CB	5.96	1.65	1.52
1	B	60	LEU	CA-CB	5.93	1.67	1.53
1	C	3	GLU	N-CA	5.91	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	47	LEU	N-CA	5.91	1.58	1.46
1	A	74	VAL	CA-CB	5.89	1.67	1.54
1	C	162	TRP	N-CA	5.89	1.58	1.46
1	A	31	LYS	N-CA	5.88	1.58	1.46
1	A	26	GLU	N-CA	5.87	1.58	1.46
1	D	157	LEU	N-CA	5.87	1.58	1.46
1	A	138	LEU	N-CA	5.83	1.58	1.46
1	D	25	ASN	N-CA	5.82	1.57	1.46
1	B	37	VAL	N-CA	5.81	1.57	1.46
1	C	180	ALA	CA-CB	5.80	1.64	1.52
1	C	138	LEU	N-CA	5.79	1.57	1.46
1	A	109	PHE	CA-CB	5.79	1.66	1.53
1	A	125	TRP	CA-CB	5.76	1.66	1.53
1	D	43	ALA	N-CA	5.75	1.57	1.46
1	D	33	HIS	N-CA	5.74	1.57	1.46
1	B	73	HIS	N-CA	5.74	1.57	1.46
1	B	71	ALA	N-CA	5.71	1.57	1.46
1	B	23	GLN	N-CA	5.68	1.57	1.46
1	D	23	GLN	N-CA	5.67	1.57	1.46
1	C	27	LEU	N-CA	5.67	1.57	1.46
1	A	66	LEU	N-CA	5.66	1.57	1.46
1	B	49	GLU	N-CA	5.65	1.57	1.46
1	A	5	THR	N-CA	5.64	1.57	1.46
1	B	75	ASN	N-CA	5.63	1.57	1.46
1	A	166	PHE	N-CA	5.62	1.57	1.46
1	A	111	ALA	N-CA	5.62	1.57	1.46
1	C	34	ALA	N-CA	5.62	1.57	1.46
1	C	179	LYS	CA-CB	5.60	1.66	1.53
1	C	116	ALA	N-CA	5.59	1.57	1.46
1	A	15	ALA	CA-CB	5.58	1.64	1.52
1	A	186	ASN	N-CA	5.57	1.57	1.46
1	C	140	PHE	CA-CB	5.57	1.66	1.53
1	D	196	ALA	CA-CB	5.55	1.64	1.52
1	A	151	LEU	CA-CB	5.54	1.66	1.53
1	C	142	VAL	CA-CB	5.54	1.66	1.54
1	C	159	LEU	N-CA	5.53	1.57	1.46
1	B	43	ALA	N-CA	5.53	1.57	1.46
1	B	139	ILE	N-CA	5.51	1.57	1.46
1	B	20	ILE	N-CA	5.50	1.57	1.46
1	B	157	LEU	N-CA	5.46	1.57	1.46
1	D	123	SER	CA-CB	5.46	1.61	1.52
1	D	4	TYR	N-CA	5.45	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	26	GLU	N-CA	5.44	1.57	1.46
1	C	109	PHE	N-CA	5.44	1.57	1.46
1	D	63	GLU	N-CA	5.43	1.57	1.46
1	C	58	ALA	N-CA	5.42	1.57	1.46
1	D	73	HIS	N-CA	5.41	1.57	1.46
1	A	3	GLU	CA-CB	5.40	1.65	1.53
1	C	42	ASP	N-CA	5.39	1.57	1.46
1	D	150	PRO	CA-CB	5.38	1.64	1.53
1	A	74	VAL	N-CA	5.37	1.57	1.46
1	C	143	TYR	CA-CB	-5.37	1.42	1.53
1	C	140	PHE	N-CA	5.36	1.57	1.46
1	C	77	THR	CA-CB	5.35	1.67	1.53
1	C	82	ASN	N-CA	5.35	1.57	1.46
1	D	17	GLU	N-CA	5.34	1.57	1.46
1	D	100	ALA	CA-CB	5.33	1.63	1.52
1	C	66	LEU	N-CA	5.31	1.56	1.46
1	C	145	GLU	N-CA	5.31	1.56	1.46
1	A	35	THR	N-CA	5.31	1.56	1.46
1	C	37	VAL	N-CA	5.30	1.56	1.46
1	B	179	LYS	N-CA	5.27	1.56	1.46
1	A	84	SER	CA-CB	5.26	1.60	1.52
1	A	70	LEU	N-CA	5.26	1.56	1.46
1	B	60	LEU	N-CA	5.26	1.56	1.46
1	D	111	ALA	CA-CB	5.26	1.63	1.52
1	B	154	VAL	N-CA	5.26	1.56	1.46
1	B	30	SER	CA-CB	5.25	1.60	1.52
1	B	42	ASP	N-CA	5.24	1.56	1.46
1	C	178	ALA	CA-CB	5.24	1.63	1.52
1	D	114	HIS	N-CA	5.22	1.56	1.46
1	B	34	ALA	N-CA	5.21	1.56	1.46
1	B	153	ILE	N-CA	5.18	1.56	1.46
1	A	73	HIS	N-CA	5.18	1.56	1.46
1	D	30	SER	CA-CB	5.18	1.60	1.52
1	D	145	GLU	N-CA	5.17	1.56	1.46
1	A	107	ASP	CA-CB	-5.16	1.42	1.53
1	A	170	TYR	N-CA	5.16	1.56	1.46
1	B	24	ILE	N-CA	5.12	1.56	1.46
1	C	62	ASN	N-CA	5.11	1.56	1.46
1	D	40	ALA	CA-CB	5.09	1.63	1.52
1	D	126	ALA	CA-CB	-5.09	1.41	1.52
1	C	179	LYS	N-CA	5.06	1.56	1.46
1	B	97	ALA	CA-CB	5.05	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	LEU	N-CA	5.05	1.56	1.46
1	D	162	TRP	CA-CB	-5.04	1.42	1.53
1	D	181	PHE	N-CA	5.04	1.56	1.46
1	B	44	VAL	CA-CB	5.03	1.65	1.54
1	B	166	PHE	N-CA	5.03	1.56	1.46
1	B	62	ASN	N-CA	5.01	1.56	1.46
1	B	58	ALA	N-CA	5.00	1.56	1.46

All (364) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	40	ALA	N-CA-CB	-12.73	92.28	110.10
1	A	92	THR	CA-CB-CG2	-11.59	96.18	112.40
1	C	153	ILE	CA-CB-CG2	10.55	131.99	110.90
1	D	117	ALA	N-CA-CB	-10.32	95.66	110.10
1	B	67	ALA	N-CA-CB	-10.23	95.78	110.10
1	A	105	SER	N-CA-CB	-10.19	95.22	110.50
1	D	145	GLU	CA-CB-CG	10.08	135.57	113.40
1	D	126	ALA	N-CA-CB	10.01	124.11	110.10
1	D	37	VAL	CA-CB-CG1	-9.88	96.08	110.90
1	C	118	THR	CA-CB-CG2	-9.80	98.67	112.40
1	B	190	VAL	CA-CB-CG1	9.56	125.24	110.90
1	A	161	MET	CG-SD-CE	9.36	115.17	100.20
1	C	185	VAL	CA-CB-CG1	-9.30	96.94	110.90
1	B	160	ASP	CB-CG-OD1	9.28	126.66	118.30
1	C	180	ALA	N-CA-CB	-9.27	97.12	110.10
1	B	117	ALA	N-CA-CB	-9.25	97.14	110.10
1	D	121	GLN	N-CA-CB	-9.21	94.02	110.60
1	C	40	ALA	N-CA-CB	-9.18	97.25	110.10
1	A	109	PHE	N-CA-CB	-9.03	94.35	110.60
1	C	186	ASN	N-CA-CB	-8.94	94.50	110.60
1	C	165	ALA	N-CA-CB	-8.86	97.70	110.10
1	A	125	TRP	CB-CA-C	-8.84	92.72	110.40
1	C	137	LEU	CB-CG-CD2	8.48	125.42	111.00
1	C	146	GLN	N-CA-CB	-8.44	95.41	110.60
1	A	114	HIS	N-CA-CB	-8.38	95.51	110.60
1	A	195	ALA	N-CA-CB	-8.37	98.38	110.10
1	A	15	ALA	N-CA-CB	-8.35	98.40	110.10
1	B	178	ALA	N-CA-CB	-8.35	98.40	110.10
1	B	74	VAL	CA-CB-CG1	8.32	123.39	110.90
1	B	61	LEU	CB-CG-CD2	-8.29	96.91	111.00
1	B	46	LYS	N-CA-CB	-8.28	95.70	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	ALA	N-CA-CB	-8.25	98.55	110.10
1	C	142	VAL	CA-CB-CG2	-8.23	98.56	110.90
1	C	92	THR	CA-CB-CG2	-8.22	100.89	112.40
1	B	158	LEU	N-CA-CB	-8.19	94.01	110.40
1	C	77	THR	CA-CB-CG2	-8.18	100.95	112.40
1	B	44	VAL	CA-CB-CG2	-8.15	98.68	110.90
1	D	161	MET	N-CA-CB	8.10	125.19	110.60
1	A	12	ASP	N-CA-CB	-8.10	96.02	110.60
1	D	161	MET	CG-SD-CE	7.99	112.98	100.20
1	C	120	VAL	CA-CB-CG1	-7.98	98.94	110.90
1	B	35	THR	CA-CB-CG2	-7.93	101.30	112.40
1	A	160	ASP	CB-CG-OD1	-7.91	111.18	118.30
1	D	111	ALA	N-CA-CB	-7.85	99.11	110.10
1	D	74	VAL	CA-CB-CG1	-7.81	99.18	110.90
1	C	179	LYS	N-CA-CB	-7.81	96.54	110.60
1	B	44	VAL	N-CA-CB	-7.76	94.42	111.50
1	D	37	VAL	CA-CB-CG2	-7.72	99.33	110.90
1	C	150	PRO	N-CA-CB	-7.64	94.13	103.30
1	A	153	ILE	CA-CB-CG1	-7.63	96.50	111.00
1	D	117	ALA	CB-CA-C	-7.62	98.68	110.10
1	C	149	PHE	CG-CD2-CE2	7.60	129.16	120.80
1	B	131	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	B	169	GLN	N-CA-CB	-7.54	97.02	110.60
1	B	52	ALA	CB-CA-C	-7.50	98.85	110.10
1	C	55	ASP	N-CA-CB	-7.49	97.12	110.60
1	C	62	ASN	N-CA-CB	-7.47	97.15	110.60
1	B	49	GLU	N-CA-CB	-7.46	97.17	110.60
1	D	73	HIS	N-CA-CB	-7.46	97.18	110.60
1	B	173	VAL	CA-CB-CG1	7.41	122.02	110.90
1	C	172	ASN	N-CA-CB	-7.41	97.26	110.60
1	C	125	TRP	CB-CA-C	-7.38	95.65	110.40
1	D	120	VAL	CG1-CB-CG2	-7.37	99.10	110.90
1	A	136	LYS	CB-CA-C	-7.35	95.70	110.40
1	A	159	LEU	CB-CG-CD1	7.31	123.42	111.00
1	B	142	VAL	N-CA-CB	-7.30	95.43	111.50
1	B	44	VAL	CA-CB-CG1	-7.30	99.95	110.90
1	A	92	THR	N-CA-CB	-7.28	96.46	110.30
1	B	125	TRP	CB-CA-C	-7.26	95.88	110.40
1	D	118	THR	CA-CB-CG2	-7.26	102.24	112.40
1	C	185	VAL	CB-CA-C	-7.25	97.62	111.40
1	C	179	LYS	CB-CA-C	-7.24	95.91	110.40
1	C	196	ALA	N-CA-CB	-7.24	99.97	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	ALA	CB-CA-C	-7.21	99.28	110.10
1	D	173	VAL	CG1-CB-CG2	-7.21	99.37	110.90
1	B	193	ARG	NE-CZ-NH1	-7.19	116.71	120.30
1	D	100	ALA	N-CA-CB	-7.19	100.04	110.10
1	B	98	ALA	CB-CA-C	7.18	120.87	110.10
1	A	74	VAL	CB-CA-C	-7.09	97.92	111.40
1	C	109	PHE	N-CA-CB	-7.05	97.90	110.60
1	D	131	ASP	N-CA-CB	-7.04	97.92	110.60
1	C	31	LYS	CD-CE-NZ	-7.04	95.51	111.70
1	A	196	ALA	N-CA-CB	-7.03	100.25	110.10
1	C	150	PRO	CB-CA-C	-7.03	94.42	112.00
1	A	43	ALA	N-CA-CB	-7.02	100.27	110.10
1	A	40	ALA	CB-CA-C	-7.00	99.60	110.10
1	C	52	ALA	N-CA-CB	-6.90	100.44	110.10
1	B	144	ASP	CB-CG-OD2	6.89	124.50	118.30
1	C	141	GLN	CA-CB-CG	-6.87	98.29	113.40
1	B	116	ALA	N-CA-CB	-6.86	100.50	110.10
1	A	198	THR	CA-CB-CG2	-6.84	102.82	112.40
1	B	11	TRP	CB-CA-C	6.77	123.93	110.40
1	D	31	LYS	N-CA-CB	-6.75	98.44	110.60
1	B	97	ALA	N-CA-CB	-6.73	100.68	110.10
1	A	186	ASN	N-CA-CB	-6.72	98.50	110.60
1	B	77	THR	CA-CB-CG2	-6.72	103.00	112.40
1	D	196	ALA	CB-CA-C	-6.71	100.03	110.10
1	C	171	LYS	C-N-CA	-6.70	104.94	121.70
1	A	92	THR	CB-CA-C	-6.68	93.56	111.60
1	B	131	ASP	N-CA-CB	-6.67	98.60	110.60
1	B	36	TYR	N-CA-CB	-6.65	98.62	110.60
1	A	126	ALA	N-CA-C	-6.64	93.07	111.00
1	D	147	THR	CA-CB-CG2	6.64	121.70	112.40
1	A	96	ALA	CB-CA-C	-6.62	100.17	110.10
1	B	125	TRP	CB-CG-CD2	-6.62	117.99	126.60
1	B	50	ALA	N-CA-CB	-6.60	100.86	110.10
1	B	116	ALA	CB-CA-C	-6.58	100.22	110.10
1	A	82	ASN	CB-CA-C	-6.57	97.26	110.40
1	A	119	THR	CA-CB-CG2	-6.56	103.21	112.40
1	B	71	ALA	N-CA-CB	-6.55	100.92	110.10
1	A	192	SER	N-CA-CB	-6.51	100.73	110.50
1	C	66	LEU	N-CA-CB	-6.51	97.38	110.40
1	D	160	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	132	THR	CA-CB-CG2	-6.50	103.30	112.40
1	D	83	LEU	CB-CG-CD1	-6.50	99.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	LYS	CB-CA-C	-6.50	97.41	110.40
1	B	184	VAL	CA-CB-CG1	-6.49	101.17	110.90
1	C	20	ILE	N-CA-C	-6.48	93.49	111.00
1	C	117	ALA	N-CA-CB	-6.47	101.05	110.10
1	D	120	VAL	CA-CB-CG1	-6.45	101.22	110.90
1	B	125	TRP	CB-CG-CD1	6.45	135.38	127.00
1	C	143	TYR	CB-CG-CD1	6.44	124.86	121.00
1	D	169	GLN	N-CA-CB	-6.43	99.02	110.60
1	D	69	ASN	N-CA-CB	-6.42	99.04	110.60
1	B	158	LEU	CB-CA-C	-6.42	98.01	110.20
1	B	186	ASN	CB-CA-C	-6.41	97.58	110.40
1	C	120	VAL	CG1-CB-CG2	-6.40	100.66	110.90
1	C	73	HIS	N-CA-CB	-6.39	99.09	110.60
1	A	143	TYR	CA-CB-CG	6.39	125.55	113.40
1	D	147	THR	N-CA-CB	-6.39	98.15	110.30
1	B	74	VAL	CG1-CB-CG2	6.38	121.11	110.90
1	B	146	GLN	CB-CG-CD	6.38	128.18	111.60
1	A	101	ASP	N-CA-CB	-6.35	99.17	110.60
1	C	177	PHE	N-CA-CB	-6.34	99.18	110.60
1	C	123	SER	N-CA-CB	-6.34	100.99	110.50
1	B	120	VAL	CG1-CB-CG2	-6.33	100.78	110.90
1	C	178	ALA	N-CA-CB	-6.32	101.26	110.10
1	B	180	ALA	CB-CA-C	-6.31	100.63	110.10
1	D	141	GLN	N-CA-C	-6.31	93.97	111.00
1	C	114	HIS	N-CA-CB	-6.30	99.26	110.60
1	A	144	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	C	77	THR	N-CA-CB	-6.27	98.38	110.30
1	C	24	ILE	CA-CB-CG2	-6.26	98.37	110.90
1	A	138	LEU	N-CA-CB	-6.26	97.88	110.40
1	D	65	ASN	N-CA-CB	-6.26	99.33	110.60
1	A	34	ALA	CB-CA-C	-6.26	100.71	110.10
1	B	57	SER	N-CA-CB	6.25	119.88	110.50
1	B	79	TRP	CA-CB-CG	6.24	125.56	113.70
1	C	54	GLU	C-N-CA	-6.24	106.11	121.70
1	B	111	ALA	N-CA-CB	-6.23	101.38	110.10
1	B	10	ASP	CB-CA-C	-6.22	97.95	110.40
1	C	149	PHE	CB-CA-C	6.19	122.78	110.40
1	C	69	ASN	N-CA-CB	-6.17	99.49	110.60
1	C	42	ASP	CB-CA-C	-6.17	98.06	110.40
1	B	51	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	C	194	TYR	N-CA-CB	-6.17	99.50	110.60
1	B	42	ASP	N-CA-CB	-6.16	99.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	168	LEU	N-CA-CB	-6.15	98.10	110.40
1	A	107	ASP	CB-CG-OD1	6.12	123.81	118.30
1	D	162	TRP	CB-CG-CD2	-6.12	118.64	126.60
1	B	185	VAL	CG1-CB-CG2	-6.12	101.11	110.90
1	D	84	SER	O-C-N	6.12	132.73	121.10
1	A	175	VAL	N-CA-CB	-6.11	98.05	111.50
1	A	3	GLU	N-CA-CB	-6.11	99.60	110.60
1	A	44	VAL	N-CA-CB	-6.11	98.07	111.50
1	A	146	GLN	N-CA-C	6.10	127.47	111.00
1	D	146	GLN	CB-CG-CD	6.10	127.45	111.60
1	A	63	GLU	N-CA-CB	-6.09	99.63	110.60
1	B	27	LEU	N-CA-CB	-6.08	98.23	110.40
1	C	176	ASP	C-N-CA	-6.08	106.49	121.70
1	B	168	LEU	C-N-CA	-6.07	106.52	121.70
1	A	130	TRP	N-CA-CB	-6.07	99.68	110.60
1	A	174	LYS	C-N-CA	-6.06	106.56	121.70
1	D	141	GLN	N-CA-CB	-6.05	99.71	110.60
1	D	37	VAL	CB-CA-C	-6.04	99.92	111.40
1	B	58	ALA	N-CA-CB	-6.01	101.68	110.10
1	D	10	ASP	CB-CA-C	-6.01	98.37	110.40
1	A	37	VAL	CG1-CB-CG2	6.00	120.51	110.90
1	D	144	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	46	LYS	CB-CA-C	-6.00	98.40	110.40
1	B	193	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	B	64	LYS	CD-CE-NZ	-5.99	97.92	111.70
1	C	109	PHE	CB-CA-C	-5.99	98.42	110.40
1	B	178	ALA	CB-CA-C	-5.98	101.13	110.10
1	D	12	ASP	CB-CG-OD1	-5.97	112.92	118.30
1	C	92	THR	CB-CA-C	-5.96	95.50	111.60
1	D	92	THR	CA-CB-CG2	5.96	120.75	112.40
1	B	11	TRP	C-N-CA	-5.96	106.79	121.70
1	B	147	THR	N-CA-CB	-5.96	98.98	110.30
1	B	60	LEU	N-CA-CB	-5.95	98.49	110.40
1	D	100	ALA	CB-CA-C	-5.95	101.18	110.10
1	C	110	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	13	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	B	197	ALA	N-CA-CB	-5.92	101.81	110.10
1	A	146	GLN	N-CA-CB	-5.91	99.96	110.60
1	C	143	TYR	CA-CB-CG	5.90	124.61	113.40
1	A	151	LEU	CB-CA-C	-5.85	99.09	110.20
1	C	85	PRO	CB-CA-C	-5.83	97.43	112.00
1	B	23	GLN	N-CA-CB	-5.81	100.14	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	164	HIS	N-CA-CB	-5.81	100.15	110.60
1	B	105	SER	N-CA-CB	-5.80	101.81	110.50
1	C	64	LYS	N-CA-CB	-5.79	100.17	110.60
1	A	83	LEU	CB-CA-C	-5.78	99.23	110.20
1	B	20	ILE	N-CA-C	-5.77	95.41	111.00
1	D	27	LEU	CB-CG-CD1	5.77	120.82	111.00
1	C	157	LEU	CB-CA-C	-5.77	99.23	110.20
1	A	83	LEU	CB-CG-CD2	5.76	120.79	111.00
1	D	30	SER	N-CA-C	5.74	126.49	111.00
1	C	109	PHE	O-C-N	5.72	131.85	122.70
1	D	163	GLU	OE1-CD-OE2	-5.72	116.44	123.30
1	B	9	LEU	CB-CG-CD2	-5.71	101.29	111.00
1	C	126	ALA	N-CA-C	-5.71	95.58	111.00
1	C	140	PHE	CB-CG-CD2	-5.71	116.81	120.80
1	B	163	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	A	125	TRP	CB-CG-CD1	5.70	134.41	127.00
1	C	120	VAL	CA-CB-CG2	-5.70	102.35	110.90
1	A	141	GLN	N-CA-C	-5.70	95.62	111.00
1	B	146	GLN	N-CA-C	5.70	126.38	111.00
1	A	151	LEU	N-CA-CB	-5.69	99.01	110.40
1	A	117	ALA	N-CA-CB	-5.69	102.13	110.10
1	B	48	GLU	CA-CB-CG	5.69	125.92	113.40
1	D	149	PHE	CG-CD2-CE2	-5.69	114.54	120.80
1	D	3	GLU	N-CA-CB	-5.69	100.36	110.60
1	B	70	LEU	CB-CG-CD2	-5.68	101.34	111.00
1	C	119	THR	CA-CB-CG2	-5.68	104.45	112.40
1	C	37	VAL	CB-CA-C	-5.67	100.63	111.40
1	C	130	TRP	N-CA-CB	-5.67	100.40	110.60
1	B	78	ILE	N-CA-CB	-5.66	97.77	110.80
1	A	125	TRP	CB-CG-CD2	-5.66	119.24	126.60
1	B	75	ASN	C-N-CA	-5.66	107.56	121.70
1	C	140	PHE	N-CA-CB	-5.63	100.46	110.60
1	B	97	ALA	CB-CA-C	-5.63	101.65	110.10
1	C	34	ALA	N-CA-CB	-5.63	102.22	110.10
1	D	79	TRP	N-CA-CB	-5.63	100.47	110.60
1	B	35	THR	N-CA-CB	-5.62	99.61	110.30
1	C	145	GLU	CA-CB-CG	5.62	125.76	113.40
1	A	113	PHE	N-CA-CB	-5.62	100.48	110.60
1	A	181	PHE	CZ-CE2-CD2	-5.61	113.37	120.10
1	D	43	ALA	N-CA-CB	-5.60	102.26	110.10
1	A	115	ALA	N-CA-CB	-5.59	102.28	110.10
1	C	147	THR	OG1-CB-CG2	-5.58	97.16	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	VAL	CA-CB-CG2	-5.58	102.54	110.90
1	C	58	ALA	N-CA-CB	-5.58	102.30	110.10
1	D	99	ILE	CB-CG1-CD1	-5.58	98.29	113.90
1	D	190	VAL	CG1-CB-CG2	5.57	119.82	110.90
1	B	20	ILE	CG1-CB-CG2	5.57	123.65	111.40
1	B	139	ILE	N-CA-CB	-5.56	98.02	110.80
1	B	37	VAL	C-N-CA	-5.55	107.83	121.70
1	C	82	ASN	C-N-CA	-5.55	107.83	121.70
1	D	69	ASN	CA-CB-CG	-5.55	101.20	113.40
1	C	180	ALA	CB-CA-C	-5.54	101.78	110.10
1	D	77	THR	CA-CB-CG2	-5.54	104.64	112.40
1	B	2	ALA	CB-CA-C	-5.54	101.79	110.10
1	A	119	THR	CB-CA-C	-5.54	96.65	111.60
1	C	149	PHE	CD1-CE1-CZ	5.53	126.74	120.10
1	D	153	ILE	CA-CB-CG2	-5.53	99.83	110.90
1	D	139	ILE	CG1-CB-CG2	-5.53	99.24	111.40
1	A	138	LEU	N-CA-C	-5.52	96.11	111.00
1	D	4	TYR	N-CA-CB	-5.51	100.68	110.60
1	A	142	VAL	CA-CB-CG1	5.49	119.13	110.90
1	C	141	GLN	CB-CA-C	-5.49	99.42	110.40
1	C	167	TYR	N-CA-CB	5.49	120.48	110.60
1	B	116	ALA	C-N-CA	-5.47	108.03	121.70
1	D	146	GLN	N-CA-CB	-5.47	100.75	110.60
1	A	195	ALA	CB-CA-C	-5.46	101.90	110.10
1	A	138	LEU	O-C-N	5.46	131.43	122.70
1	B	156	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	A	26	GLU	N-CA-CB	-5.42	100.84	110.60
1	D	175	VAL	CA-CB-CG1	-5.42	102.78	110.90
1	C	48	GLU	N-CA-CB	-5.41	100.87	110.60
1	B	184	VAL	N-CA-CB	-5.41	99.61	111.50
1	A	148	ASN	N-CA-C	5.40	125.58	111.00
1	D	40	ALA	CB-CA-C	-5.40	102.00	110.10
1	C	116	ALA	CB-CA-C	-5.39	102.01	110.10
1	B	86	ASN	CB-CA-C	-5.39	99.62	110.40
1	B	120	VAL	CA-CB-CG2	-5.38	102.83	110.90
1	A	30	SER	N-CA-CB	-5.38	102.44	110.50
1	B	143	TYR	N-CA-C	-5.38	96.49	111.00
1	C	37	VAL	CA-CB-CG1	-5.37	102.84	110.90
1	A	161	MET	N-CA-CB	5.37	120.27	110.60
1	A	74	VAL	CA-CB-CG2	-5.36	102.86	110.90
1	D	123	SER	N-CA-CB	-5.35	102.47	110.50
1	B	45	ALA	CB-CA-C	-5.35	102.08	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	149	PHE	CZ-CE2-CD2	-5.34	113.69	120.10
1	D	125	TRP	CB-CA-C	-5.34	99.71	110.40
1	C	35	THR	N-CA-CB	-5.34	100.15	110.30
1	C	137	LEU	N-CA-C	-5.34	96.57	111.00
1	C	188	ALA	N-CA-CB	-5.33	102.63	110.10
1	D	181	PHE	CB-CA-C	-5.33	99.75	110.40
1	D	192	SER	N-CA-CB	-5.32	102.51	110.50
1	A	157	LEU	CB-CG-CD1	5.32	120.04	111.00
1	B	125	TRP	N-CA-CB	-5.29	101.07	110.60
1	A	64	LYS	CD-CE-NZ	-5.29	99.53	111.70
1	C	101	ASP	CB-CA-C	-5.29	99.82	110.40
1	C	166	PHE	CG-CD2-CE2	5.29	126.62	120.80
1	D	150	PRO	CB-CA-C	-5.28	98.80	112.00
1	C	95	LEU	N-CA-CB	-5.28	99.84	110.40
1	D	157	LEU	CB-CG-CD2	5.25	119.93	111.00
1	A	45	ALA	N-CA-CB	-5.25	102.75	110.10
1	D	70	LEU	CB-CG-CD1	5.25	119.92	111.00
1	D	114	HIS	N-CA-CB	-5.25	101.15	110.60
1	C	120	VAL	CB-CA-C	-5.25	101.43	111.40
1	A	73	HIS	N-CA-CB	-5.24	101.16	110.60
1	B	144	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	A	153	ILE	N-CA-CB	-5.24	98.74	110.80
1	C	156	LEU	CB-CG-CD1	5.24	119.91	111.00
1	D	181	PHE	N-CA-CB	-5.23	101.18	110.60
1	D	38	LYS	CA-CB-CG	-5.23	101.90	113.40
1	C	138	LEU	N-CA-CB	-5.22	99.96	110.40
1	B	146	GLN	N-CA-CB	-5.22	101.20	110.60
1	D	71	ALA	N-CA-CB	-5.22	102.80	110.10
1	D	99	ILE	CA-CB-CG2	5.21	121.31	110.90
1	A	33	HIS	N-CA-CB	-5.20	101.23	110.60
1	A	128	LEU	N-CA-C	-5.20	96.96	111.00
1	A	147	THR	OG1-CB-CG2	5.20	121.95	110.00
1	A	6	LEU	N-CA-CB	-5.19	100.02	110.40
1	B	142	VAL	CB-CA-C	-5.19	101.54	111.40
1	D	185	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	C	182	TRP	N-CA-CB	-5.17	101.30	110.60
1	D	117	ALA	C-N-CA	-5.16	108.80	121.70
1	D	84	SER	N-CA-CB	5.16	118.23	110.50
1	B	77	THR	N-CA-CB	-5.15	100.51	110.30
1	A	9	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	D	102	ALA	CB-CA-C	5.15	117.83	110.10
1	A	3	GLU	CA-CB-CG	-5.15	102.07	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	LEU	CB-CG-CD2	5.14	119.74	111.00
1	A	90	LYS	CA-CB-CG	-5.14	102.09	113.40
1	D	162	TRP	CB-CG-CD1	5.14	133.68	127.00
1	B	96	ALA	CB-CA-C	-5.14	102.39	110.10
1	C	11	TRP	CB-CA-C	5.12	120.64	110.40
1	D	165	ALA	CB-CA-C	5.12	117.78	110.10
1	D	15	ALA	N-CA-C	5.12	124.81	111.00
1	A	8	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	74	VAL	N-CA-CB	-5.11	100.26	111.50
1	A	36	TYR	N-CA-CB	-5.11	101.41	110.60
1	A	20	ILE	N-CA-C	-5.10	97.22	111.00
1	D	82	ASN	CB-CA-C	-5.09	100.22	110.40
1	D	137	LEU	CB-CG-CD2	5.09	119.66	111.00
1	D	89	ASP	N-CA-CB	-5.09	101.44	110.60
1	D	21	SER	CB-CA-C	-5.08	100.45	110.10
1	D	176	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	C	156	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	37	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	C	109	PHE	N-CA-C	-5.08	97.30	111.00
1	A	103	PHE	CG-CD2-CE2	-5.07	115.22	120.80
1	B	190	VAL	CG1-CB-CG2	5.07	119.01	110.90
1	C	6	LEU	CB-CG-CD2	-5.07	102.39	111.00
1	A	113	PHE	C-N-CA	-5.06	109.04	121.70
1	C	64	LYS	CD-CE-NZ	-5.06	100.06	111.70
1	C	59	ILE	CG1-CB-CG2	5.05	122.52	111.40
1	D	151	LEU	CB-CG-CD1	5.05	119.59	111.00
1	C	115	ALA	N-CA-CB	-5.04	103.04	110.10
1	D	120	VAL	C-N-CA	-5.04	109.09	121.70
1	B	175	VAL	CA-CB-CG1	-5.04	103.34	110.90
1	B	170	TYR	CB-CG-CD2	5.03	124.02	121.00
1	B	114	HIS	N-CA-CB	-5.03	101.55	110.60
1	B	145	GLU	N-CA-CB	-5.03	101.55	110.60
1	C	142	VAL	CG1-CB-CG2	-5.02	102.86	110.90
1	C	60	LEU	CA-CB-CG	-5.02	103.75	115.30
1	A	5	THR	CB-CA-C	-5.02	98.06	111.60
1	D	142	VAL	N-CA-CB	-5.02	100.46	111.50
1	C	10	ASP	CB-CG-OD1	5.01	122.81	118.30
1	C	59	ILE	CA-CB-CG2	5.01	120.92	110.90
1	D	118	THR	CA-CB-OG1	-5.01	98.49	109.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	20	ILE	CB
1	C	153	ILE	CB
1	D	161	MET	CA

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	1567	0	1488	44	0
1	B	1567	0	1488	44	0
1	C	1567	0	1488	53	0
1	D	1567	0	1488	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	70	0	0	1	0
3	B	81	0	0	0	0
3	C	69	0	0	5	0
3	D	68	0	0	3	0
All	All	6560	0	5952	180	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 (180) 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:C:88:GLY:O	1:C:89:ASP:HB2	1.39	1.07
1:B:95:LEU:HD21	1:B:190:VAL:HG12	1.41	1.02
1:A:88:GLY:O	1:A:89:ASP:HB2	1.66	0.92
1:C:88:GLY:O	1:C:89:ASP:CB	2.22	0.86
1:B:95:LEU:CD2	1:B:190:VAL:HG12	2.06	0.86
1:A:95:LEU:HD23	1:A:191:GLN:HG3	1.58	0.84
1:A:157:LEU:O	1:A:158:LEU:HD23	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:SER:OG	1:D:85:PRO:HD2	1.79	0.82
1:A:51:ARG:HG2	3:C:2039:HOH:O	1.82	0.78
1:D:146:GLN:N	1:D:146:GLN:OE1	2.17	0.78
1:C:84:SER:OG	1:C:85:PRO:HD2	1.84	0.77
1:D:88:GLY:O	1:D:89:ASP:HB2	1.87	0.74
1:B:64:LYS:HE3	3:D:2052:HOH:O	1.86	0.74
1:A:92:THR:CG2	1:A:93:GLY:N	2.49	0.74
1:B:27:LEU:O	1:B:31:LYS:HB2	1.88	0.74
1:C:64:LYS:HE3	3:C:2055:HOH:O	1.89	0.72
1:B:9:LEU:HD13	1:B:11:TRP:CZ3	2.25	0.72
1:C:63:GLU:HA	1:C:63:GLU:OE1	1.88	0.72
1:C:91:PRO:HD3	1:C:106:PHE:CE1	2.25	0.71
1:B:14:GLY:O	1:B:17:GLU:HG3	1.90	0.71
1:A:92:THR:HG22	1:A:93:GLY:N	1.94	0.71
1:D:92:THR:H	1:D:191:GLN:NE2	1.89	0.71
1:C:172:ASN:OD1	1:C:172:ASN:N	2.24	0.71
1:C:92:THR:HG22	1:C:93:GLY:N	2.01	0.70
1:B:181:PHE:O	1:B:184:VAL:HG22	1.92	0.70
1:B:53:LYS:O	1:B:54:GLU:HB2	1.92	0.70
1:C:51:ARG:HG2	3:C:2027:HOH:O	1.92	0.69
1:A:95:LEU:HD22	1:A:191:GLN:HA	1.74	0.68
1:A:70:LEU:O	1:A:70:LEU:HD12	1.94	0.67
1:D:9:LEU:HD21	1:D:29:HIS:CD2	2.29	0.67
1:C:106:PHE:CE2	1:C:110:ARG:HD3	2.30	0.67
1:D:38:LYS:HG3	1:D:38:LYS:O	1.95	0.67
1:B:91:PRO:HG2	1:B:99:ILE:HD12	1.77	0.67
1:A:64:LYS:HE3	3:C:2056:HOH:O	1.96	0.66
1:C:170:TYR:O	1:C:173:VAL:HG23	1.95	0.65
1:C:92:THR:CG2	1:C:93:GLY:N	2.58	0.65
1:A:95:LEU:CD2	1:A:191:GLN:HG3	2.25	0.64
1:D:19:HIS:CE1	1:D:183:ASN:HD22	2.15	0.64
1:B:88:GLY:O	1:B:89:ASP:HB2	1.96	0.63
1:C:33:HIS:O	1:C:37:VAL:HG23	1.98	0.63
1:D:95:LEU:HD21	1:D:190:VAL:HG12	1.80	0.62
1:B:51:ARG:HD3	1:D:112:GLN:OE1	1.99	0.62
1:C:169:GLN:HG2	1:C:170:TYR:CD2	2.35	0.61
1:B:95:LEU:HD21	1:B:190:VAL:CG1	2.27	0.59
1:D:9:LEU:HD21	1:D:29:HIS:HD2	1.66	0.59
1:C:64:LYS:HE2	1:D:121:GLN:OE1	2.03	0.59
1:C:53:LYS:O	1:C:54:GLU:HB2	2.02	0.58
1:D:95:LEU:HD22	1:D:191:GLN:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:GLN:HG2	1:C:146:GLN:O	2.04	0.57
1:D:64:LYS:O	1:D:64:LYS:HG3	2.05	0.57
1:C:14:GLY:O	1:C:17:GLU:HG2	2.05	0.56
1:A:147:THR:HG22	1:A:148:ASN:N	2.19	0.56
1:C:121:GLN:OE1	1:D:64:LYS:HE2	2.05	0.56
1:B:9:LEU:HD21	1:B:29:HIS:CD2	2.40	0.56
1:B:83:LEU:HD22	1:B:184:VAL:HG23	1.87	0.56
1:A:95:LEU:HD22	1:A:191:GLN:CA	2.36	0.55
1:B:161:MET:HE3	1:B:174:LYS:HB2	1.88	0.55
1:B:95:LEU:HD23	1:B:191:GLN:HG3	1.89	0.54
1:C:56:HIS:O	1:C:59:ILE:HG22	2.07	0.54
1:B:6:LEU:HD12	1:B:7:PRO:HD2	1.89	0.54
1:A:9:LEU:HD11	1:A:13:TYR:HE1	1.73	0.54
1:D:146:GLN:H	1:D:146:GLN:CD	2.09	0.54
1:B:99:ILE:HG22	1:B:100:ALA:N	2.23	0.54
1:B:194:TYR:CE1	1:B:198:THR:HG21	2.42	0.54
1:D:90:LYS:HB3	1:D:91:PRO:HD2	1.90	0.53
1:A:147:THR:HG23	1:C:147:THR:OG1	2.08	0.53
1:B:9:LEU:CD1	1:B:11:TRP:CZ3	2.91	0.53
1:C:9:LEU:HD13	1:C:11:TRP:CZ3	2.43	0.53
1:A:63:GLU:OE1	1:A:63:GLU:HA	2.09	0.53
1:C:90:LYS:HB3	1:C:91:PRO:HD2	1.90	0.53
1:D:89:ASP:O	1:D:90:LYS:HG2	2.09	0.52
1:A:186:ASN:C	1:A:186:ASN:OD1	2.47	0.52
1:A:9:LEU:HD11	1:A:13:TYR:CE1	2.44	0.52
1:D:19:HIS:CE1	1:D:183:ASN:ND2	2.77	0.52
1:B:70:LEU:O	1:B:74:VAL:HG23	2.10	0.52
1:D:27:LEU:O	1:D:31:LYS:HB2	2.10	0.52
1:C:123:SER:HB3	1:C:162:TRP:CE2	2.44	0.52
1:C:164:HIS:HB3	1:D:163:GLU:CD	2.30	0.51
1:D:130:TRP:CZ2	1:D:135:ASN:HB3	2.45	0.51
1:C:33:HIS:O	1:C:33:HIS:CD2	2.63	0.51
1:D:11:TRP:CH2	1:D:16:LEU:HD11	2.46	0.50
1:A:78:ILE:O	1:A:78:ILE:HG22	2.09	0.50
1:C:147:THR:O	1:C:148:ASN:CB	2.59	0.50
1:B:161:MET:CE	1:B:174:LYS:HB2	2.40	0.50
1:B:19:HIS:CE1	1:B:183:ASN:HD22	2.29	0.50
1:A:146:GLN:OE1	1:A:146:GLN:N	2.40	0.50
1:A:84:SER:HB2	1:A:186:ASN:HB2	1.93	0.50
1:C:83:LEU:O	1:C:84:SER:HB2	2.11	0.49
1:C:33:HIS:O	1:C:33:HIS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:GLY:O	1:D:17:GLU:HG3	2.12	0.49
1:D:88:GLY:O	1:D:89:ASP:CB	2.52	0.49
1:B:150:PRO:HD2	1:B:153:ILE:HG13	1.93	0.49
1:C:106:PHE:O	1:C:109:PHE:HB3	2.13	0.48
1:C:14:GLY:O	1:C:17:GLU:CG	2.61	0.48
1:B:97:ALA:O	1:B:101:ASP:HB2	2.14	0.48
1:D:84:SER:OG	1:D:85:PRO:CD	2.57	0.48
1:D:153:ILE:O	1:D:155:PRO:HD3	2.13	0.48
1:A:84:SER:OG	1:A:85:PRO:CD	2.62	0.48
1:B:92:THR:HG22	1:B:93:GLY:N	2.29	0.48
1:A:169:GLN:NE2	1:A:170:TYR:CE2	2.82	0.48
1:A:147:THR:CG2	1:A:148:ASN:N	2.78	0.47
1:A:63:GLU:CA	1:A:63:GLU:OE1	2.62	0.47
1:A:16:LEU:HB2	3:A:2015:HOH:O	2.15	0.47
1:D:154:VAL:HA	1:D:155:PRO:HD2	1.69	0.47
1:C:42:ASP:HB3	3:C:2019:HOH:O	2.13	0.47
1:C:78:ILE:HG22	1:C:78:ILE:O	2.13	0.47
1:B:78:ILE:O	1:B:78:ILE:HG22	2.14	0.47
1:D:140:PHE:CE2	1:D:153:ILE:HD12	2.49	0.47
1:A:16:LEU:HD12	1:A:25:ASN:HD21	1.79	0.47
1:A:9:LEU:CD1	1:A:13:TYR:CE1	2.98	0.46
1:C:89:ASP:O	1:C:90:LYS:HG2	2.15	0.46
1:D:6:LEU:HA	1:D:7:PRO:HD2	1.82	0.46
1:A:137:LEU:O	1:A:138:LEU:HD23	2.16	0.46
1:C:91:PRO:CD	1:C:106:PHE:CE1	2.97	0.46
1:D:95:LEU:HD22	1:D:191:GLN:CA	2.46	0.46
1:B:153:ILE:HD13	1:B:153:ILE:HA	1.77	0.45
1:B:123:SER:HB3	1:B:162:TRP:CD2	2.51	0.45
1:D:99:ILE:HG21	1:D:99:ILE:HD13	1.45	0.45
1:B:106:PHE:HE1	1:B:187:TRP:CZ2	2.34	0.45
1:D:36:TYR:CE2	1:D:76:HIS:CE1	3.04	0.45
1:C:104:GLY:O	1:C:105:SER:HB3	2.16	0.45
1:D:153:ILE:HG23	1:D:153:ILE:HD13	1.74	0.45
1:B:90:LYS:HB3	1:B:91:PRO:CD	2.47	0.45
1:B:171:LYS:HB3	1:B:172:ASN:H	1.65	0.45
1:A:49:GLU:O	1:A:53:LYS:HG3	2.17	0.45
1:C:84:SER:HA	1:C:85:PRO:HD3	1.86	0.44
1:C:164:HIS:CD2	1:C:164:HIS:C	2.91	0.44
1:A:157:LEU:C	1:A:158:LEU:HD23	2.38	0.44
1:B:9:LEU:HD13	1:B:11:TRP:CH2	2.52	0.44
1:C:13:TYR:O	1:C:22:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLN:O	1:A:115:ALA:HB3	2.18	0.44
1:D:186:ASN:ND2	1:D:189:ASP:HB2	2.33	0.44
1:D:131:ASP:O	1:D:135:ASN:HA	2.18	0.44
1:B:16:LEU:HD13	1:B:83:LEU:HD13	2.00	0.43
1:B:56:HIS:CE1	1:D:112:GLN:HG3	2.54	0.43
1:D:168:LEU:HA	1:D:168:LEU:HD23	1.66	0.43
1:C:28:HIS:HB3	1:C:80:TRP:HH2	1.83	0.43
1:C:110:ARG:HG3	1:C:182:TRP:CZ2	2.52	0.43
1:D:9:LEU:CD2	1:D:29:HIS:CD2	3.01	0.43
1:A:53:LYS:O	1:A:54:GLU:HB2	2.19	0.43
1:C:27:LEU:O	1:C:31:LYS:HB2	2.18	0.43
1:A:123:SER:HB3	1:A:162:TRP:CD2	2.54	0.43
1:A:19:HIS:CD2	1:A:183:ASN:HD22	2.37	0.43
1:D:143:TYR:O	1:D:144:ASP:HB2	2.19	0.43
1:B:166:PHE:C	1:B:166:PHE:CD1	2.92	0.43
1:A:189:ASP:O	1:A:192:SER:HB3	2.19	0.43
1:B:95:LEU:HB3	1:B:191:GLN:HG2	2.00	0.43
1:D:6:LEU:HD21	1:D:29:HIS:CE1	2.54	0.43
1:A:95:LEU:CB	1:A:191:GLN:HG2	2.49	0.42
1:B:143:TYR:HB2	1:B:147:THR:HB	2.01	0.42
1:A:64:LYS:HG3	1:A:64:LYS:O	2.20	0.42
1:B:118:THR:O	1:B:174:LYS:HE3	2.20	0.42
1:C:24:ILE:O	1:C:24:ILE:CG2	2.64	0.42
1:D:81:LYS:HE2	3:D:2031:HOH:O	2.18	0.42
1:A:95:LEU:CD2	1:A:191:GLN:CG	2.97	0.42
1:B:106:PHE:CE1	1:B:187:TRP:CZ2	3.07	0.42
1:C:104:GLY:O	1:C:105:SER:CB	2.68	0.42
1:D:40:ALA:N	1:D:69:ASN:HB3	2.35	0.42
1:D:36:TYR:HE2	1:D:76:HIS:CE1	2.38	0.41
1:C:137:LEU:CD2	1:C:156:LEU:CD1	2.98	0.41
1:D:75:ASN:HB3	1:D:125:TRP:CZ2	2.55	0.41
1:D:91:PRO:HG2	3:D:2033:HOH:O	2.20	0.41
1:B:60:LEU:O	1:B:60:LEU:HD13	2.20	0.41
1:B:11:TRP:CD1	1:B:85:PRO:HD3	2.55	0.41
1:C:174:LYS:O	1:C:177:PHE:HB3	2.20	0.41
1:A:6:LEU:HD12	1:A:6:LEU:HA	1.85	0.41
1:A:147:THR:HG23	1:C:147:THR:HG23	2.03	0.41
1:C:81:LYS:C	1:C:83:LEU:H	2.23	0.41
1:D:149:PHE:HA	1:D:150:PRO:HD3	1.88	0.41
1:C:103:PHE:CE1	1:C:139:ILE:HD12	2.55	0.41
1:B:9:LEU:HD23	1:B:9:LEU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ILE:O	1:C:78:ILE:CG2	2.68	0.41
1:C:95:LEU:HA	1:C:95:LEU:HD12	1.77	0.41
1:C:109:PHE:HB3	1:C:110:ARG:H	1.66	0.40
1:A:67:ALA:O	1:A:71:ALA:HB2	2.21	0.40
1:C:6:LEU:HA	1:C:7:PRO:HD2	1.93	0.40
1:A:125:TRP:CE3	1:A:158:LEU:HB3	2.56	0.40
1:A:173:VAL:O	1:A:176:ASP:HB2	2.21	0.40
1:B:110:ARG:HH11	1:B:110:ARG:HD2	1.74	0.40
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.84	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	196/207 (95%)	177 (90%)	17 (9%)	2 (1%)	19	34
1	B	196/207 (95%)	184 (94%)	10 (5%)	2 (1%)	19	34
1	C	196/207 (95%)	175 (89%)	20 (10%)	1 (0%)	34	55
1	D	196/207 (95%)	182 (93%)	12 (6%)	2 (1%)	19	34
All	All	784/828 (95%)	718 (92%)	59 (8%)	7 (1%)	21	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	ASP
1	A	89	ASP
1	B	148	ASN
1	D	148	ASN
1	B	166	PHE
1	D	13	TYR

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Mol	Chain	Res	Type
1	A	173	VAL

5.3.2 Protein sidechains

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	156/163 (96%)	140 (90%)	16 (10%)	9 17
1	B	156/163 (96%)	141 (90%)	15 (10%)	10 19
1	C	156/163 (96%)	142 (91%)	14 (9%)	12 22
1	D	156/163 (96%)	141 (90%)	15 (10%)	10 19
All	All	624/652 (96%)	564 (90%)	60 (10%)	10 19

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TRP
1	A	17	GLU
1	A	21	SER
1	A	38	LYS
1	A	48	GLU
1	A	60	LEU
1	A	64	LYS
1	A	92	THR
1	A	101	ASP
1	A	110	ARG
1	A	137	LEU
1	A	153	ILE
1	A	159	LEU
1	A	164	HIS
1	A	198	THR
1	A	199	SER
1	B	11	TRP
1	B	21	SER
1	B	48	GLU
1	B	51	ARG

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Mol	Chain	Res	Type
1	B	64	LYS
1	B	73	HIS
1	B	74	VAL
1	B	82	ASN
1	B	83	LEU
1	B	89	ASP
1	B	101	ASP
1	B	105	SER
1	B	167	TYR
1	B	171	LYS
1	B	199	SER
1	C	21	SER
1	C	28	HIS
1	C	30	SER
1	C	48	GLU
1	C	64	LYS
1	C	137	LEU
1	C	139	ILE
1	C	150	PRO
1	C	159	LEU
1	C	164	HIS
1	C	167	TYR
1	C	173	VAL
1	C	192	SER
1	C	199	SER
1	D	38	LYS
1	D	48	GLU
1	D	53	LYS
1	D	59	ILE
1	D	60	LEU
1	D	64	LYS
1	D	89	ASP
1	D	105	SER
1	D	109	PHE
1	D	110	ARG
1	D	146	GLN
1	D	151	LEU
1	D	153	ILE
1	D	161	MET
1	D	179	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	183	ASN
1	B	19	HIS
1	B	62	ASN
1	B	82	ASN
1	B	114	HIS
1	C	62	ASN
1	C	183	ASN
1	D	19	HIS
1	D	62	ASN
1	D	183	ASN
1	D	191	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	198/207 (95%)	-1.04	0	100	100	4, 20, 49, 89	0
1	B	198/207 (95%)	-0.88	0	100	100	7, 27, 61, 86	0
1	C	198/207 (95%)	-1.00	0	100	100	5, 20, 53, 84	0
1	D	198/207 (95%)	-0.95	0	100	100	7, 23, 57, 110	0
All	All	792/828 (95%)	-0.97	0	100	100	4, 22, 56, 110	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	A	1200	1/1	0.99	0.07	-0.75	13,13,13,13	0
2	MN	C	1200	1/1	0.99	0.06	-1.48	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	D	1200	1/1	0.99	0.06	-2.80	18,18,18,18	0
2	MN	B	1200	1/1	0.98	0.04	-6.17	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.