Full wwPDB NMR Structure Validation Report (i)

Feb 14, 2022 – 09:05 AM EST

PDB ID	:	1JI8
Title	:	Solution Structure of Pyrobaculum Aerophilum DsrC/gamma subunit of dissimilatory sulfite reductase
Authors	:	Cort, J.R.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2001-06-29

This is a Full wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

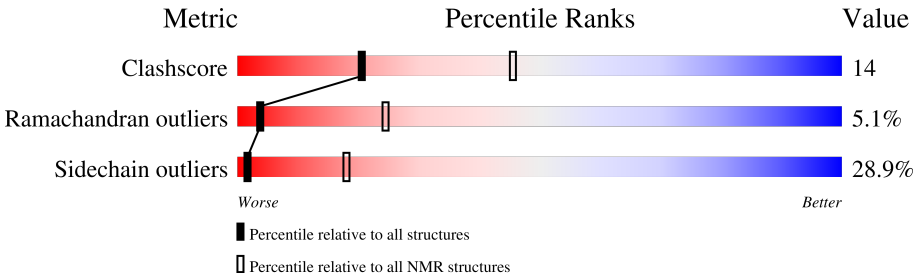
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	111	38% 52% • 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average,fewest violations,lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:3-A:104 (102)	0.66	15

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 6, 7, 8, 10, 12, 13, 15, 16, 18
2	4, 5, 20
3	2, 9, 14
4	17, 19
Single-model clusters	11

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1757 atoms, of which 868 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called dissimilatory siroheme-sulfite reductase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	111	1757	573	868	142	165	9	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLN	LYS	conflict	UNP Q8ZUX1
A	13	GLY	ASP	conflict	UNP Q8ZUX1
A	14	LYS	VAL	conflict	UNP Q8ZUX1
A	15	LYS	THR	conflict	UNP Q8ZUX1
A	16	VAL	ILE	conflict	UNP Q8ZUX1
A	21	ASP	GLU	conflict	UNP Q8ZUX1
A	24	MET	LEU	conflict	UNP Q8ZUX1
A	25	GLN	SER	conflict	UNP Q8ZUX1
A	29	ASP	VAL	conflict	UNP Q8ZUX1
A	31	ASP	ASN	conflict	UNP Q8ZUX1
A	38	LEU	MET	conflict	UNP Q8ZUX1
A	51	GLU	ASP	conflict	UNP Q8ZUX1
A	55	LEU	VAL	conflict	UNP Q8ZUX1
A	66	PHE	TYR	conflict	UNP Q8ZUX1
A	68	THR	VAL	conflict	UNP Q8ZUX1
A	75	VAL	LEU	conflict	UNP Q8ZUX1
A	76	THR	LEU	conflict	UNP Q8ZUX1
A	82	SER	THR	conflict	UNP Q8ZUX1
A	85	LYS	GLN	conflict	UNP Q8ZUX1
A	96	HIS	ASN	conflict	UNP Q8ZUX1

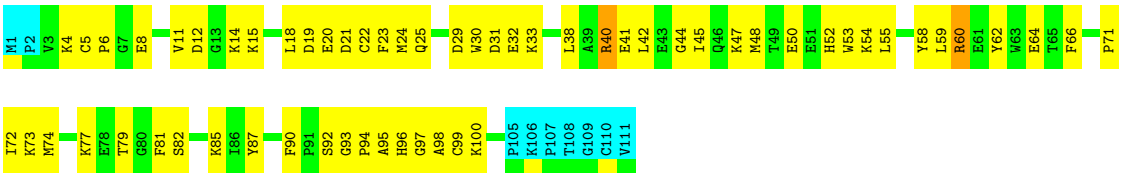
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 38% 52% • 8%



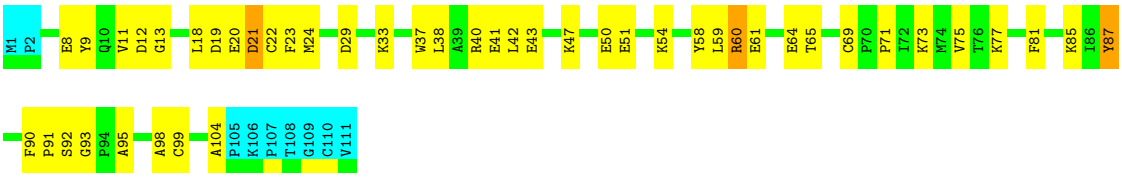
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: dissimilatory siroheme-sulfite reductase

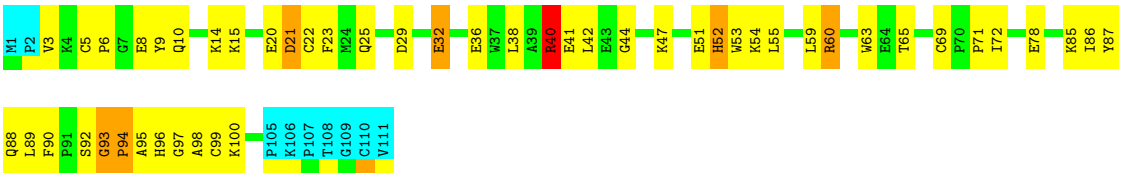
Chain A: 50% 39% • 8%



4.2.2 Score per residue for model 2

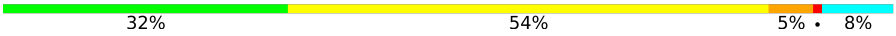
• Molecule 1: dissimilatory siroheme-sulfite reductase

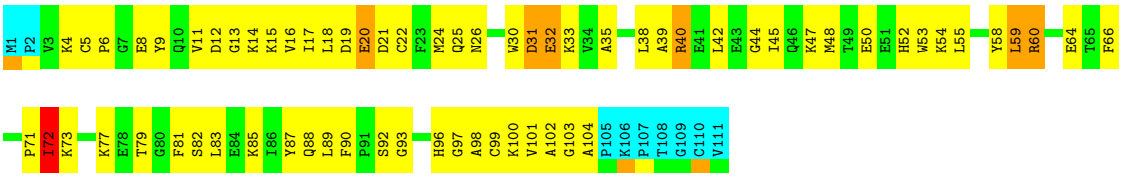
Chain A: 47% 39% 5% • 8%



4.2.3 Score per residue for model 3

- Molecule 1: dissimilatory siroheme-sulfite reductase

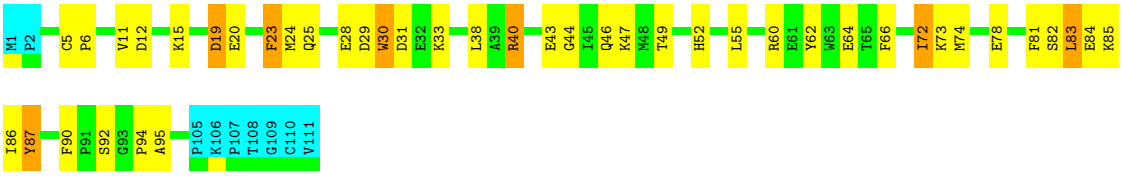
Chain A: 



4.2.4 Score per residue for model 4

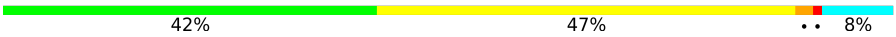
- Molecule 1: dissimilatory siroheme-sulfite reductase

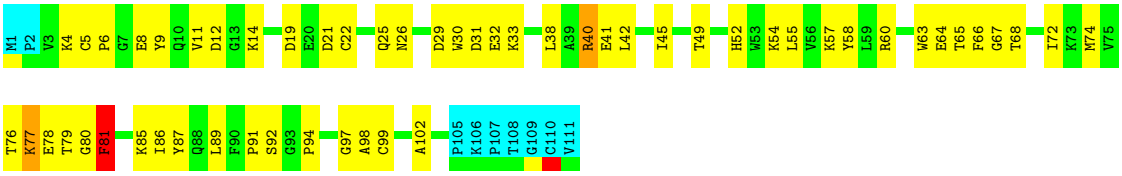
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 



4.2.6 Score per residue for model 6

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 36% 50% 6% 8%

M1 P2 V3 K4 C5 P6 G7 E8 Y9 Q10 V11 D12 G13 K14 I17 L18 D19 E20 D21 C22 F23 M24 Q25 N26 P27 E28 D29 W30 D31 E32 K33 V34 A35 E36 W37 L38 A39 R40 E41 G44 I45 Q46 K47 M48 E51 H52 W53 K54 L55 Y58 L59 R60 E61 Y62 W63 E64

G67 T68 P71 I72 K73 M74 V75 T79 G80 F81 S82 K85 I86 Y87 Q88 L89 F90 P91 S92 G93 H96 G97 A98 C99 P105 K106 P107 T108 G109 C110 V111

4.2.7 Score per residue for model 7

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 40% 43% 9% 8%

M1 P2 V3 K4 C5 P6 G7 E8 V11 D12 G13 K14 K15 D19 E20 D21 Q25 D31 E32 A35 L38 A39 R40 E41 L42 E43 G44 I45 Q46 E51 H52 W53 K54 L55 R60 E61 Y62 W63 F66 G67 T68 C69 I72 K73 M74 V75 T76 K77 E78 T79

G80 F81 S82 L83 E84 K85 I86 Y87 Q88 L89 F90 P91 S92 A95 H96 G97 A98 C99 K100 P105 K106 P107 T108 G109 C110 V111

4.2.8 Score per residue for model 8

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 55% 32% 5% 8%

M1 P2 C5 P6 G7 E8 Y9 Q10 K14 K15 L18 D19 E20 D21 C22 F23 D29 W30 D31 E32 K33 R40 E41 L42 K47 M48 T49 H52 W53 K54 L55 V56 K57 R60 W63 E64 I72 K73 K77 S82 K85 I86 Y87 Q88 L89 F90

P94 A95 A98 C99 K100 A104 P105 K106 P107 T108 G109 C110 V111

4.2.9 Score per residue for model 9

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 48% 41% 8%

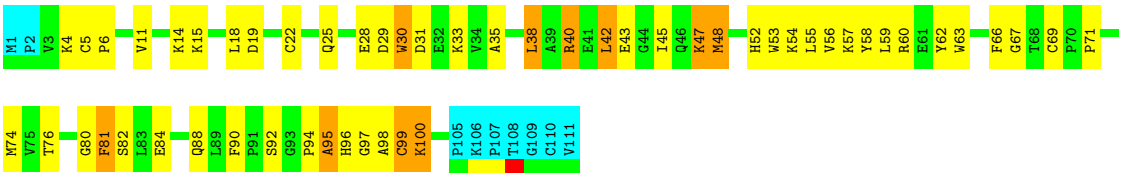
M1 P2 V3 K4 C5 P6 V11 D12 G13 L18 C22 F23 M24 E28 D31 L38 A39 R40 E43 Q46 K47 M48 T49 E50 E51 H52 V56 K57 Y58 L59 R60 E61 Y62 W63 E64 T65 F66 G67 T68 P71 I72 T76 K77 E78 T79 G80 F81 S82 L83

E84 K85 Q88 L89 F90 P91 S92 G93 P94 A95 C99 K100 V101 P105 K106 P107 T108 G109 C110 V111

4.2.10 Score per residue for model 10

- Molecule 1: dissimilatory siroheme-sulfite reductase

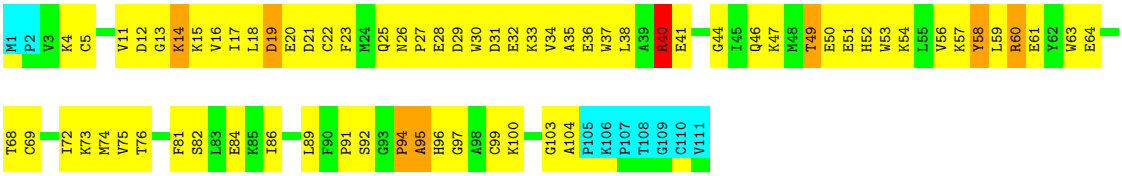
Chain A: 43% 40% 9% 8%



4.2.11 Score per residue for model 11

- Molecule 1: dissimilatory siroheme-sulfite reductase

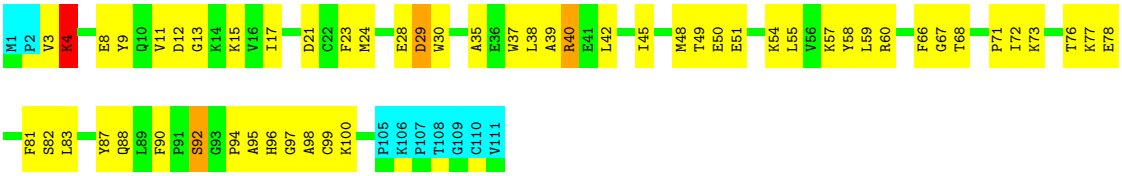
Chain A: 29% 56% 6% • 8%



4.2.12 Score per residue for model 12

- Molecule 1: dissimilatory siroheme-sulfite reductase

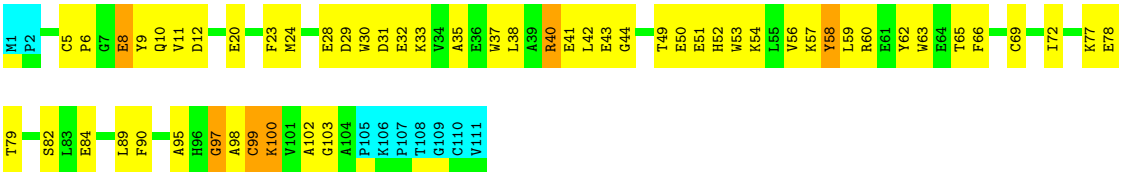
Chain A: 42% 46% • • 8%



4.2.13 Score per residue for model 13

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 42% 44% 5% 8%



4.2.14 Score per residue for model 14

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 50% 37% 5% 8%

M1 P2 V3 K4 C5 P6 G7 E8 V11 D12 G13 L18 D19 E20 D21 C22 D29 W30 D31 E32 E36 W37 L38 A39 R40 E41 L42 E43 G44 I45 M48 H52 L59 R60 E61 Y62 W63 E64 T65 F66 M74 K77 E78 S82 I86 Y87 P91 S92

G93 P94 A95 H96 G97 A98 P105 K106 P107 T108 G109 C110 V111

4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 45% 40% 6% • 8%

M1 P2 V3 K4 C5 P6 Q10 V11 K14 K15 V16 I17 L18 D19 E20 D21 Q25 D29 W30 D31 E32 K33 Y34 A35 E36 W37 L38 A39 R40 E41 L42 E43 G44 I45 M48 T49 E50 E51 H52 W53 K54 K57 Y58 L59 R60 E61 Y62 W63 E64 P71 I72 K73 M74

V75 T79 S82 L83 E84 K85 I86 Y87 Q88 L89 F90 P91 S92 G93 P94 A95 K100 P105 K106 P107 T108 G109 C110 V111

4.2.16 Score per residue for model 16

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 44% 41% 5% • 8%

M1 P2 V3 K4 C5 P6 G7 E8 Y9 Q10 V11 D12 G13 K14 K15 V16 I17 L18 D19 M24 Q25 N26 P27 E28 D31 E32 L38 A39 R40 E41 L42 E43 G44 I45 Q46 K47 M48 W53 K54 L55 Y58 L59 R60 E61 Y62 W63 E64 T65 F66 G67 T68 C69 P70 P71 I72

K73 M74 K77 K85 I86 F90 P94 A95 H96 C99 K100 P105 K106 P107 T108 G109 C110 V111

4.2.17 Score per residue for model 17

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 41% 43% 8% 8%

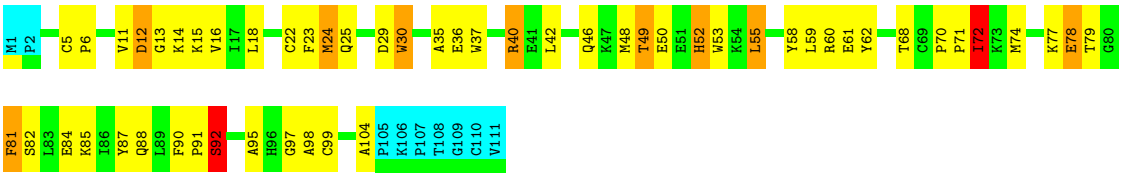
M1 P2 V3 K4 C5 P6 Q10 V11 D12 G13 K14 L18 D19 E20 M24 Q25 N26 P27 E28 D29 W30 D31 E36 W37 R40 E41 L42 E43 G44 I45 Q46 K47 E50 W53 K54 L55 V56 K57 Y58 L59 R60 E61 Y62 W63 E64 P70 M74 K77 E78 T79

G80 F81 S82 K85 I86 Y87 Q88 L89 F90 P91 S92 G93 P94 A95 H96 G97 A98 C99 K100 V101 P105 K106 P107 T108 G109 C110 V111

4.2.18 Score per residue for model 18

- Molecule 1: dissimilatory siroheme-sulfite reductase

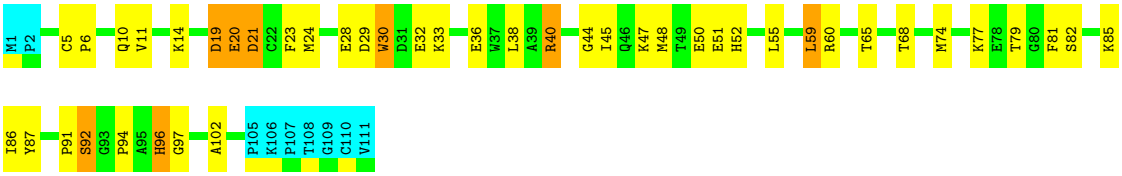
Chain A: 43% 39% 8% • 8%



4.2.19 Score per residue for model 19

- Molecule 1: dissimilatory siroheme-sulfite reductase

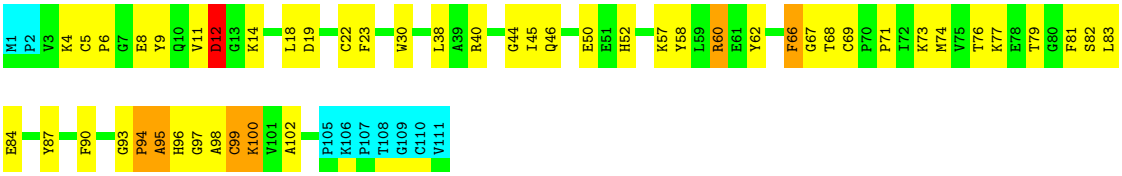
Chain A: 52% 32% 7% 8%



4.2.20 Score per residue for model 20

- Molecule 1: dissimilatory siroheme-sulfite reductase

Chain A: 48% 38% 5% • 8%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry and simulated annealing.*

Of the 24 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations,structures with the lowest energy.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	structure solution	3.84
X-PLOR	refinement	3.84

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

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	Planarity
1	A	0.0±0.0	2.0±0.0
All	All	0	40

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	40	ARG	Sidechain	20
1	A	60	ARG	Sidechain	20

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	826	799	799	22±7
All	All	16520	15980	15980	440

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 14.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:THR:HG22	1:A:52:HIS:ND1	0.89	1.81	13	2
1:A:82:SER:O	1:A:86:ILE:HD12	0.82	1.75	7	2
1:A:58:TYR:CE2	1:A:75:VAL:HG13	0.81	2.10	6	1
1:A:79:THR:HG22	1:A:81:PHE:CD1	0.78	2.14	17	1
1:A:52:HIS:O	1:A:56:VAL:HG23	0.75	1.81	10	4
1:A:55:LEU:O	1:A:59:LEU:HD12	0.71	1.86	19	1
1:A:24:MET:SD	1:A:38:LEU:HD11	0.70	2.27	19	1
1:A:17:ILE:O	1:A:17:ILE:HG23	0.70	1.85	11	1
1:A:52:HIS:CE1	1:A:89:LEU:HD22	0.69	2.22	15	5
1:A:72:ILE:HG21	1:A:86:ILE:CD1	0.69	2.17	16	1
1:A:18:LEU:HD22	1:A:22:CYS:C	0.68	2.09	9	4
1:A:39:ALA:HB1	1:A:45:ILE:HD12	0.66	1.65	12	4
1:A:99:CYS:SG	1:A:104:ALA:HB3	0.63	2.33	18	2
1:A:94:PRO:O	1:A:98:ALA:HB3	0.63	1.94	8	1
1:A:52:HIS:NE2	1:A:89:LEU:HD22	0.62	2.10	11	2
1:A:52:HIS:CE1	1:A:89:LEU:CD2	0.61	2.83	11	2
1:A:56:VAL:HG21	1:A:101:VAL:HG11	0.60	1.72	17	1
1:A:35:ALA:HB3	1:A:53:TRP:CH2	0.59	2.32	10	4
1:A:94:PRO:O	1:A:95:ALA:HB3	0.59	1.98	16	3
1:A:30:TRP:CZ2	1:A:35:ALA:HB2	0.59	2.33	12	4
1:A:30:TRP:CD2	1:A:31:ASP:N	0.58	2.72	17	4
1:A:63:TRP:NE1	1:A:104:ALA:HB1	0.57	2.13	8	1
1:A:11:VAL:HG22	1:A:37:TRP:CD2	0.57	2.34	11	2
1:A:45:ILE:O	1:A:45:ILE:HG22	0.57	1.98	5	2
1:A:63:TRP:O	1:A:63:TRP:CE3	0.57	2.58	17	4
1:A:11:VAL:CG2	1:A:37:TRP:CD2	0.57	2.87	11	1
1:A:18:LEU:HD22	1:A:22:CYS:CA	0.57	2.30	9	3
1:A:14:LYS:CD	1:A:34:VAL:HG21	0.56	2.29	11	1
1:A:48:MET:SD	1:A:53:TRP:CZ2	0.56	2.99	3	2
1:A:55:LEU:CD1	1:A:81:PHE:CE2	0.56	2.88	18	1
1:A:8:GLU:O	1:A:9:TYR:CD2	0.56	2.60	12	3
1:A:17:ILE:HD12	1:A:17:ILE:N	0.55	2.15	3	2
1:A:39:ALA:HB1	1:A:45:ILE:CD1	0.55	2.31	14	1
1:A:8:GLU:O	1:A:9:TYR:CG	0.55	2.60	6	3
1:A:30:TRP:CE3	1:A:31:ASP:N	0.55	2.75	5	5
1:A:32:GLU:OE2	1:A:53:TRP:CZ2	0.54	2.61	3	1
1:A:30:TRP:CD1	1:A:102:ALA:O	0.54	2.61	5	2
1:A:23:PHE:CD2	1:A:24:MET:O	0.54	2.61	18	1
1:A:93:GLY:O	1:A:96:HIS:CD2	0.54	2.60	3	1
1:A:83:LEU:HD21	1:A:87:TYR:CE2	0.54	2.38	4	1
1:A:3:VAL:HG11	1:A:18:LEU:CD1	0.54	2.33	17	2
1:A:72:ILE:HG21	1:A:86:ILE:HD13	0.54	1.80	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:GLU:O	1:A:9:TYR:CD1	0.53	2.62	13	3
1:A:3:VAL:O	1:A:3:VAL:HG13	0.53	2.02	2	1
1:A:58:TYR:CD1	1:A:58:TYR:C	0.53	2.82	20	2
1:A:18:LEU:HD22	1:A:22:CYS:HA	0.53	1.81	3	6
1:A:72:ILE:HG13	1:A:76:THR:HG23	0.53	1.81	7	1
1:A:32:GLU:OE2	1:A:53:TRP:CE2	0.52	2.62	3	1
1:A:35:ALA:HB3	1:A:53:TRP:HH2	0.52	1.64	10	3
1:A:14:LYS:CD	1:A:34:VAL:CG2	0.52	2.87	11	1
1:A:24:MET:HG2	1:A:38:LEU:HD11	0.52	1.81	6	1
1:A:17:ILE:O	1:A:17:ILE:CG2	0.52	2.57	11	1
1:A:55:LEU:HD13	1:A:81:PHE:CE2	0.52	2.39	18	1
1:A:72:ILE:HG12	1:A:83:LEU:HD11	0.52	1.82	9	1
1:A:96:HIS:CD2	1:A:97:GLY:N	0.52	2.78	14	2
1:A:94:PRO:O	1:A:96:HIS:N	0.51	2.43	20	4
1:A:8:GLU:C	1:A:9:TYR:CD2	0.51	2.84	6	1
1:A:30:TRP:NE1	1:A:102:ALA:O	0.51	2.44	20	1
1:A:11:VAL:O	1:A:13:GLY:N	0.51	2.43	12	7
1:A:48:MET:SD	1:A:53:TRP:CE2	0.51	3.03	3	1
1:A:58:TYR:CE2	1:A:79:THR:HG23	0.51	2.39	13	1
1:A:11:VAL:O	1:A:14:LYS:CG	0.51	2.58	16	1
1:A:6:PRO:CB	1:A:18:LEU:O	0.51	2.59	18	1
1:A:72:ILE:HG22	1:A:72:ILE:O	0.51	2.06	13	2
1:A:72:ILE:O	1:A:72:ILE:HG23	0.51	2.06	2	5
1:A:72:ILE:O	1:A:72:ILE:CG1	0.51	2.59	18	3
1:A:26:ASN:N	1:A:27:PRO:CD	0.51	2.74	17	2
1:A:18:LEU:HD23	1:A:23:PHE:O	0.50	2.07	6	1
1:A:3:VAL:HG12	1:A:9:TYR:CE2	0.50	2.41	16	1
1:A:5:CYS:SG	1:A:22:CYS:N	0.50	2.85	3	3
1:A:94:PRO:HB2	1:A:98:ALA:HB2	0.50	1.82	2	1
1:A:16:VAL:C	1:A:17:ILE:HD12	0.49	2.26	3	1
1:A:11:VAL:HG22	1:A:37:TRP:CE2	0.49	2.41	12	1
1:A:49:THR:HG22	1:A:52:HIS:CE1	0.49	2.42	13	1
1:A:72:ILE:HD11	1:A:83:LEU:CD1	0.49	2.37	9	1
1:A:32:GLU:HG3	1:A:33:LYS:N	0.49	2.22	11	1
1:A:29:ASP:OD1	1:A:29:ASP:N	0.49	2.45	12	2
1:A:76:THR:O	1:A:80:GLY:N	0.49	2.46	10	1
1:A:48:MET:SD	1:A:52:HIS:CG	0.49	3.06	18	2
1:A:63:TRP:O	1:A:63:TRP:CD2	0.49	2.66	16	2
1:A:5:CYS:SG	1:A:18:LEU:HD13	0.49	2.48	11	1
1:A:49:THR:CG2	1:A:52:HIS:ND1	0.48	2.67	13	1
1:A:72:ILE:HD11	1:A:86:ILE:HD13	0.48	1.84	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:TRP:NE1	1:A:35:ALA:HB2	0.48	2.22	6	1
1:A:32:GLU:CG	1:A:33:LYS:N	0.48	2.76	11	1
1:A:20:GLU:O	1:A:21:ASP:CB	0.48	2.62	8	5
1:A:24:MET:CG	1:A:38:LEU:HD11	0.48	2.39	6	1
1:A:65:THR:HG22	1:A:66:PHE:CD2	0.48	2.43	9	1
1:A:37:TRP:CE2	1:A:41:GLU:OE1	0.48	2.67	1	1
1:A:40:ARG:O	1:A:44:GLY:N	0.48	2.46	11	2
1:A:3:VAL:HG23	1:A:9:TYR:CE2	0.48	2.44	2	1
1:A:103:GLY:O	1:A:104:ALA:HB2	0.48	2.08	3	1
1:A:63:TRP:CD1	1:A:67:GLY:HA2	0.47	2.44	5	2
1:A:62:TYR:CG	1:A:70:PRO:HG3	0.47	2.44	17	1
1:A:3:VAL:HG12	1:A:4:LYS:N	0.47	2.24	7	1
1:A:49:THR:HG23	1:A:50:GLU:N	0.47	2.24	18	1
1:A:17:ILE:O	1:A:25:GLN:CB	0.47	2.62	6	1
1:A:3:VAL:HG11	1:A:41:GLU:OE1	0.47	2.09	2	1
1:A:58:TYR:CE1	1:A:79:THR:CG2	0.47	2.98	9	1
1:A:72:ILE:CG1	1:A:83:LEU:CD1	0.47	2.92	9	1
1:A:30:TRP:O	1:A:30:TRP:CE3	0.47	2.68	18	1
1:A:21:ASP:HB3	1:A:23:PHE:CD1	0.47	2.45	6	1
1:A:55:LEU:CD1	1:A:81:PHE:CD2	0.47	2.98	18	1
1:A:87:TYR:O	1:A:90:PHE:O	0.47	2.33	4	4
1:A:38:LEU:HD23	1:A:42:LEU:CD1	0.47	2.40	7	1
1:A:94:PRO:O	1:A:95:ALA:O	0.47	2.33	17	1
1:A:26:ASN:O	1:A:26:ASN:ND2	0.46	2.49	3	1
1:A:29:ASP:O	1:A:30:TRP:O	0.46	2.33	18	5
1:A:11:VAL:HG22	1:A:37:TRP:CG	0.46	2.45	11	1
1:A:16:VAL:HG22	1:A:26:ASN:HD21	0.46	1.70	11	1
1:A:23:PHE:CE2	1:A:24:MET:O	0.46	2.68	18	1
1:A:30:TRP:CE3	1:A:31:ASP:CA	0.46	2.98	3	2
1:A:94:PRO:O	1:A:98:ALA:CB	0.46	2.63	8	1
1:A:92:SER:O	1:A:92:SER:OG	0.46	2.34	17	1
1:A:38:LEU:HD23	1:A:38:LEU:O	0.46	2.10	15	1
1:A:37:TRP:O	1:A:41:GLU:OE1	0.46	2.34	6	2
1:A:32:GLU:HG3	1:A:53:TRP:CZ2	0.46	2.45	13	2
1:A:58:TYR:CZ	1:A:79:THR:HG22	0.46	2.45	9	1
1:A:80:GLY:O	1:A:82:SER:N	0.46	2.48	10	1
1:A:86:ILE:CG2	1:A:94:PRO:HB3	0.46	2.40	5	3
1:A:95:ALA:O	1:A:99:CYS:SG	0.46	2.74	11	2
1:A:75:VAL:O	1:A:79:THR:OG1	0.46	2.34	15	2
1:A:37:TRP:CZ2	1:A:41:GLU:OE1	0.45	2.68	1	1
1:A:63:TRP:CG	1:A:67:GLY:HA2	0.45	2.46	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LEU:CD2	1:A:22:CYS:C	0.45	2.81	9	2
1:A:11:VAL:O	1:A:12:ASP:CB	0.45	2.63	13	2
1:A:63:TRP:O	1:A:63:TRP:CG	0.45	2.68	13	1
1:A:92:SER:O	1:A:93:GLY:O	0.45	2.33	14	3
1:A:58:TYR:CE1	1:A:75:VAL:HG13	0.45	2.47	1	1
1:A:49:THR:HG23	1:A:52:HIS:H	0.45	1.70	8	2
1:A:68:THR:HG22	1:A:69:CYS:H	0.45	1.70	20	1
1:A:75:VAL:O	1:A:79:THR:CB	0.45	2.65	7	1
1:A:58:TYR:CD2	1:A:75:VAL:HG13	0.45	2.46	11	2
1:A:52:HIS:O	1:A:56:VAL:CG2	0.45	2.65	9	2
1:A:19:ASP:CB	1:A:25:GLN:OE1	0.45	2.64	3	1
1:A:17:ILE:O	1:A:25:GLN:HB3	0.45	2.12	6	1
1:A:16:VAL:HG13	1:A:24:MET:HB3	0.45	1.89	16	1
1:A:91:PRO:O	1:A:92:SER:CB	0.45	2.64	18	1
1:A:95:ALA:O	1:A:97:GLY:N	0.45	2.50	14	1
1:A:18:LEU:O	1:A:19:ASP:O	0.45	2.34	17	1
1:A:55:LEU:HD12	1:A:81:PHE:CZ	0.45	2.46	18	1
1:A:11:VAL:O	1:A:14:LYS:HG3	0.45	2.12	16	2
1:A:30:TRP:CE3	1:A:30:TRP:C	0.44	2.90	14	2
1:A:37:TRP:CZ2	1:A:41:GLU:OE2	0.44	2.70	15	1
1:A:8:GLU:OE2	1:A:17:ILE:CG1	0.44	2.64	16	1
1:A:40:ARG:CD	1:A:41:GLU:OE2	0.44	2.64	8	1
1:A:91:PRO:O	1:A:92:SER:C	0.44	2.56	1	3
1:A:14:LYS:HD3	1:A:34:VAL:HG21	0.44	1.90	11	1
1:A:16:VAL:HG13	1:A:24:MET:HG2	0.44	1.90	18	1
1:A:81:PHE:N	1:A:81:PHE:CD1	0.44	2.85	3	1
1:A:6:PRO:CA	1:A:18:LEU:O	0.44	2.66	18	1
1:A:8:GLU:C	1:A:9:TYR:CG	0.44	2.91	3	2
1:A:69:CYS:O	1:A:69:CYS:SG	0.44	2.75	13	1
1:A:19:ASP:N	1:A:19:ASP:OD1	0.44	2.49	7	1
1:A:50:GLU:HG3	1:A:51:GLU:N	0.44	2.28	12	1
1:A:29:ASP:O	1:A:29:ASP:OD1	0.44	2.36	2	1
1:A:55:LEU:HD11	1:A:81:PHE:CD2	0.44	2.48	6	1
1:A:44:GLY:O	1:A:46:GLN:N	0.43	2.51	20	2
1:A:48:MET:HB3	1:A:53:TRP:NE1	0.43	2.27	16	1
1:A:15:LYS:HG2	1:A:17:ILE:HD11	0.43	1.89	3	1
1:A:12:ASP:O	1:A:13:GLY:C	0.43	2.57	14	2
1:A:36:GLU:HG3	1:A:48:MET:CG	0.43	2.44	14	1
1:A:38:LEU:O	1:A:42:LEU:HD13	0.43	2.14	16	1
1:A:21:ASP:O	1:A:22:CYS:C	0.43	2.57	5	4
1:A:50:GLU:CG	1:A:51:GLU:N	0.43	2.81	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:THR:HB	1:A:81:PHE:CD1	0.43	2.48	3	1
1:A:97:GLY:O	1:A:98:ALA:C	0.43	2.57	3	11
1:A:79:THR:O	1:A:80:GLY:C	0.43	2.57	5	1
1:A:26:ASN:N	1:A:27:PRO:HD3	0.43	2.28	11	2
1:A:30:TRP:CE2	1:A:35:ALA:HB2	0.43	2.48	6	2
1:A:47:LYS:O	1:A:48:MET:C	0.43	2.57	10	3
1:A:63:TRP:CD2	1:A:63:TRP:O	0.43	2.72	9	1
1:A:81:PHE:O	1:A:82:SER:C	0.43	2.57	10	1
1:A:76:THR:HG23	1:A:77:LYS:N	0.43	2.29	5	1
1:A:19:ASP:O	1:A:20:GLU:C	0.43	2.57	19	2
1:A:86:ILE:H	1:A:86:ILE:HD12	0.43	1.73	19	1
1:A:18:LEU:HD22	1:A:22:CYS:O	0.43	2.13	9	1
1:A:72:ILE:HD11	1:A:83:LEU:HD12	0.43	1.91	9	1
1:A:96:HIS:O	1:A:97:GLY:C	0.43	2.57	11	2
1:A:16:VAL:HG13	1:A:24:MET:CB	0.43	2.42	16	1
1:A:24:MET:SD	1:A:26:ASN:CB	0.42	3.07	6	1
1:A:20:GLU:O	1:A:21:ASP:HB3	0.42	2.13	8	2
1:A:99:CYS:O	1:A:100:LYS:C	0.42	2.57	20	6
1:A:30:TRP:O	1:A:31:ASP:OD1	0.42	2.37	14	2
1:A:72:ILE:HG21	1:A:83:LEU:HD13	0.42	1.92	7	1
1:A:90:PHE:CE1	1:A:101:VAL:HG21	0.42	2.48	9	1
1:A:94:PRO:O	1:A:95:ALA:CB	0.42	2.65	16	1
1:A:11:VAL:O	1:A:12:ASP:C	0.42	2.57	1	4
1:A:53:TRP:HA	1:A:53:TRP:CE3	0.42	2.48	6	3
1:A:11:VAL:O	1:A:14:LYS:HB2	0.42	2.13	10	2
1:A:10:GLN:HA	1:A:14:LYS:O	0.42	2.15	2	2
1:A:6:PRO:HA	1:A:18:LEU:O	0.42	2.14	18	1
1:A:19:ASP:OD2	1:A:25:GLN:OE1	0.42	2.37	7	1
1:A:10:GLN:C	1:A:11:VAL:HG23	0.42	2.33	15	1
1:A:37:TRP:O	1:A:41:GLU:HG3	0.42	2.14	17	1
1:A:53:TRP:CE3	1:A:53:TRP:HA	0.42	2.49	17	1
1:A:78:GLU:O	1:A:79:THR:C	0.42	2.57	18	1
1:A:86:ILE:HG23	1:A:94:PRO:HG3	0.42	1.91	2	1
1:A:23:PHE:O	1:A:24:MET:C	0.42	2.57	4	2
1:A:12:ASP:C	1:A:12:ASP:OD1	0.42	2.57	9	1
1:A:80:GLY:O	1:A:81:PHE:C	0.42	2.58	10	1
1:A:90:PHE:CE1	1:A:97:GLY:HA3	0.42	2.50	2	1
1:A:59:LEU:O	1:A:60:ARG:C	0.42	2.58	3	1
1:A:71:PRO:HB3	1:A:95:ALA:HB2	0.42	1.91	16	1
1:A:73:LYS:O	1:A:76:THR:OG1	0.42	2.38	7	2
1:A:103:GLY:O	1:A:104:ALA:C	0.42	2.57	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:VAL:O	1:A:4:LYS:CB	0.42	2.68	12	1
1:A:82:SER:O	1:A:84:GLU:N	0.42	2.53	15	1
1:A:91:PRO:O	1:A:92:SER:HB2	0.42	2.14	7	1
1:A:86:ILE:CG2	1:A:94:PRO:HG3	0.42	2.45	11	1
1:A:55:LEU:O	1:A:59:LEU:CD1	0.42	2.65	19	1
1:A:98:ALA:O	1:A:99:CYS:C	0.42	2.57	1	1
1:A:5:CYS:HA	1:A:6:PRO:C	0.42	2.34	18	17
1:A:17:ILE:N	1:A:17:ILE:CD1	0.42	2.83	3	1
1:A:79:THR:O	1:A:81:PHE:N	0.42	2.53	5	1
1:A:3:VAL:HG11	1:A:37:TRP:CH2	0.42	2.50	14	1
1:A:63:TRP:CE3	1:A:63:TRP:C	0.42	2.94	17	1
1:A:17:ILE:O	1:A:24:MET:O	0.41	2.38	6	1
1:A:42:LEU:CD2	1:A:100:LYS:NZ	0.41	2.83	16	1
1:A:38:LEU:HD23	1:A:42:LEU:HD13	0.41	1.91	10	2
1:A:11:VAL:O	1:A:12:ASP:O	0.41	2.38	20	2
1:A:17:ILE:HG12	1:A:18:LEU:N	0.41	2.30	15	1
1:A:8:GLU:OE2	1:A:17:ILE:HG12	0.41	2.16	16	1
1:A:16:VAL:HG22	1:A:24:MET:CE	0.41	2.44	18	1
1:A:96:HIS:O	1:A:100:LYS:HB2	0.41	2.14	7	1
1:A:21:ASP:HB3	1:A:23:PHE:CD2	0.41	2.50	8	1
1:A:68:THR:HG22	1:A:69:CYS:N	0.41	2.30	20	1
1:A:52:HIS:NE2	1:A:89:LEU:HB3	0.41	2.29	3	1
1:A:72:ILE:CG1	1:A:83:LEU:HD11	0.41	2.45	9	1
1:A:6:PRO:HD3	1:A:20:GLU:CG	0.41	2.46	4	1
1:A:29:ASP:O	1:A:30:TRP:HB3	0.41	2.15	4	2
1:A:82:SER:O	1:A:83:LEU:C	0.41	2.57	15	1
1:A:68:THR:O	1:A:70:PRO:HD3	0.41	2.16	18	1
1:A:51:GLU:N	1:A:51:GLU:CD	0.41	2.74	1	1
1:A:101:VAL:O	1:A:102:ALA:C	0.41	2.59	3	1
1:A:3:VAL:CG2	1:A:41:GLU:HG3	0.41	2.45	7	1
1:A:65:THR:HG22	1:A:66:PHE:CE2	0.41	2.50	9	1
1:A:49:THR:HG22	1:A:50:GLU:H	0.41	1.76	11	1
1:A:63:TRP:O	1:A:67:GLY:N	0.41	2.54	10	1
1:A:29:ASP:O	1:A:30:TRP:C	0.41	2.59	14	1
1:A:3:VAL:HG21	1:A:41:GLU:CG	0.41	2.46	15	1
1:A:69:CYS:N	1:A:70:PRO:CD	0.41	2.84	16	1
1:A:71:PRO:CA	1:A:95:ALA:HB2	0.41	2.45	16	1
1:A:94:PRO:O	1:A:95:ALA:C	0.41	2.59	20	1
1:A:40:ARG:O	1:A:42:LEU:N	0.41	2.53	2	1
1:A:76:THR:CG2	1:A:77:LYS:N	0.41	2.82	5	1
1:A:8:GLU:OE1	1:A:8:GLU:O	0.41	2.39	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ILE:HG13	1:A:72:ILE:O	0.41	2.16	7	1
1:A:95:ALA:O	1:A:96:HIS:C	0.41	2.57	14	1
1:A:72:ILE:O	1:A:72:ILE:HG13	0.41	2.15	15	1
1:A:76:THR:O	1:A:77:LYS:C	0.41	2.59	20	1
1:A:11:VAL:O	1:A:14:LYS:CB	0.41	2.69	10	1
1:A:53:TRP:O	1:A:57:LYS:HB2	0.41	2.17	11	1
1:A:97:GLY:O	1:A:99:CYS:N	0.41	2.53	13	1
1:A:11:VAL:HG21	1:A:37:TRP:CZ3	0.41	2.50	18	1
1:A:99:CYS:SG	1:A:104:ALA:CB	0.41	3.06	18	1
1:A:3:VAL:HG13	1:A:9:TYR:CE2	0.40	2.51	6	1
1:A:52:HIS:CG	1:A:89:LEU:HD22	0.40	2.51	9	1
1:A:10:GLN:C	1:A:11:VAL:CG2	0.40	2.89	15	1
1:A:38:LEU:HD23	1:A:38:LEU:C	0.40	2.35	15	1
1:A:33:LYS:O	1:A:37:TRP:HB2	0.40	2.16	1	1
1:A:64:GLU:O	1:A:65:THR:C	0.40	2.60	5	1
1:A:45:ILE:O	1:A:46:GLN:C	0.40	2.58	6	1
1:A:48:MET:HB3	1:A:53:TRP:CD1	0.40	2.52	16	1
1:A:11:VAL:O	1:A:12:ASP:HB3	0.40	2.17	9	1
1:A:74:MET:SD	1:A:74:MET:C	0.40	2.99	17	1
1:A:43:GLU:OE1	1:A:45:ILE:CD1	0.40	2.69	15	1
1:A:95:ALA:O	1:A:99:CYS:HB2	0.40	2.16	16	1
1:A:66:PHE:O	1:A:67:GLY:C	0.40	2.60	12	1
1:A:30:TRP:CZ2	1:A:102:ALA:HA	0.40	2.51	19	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	102/111 (92%)	80±4 (79±4%)	16±4 (16±4%)	5±2 (5±2%)	4 24
All	All	2040/2220 (92%)	1608 (79%)	328 (16%)	104 (5%)	4 24

All 23 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	95	ALA	14
1	A	71	PRO	10
1	A	12	ASP	10
1	A	93	GLY	8
1	A	44	GLY	8
1	A	19	ASP	8
1	A	72	ILE	6
1	A	30	TRP	6
1	A	91	PRO	5
1	A	92	SER	5
1	A	94	PRO	4
1	A	81	PHE	3
1	A	67	GLY	3
1	A	45	ILE	3
1	A	4	LYS	2
1	A	66	PHE	2
1	A	48	MET	1
1	A	97	GLY	1
1	A	99	CYS	1
1	A	103	GLY	1
1	A	73	LYS	1
1	A	49	THR	1
1	A	79	THR	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	88/96 (92%)	63±3 (71±3%)	25±3 (29±3%)	2 18
All	All	1760/1920 (92%)	1251 (71%)	509 (29%)	2 18

All 64 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	38	LEU	14
1	A	85	LYS	14
1	A	87	TYR	14

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Mol	Chain	Res	Type	Models (Total)
1	A	59	LEU	12
1	A	77	LYS	12
1	A	40	ARG	12
1	A	31	ASP	12
1	A	74	MET	12
1	A	54	LYS	11
1	A	64	GLU	11
1	A	82	SER	11
1	A	62	TYR	11
1	A	23	PHE	10
1	A	42	LEU	10
1	A	73	LYS	10
1	A	81	PHE	10
1	A	15	LYS	10
1	A	25	GLN	10
1	A	55	LEU	10
1	A	88	GLN	10
1	A	4	LYS	10
1	A	14	LYS	10
1	A	100	LYS	10
1	A	28	GLU	10
1	A	47	LYS	9
1	A	60	ARG	9
1	A	33	LYS	9
1	A	92	SER	9
1	A	57	LYS	9
1	A	90	PHE	9
1	A	24	MET	8
1	A	50	GLU	8
1	A	78	GLU	8
1	A	58	TYR	8
1	A	84	GLU	8
1	A	68	THR	8
1	A	19	ASP	7
1	A	29	ASP	7
1	A	43	GLU	7
1	A	20	GLU	7
1	A	32	GLU	7
1	A	36	GLU	7
1	A	52	HIS	7
1	A	66	PHE	7
1	A	99	CYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	21	ASP	6
1	A	69	CYS	6
1	A	51	GLU	6
1	A	72	ILE	6
1	A	46	GLN	6
1	A	61	GLU	5
1	A	65	THR	5
1	A	8	GLU	5
1	A	41	GLU	5
1	A	83	LEU	4
1	A	48	MET	4
1	A	26	ASN	3
1	A	79	THR	3
1	A	96	HIS	3
1	A	10	GLN	3
1	A	12	ASP	3
1	A	76	THR	2
1	A	49	THR	2
1	A	89	LEU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided