



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:16 AM GMT

PDB ID : 2Q44  
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At1g77540  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 1.15 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

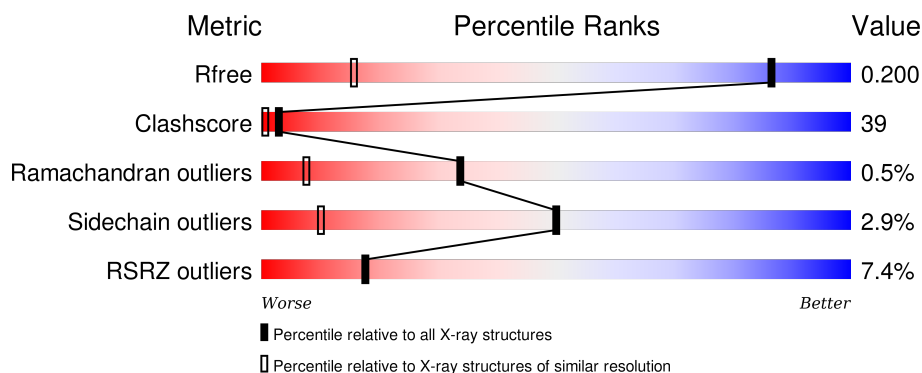
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.15 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	1495 (1.20-1.08)
Clashscore	102246	1593 (1.20-1.08)
Ramachandran outliers	100387	1521 (1.20-1.08)
Sidechain outliers	100360	1518 (1.20-1.08)
RSRZ outliers	91569	1498 (1.20-1.08)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	1-A	103	<div> <div>7%</div> <div>16%</div> <div>43%</div> <div>25%</div> <div>9%</div> <div>8%</div> </div>
1	2-A	103	<div> <div>7%</div> <div>17%</div> <div>41%</div> <div>25%</div> <div>10%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BR	1-A	202	-	-	X	-
3	BR	1-A	205	-	-	X	X
3	BR	1-A	206	-	-	X	-
3	BR	1-A	207	-	-	X	X
3	BR	1-A	210	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1797 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 Uncharacterized protein At1g77540.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	95	Total	C	N	O	S	0	0	0
			768	494	134	136	4			
1	2-A	95	Total	C	N	O	S	0	0	0
			768	494	134	136	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9CAQ2

- Molecule 2 is BROMIDE ION (three-letter code: HOH, BR) (formula: H<sub>2</sub>O, Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	11	Total	Br	0	0
			11	11		

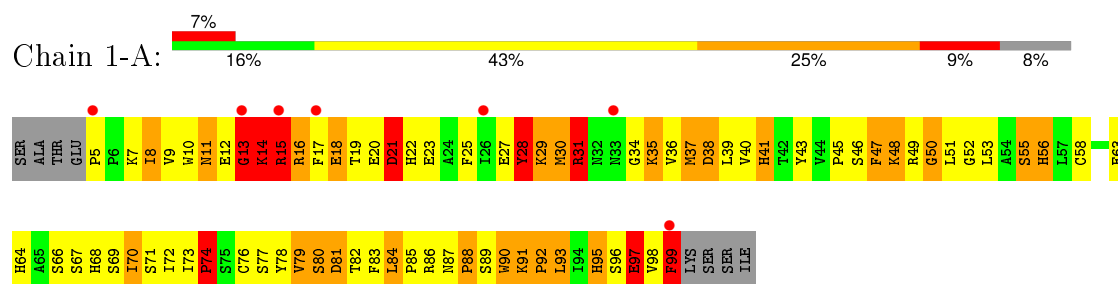
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	125	Total	O	0	0
			125	125		

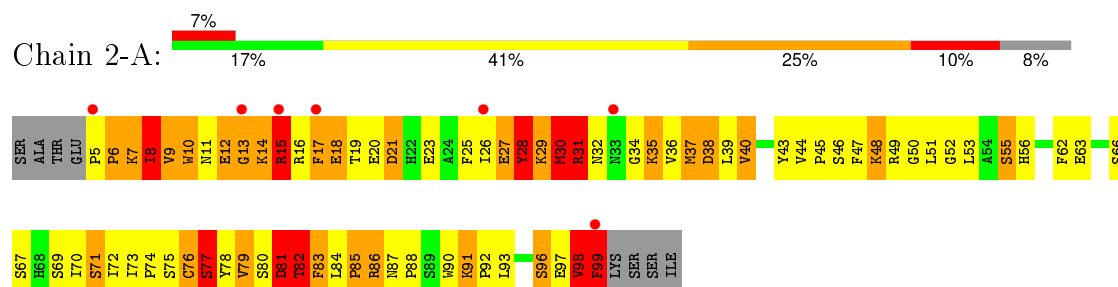
### 3 Residue-property plots [i](#)

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: Uncharacterized protein At1g77540



#### • Molecule 1: Uncharacterized protein At1g77540



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	27.35Å 60.60Å 29.42Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	20.29 – 1.15 20.29 – 1.15	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.29-1.15) 95.9 (20.29-1.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 1.15Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.165 , 0.190 0.173 , 0.200	Depositor DCC
$R_{free}$ test set	1658 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.5	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 50.3	EDS
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32689 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	1797	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: BR

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	1-A	4.13	135/793 (17.0%)	3.10	89/1074 (8.3%)
1	2-A	3.93	124/793 (15.6%)	3.10	99/1074 (9.2%)
All	All	4.03	259/1586 (16.3%)	3.10	188/2148 (8.8%)

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	1-A	0	9
1	2-A	0	10
All	All	0	19

All (259) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	12	GLU	CB-CG	-21.43	1.11	1.52
1	1-A	31	ARG	CG-CD	21.32	2.05	1.51
1	1-A	83	PHE	CG-CD2	-20.12	1.08	1.38
1	2-A	96	SER	CB-OG	17.50	1.65	1.42
1	2-A	8	ILE	CB-CG1	17.43	2.02	1.54
1	2-A	83	PHE	CG-CD2	16.74	1.63	1.38
1	2-A	76	CYS	CB-SG	-16.28	1.54	1.82
1	1-A	80	SER	CB-OG	-16.18	1.21	1.42
1	2-A	99	PHE	C-O	16.07	1.53	1.23
1	2-A	83	PHE	CB-CG	15.24	1.77	1.51
1	1-A	89	SER	CB-OG	-15.06	1.22	1.42
1	1-A	80	SER	CA-CB	15.05	1.75	1.52
1	1-A	83	PHE	CG-CD1	14.73	1.60	1.38
1	2-A	29	LYS	CG-CD	14.31	2.01	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	90	TRP	CD2-CE2	-13.34	1.25	1.41
1	1-A	38	ASP	CG-OD2	13.21	1.55	1.25
1	2-A	80	SER	CA-CB	-13.18	1.33	1.52
1	2-A	83	PHE	CG-CD1	-12.73	1.19	1.38
1	1-A	83	PHE	CB-CG	-12.71	1.29	1.51
1	2-A	30	MET	CG-SD	12.58	2.13	1.81
1	1-A	67	SER	CA-CB	12.54	1.71	1.52
1	2-A	91	LYS	CE-NZ	12.43	1.80	1.49
1	2-A	78	TYR	CE2-CZ	-12.40	1.22	1.38
1	2-A	39	LEU	C-O	12.12	1.46	1.23
1	1-A	71	SER	CA-CB	-11.97	1.34	1.52
1	1-A	20	GLU	CG-CD	11.92	1.69	1.51
1	1-A	90	TRP	CZ3-CH2	-11.87	1.21	1.40
1	2-A	23	GLU	CG-CD	-11.59	1.34	1.51
1	1-A	23	GLU	CD-OE2	11.46	1.38	1.25
1	1-A	96	SER	CA-CB	11.28	1.69	1.52
1	1-A	27	GLU	CD-OE1	11.15	1.38	1.25
1	2-A	48	LYS	CB-CG	-11.06	1.22	1.52
1	1-A	15	ARG	CZ-NH1	11.03	1.47	1.33
1	1-A	16	ARG	CG-CD	11.01	1.79	1.51
1	2-A	46	SER	CA-CB	10.96	1.69	1.52
1	2-A	67	SER	CB-OG	-10.93	1.28	1.42
1	1-A	10	TRP	CZ3-CH2	-10.80	1.22	1.40
1	1-A	18	GLU	CD-OE2	10.63	1.37	1.25
1	1-A	16	ARG	CZ-NH2	10.61	1.46	1.33
1	1-A	31	ARG	NE-CZ	10.46	1.46	1.33
1	2-A	29	LYS	CE-NZ	-10.40	1.23	1.49
1	1-A	74	PRO	CG-CD	10.36	1.84	1.50
1	1-A	96	SER	CB-OG	-10.29	1.28	1.42
1	1-A	29	LYS	CD-CE	10.25	1.76	1.51
1	1-A	46	SER	CA-CB	-10.24	1.37	1.52
1	1-A	28	TYR	CG-CD1	10.17	1.52	1.39
1	2-A	99	PHE	CE1-CZ	-9.95	1.18	1.37
1	1-A	43	TYR	CB-CG	-9.91	1.36	1.51
1	1-A	91	LYS	CE-NZ	9.90	1.73	1.49
1	1-A	30	MET	SD-CE	-9.89	1.22	1.77
1	2-A	34	GLY	C-O	9.75	1.39	1.23
1	1-A	70	ILE	C-O	9.73	1.41	1.23
1	2-A	76	CYS	CA-CB	9.69	1.75	1.53
1	1-A	99	PHE	CA-C	9.63	1.77	1.52
1	1-A	99	PHE	CD1-CE1	9.59	1.58	1.39
1	1-A	14	LYS	CA-C	9.51	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	47	PHE	CD1-CE1	-9.21	1.20	1.39
1	1-A	21	ASP	CG-OD2	9.15	1.46	1.25
1	2-A	13	GLY	N-CA	9.13	1.59	1.46
1	2-A	31	ARG	CZ-NH2	9.10	1.44	1.33
1	1-A	16	ARG	CB-CG	-9.06	1.28	1.52
1	1-A	99	PHE	CB-CG	9.05	1.66	1.51
1	1-A	97	GLU	CG-CD	9.03	1.65	1.51
1	2-A	29	LYS	CA-C	-8.99	1.29	1.52
1	2-A	90	TRP	CB-CG	-8.93	1.34	1.50
1	2-A	28	TYR	CG-CD2	-8.92	1.27	1.39
1	1-A	81	ASP	CG-OD2	-8.91	1.04	1.25
1	1-A	78	TYR	CD2-CE2	8.86	1.52	1.39
1	1-A	34	GLY	C-O	8.80	1.37	1.23
1	1-A	98	VAL	CA-CB	8.68	1.73	1.54
1	2-A	9	VAL	CB-CG1	8.65	1.71	1.52
1	2-A	47	PHE	CG-CD1	8.65	1.51	1.38
1	2-A	19	THR	C-O	-8.63	1.06	1.23
1	1-A	9	VAL	CB-CG1	-8.62	1.34	1.52
1	1-A	28	TYR	CE1-CZ	8.57	1.49	1.38
1	2-A	12	GLU	CD-OE1	-8.49	1.16	1.25
1	1-A	97	GLU	CD-OE2	-8.47	1.16	1.25
1	1-A	47	PHE	CD2-CE2	-8.41	1.22	1.39
1	1-A	46	SER	CB-OG	-8.34	1.31	1.42
1	2-A	71	SER	CB-OG	-8.33	1.31	1.42
1	2-A	18	GLU	CG-CD	8.30	1.64	1.51
1	2-A	97	GLU	CD-OE1	8.26	1.34	1.25
1	1-A	99	PHE	C-O	8.25	1.39	1.23
1	1-A	47	PHE	CD1-CE1	8.23	1.55	1.39
1	2-A	75	SER	CB-OG	-8.22	1.31	1.42
1	1-A	48	LYS	CB-CG	8.20	1.74	1.52
1	1-A	88	PRO	CG-CD	-8.13	1.23	1.50
1	1-A	27	GLU	CB-CG	-8.02	1.36	1.52
1	2-A	36	VAL	CB-CG2	-8.01	1.36	1.52
1	2-A	9	VAL	CB-CG2	8.01	1.69	1.52
1	2-A	16	ARG	CA-CB	-7.90	1.36	1.53
1	2-A	15	ARG	CZ-NH1	7.90	1.43	1.33
1	1-A	77	SER	CB-OG	7.89	1.52	1.42
1	2-A	74	PRO	CA-C	-7.88	1.37	1.52
1	1-A	27	GLU	CD-OE2	7.87	1.34	1.25
1	1-A	74	PRO	N-CD	7.86	1.58	1.47
1	1-A	41	HIS	C-N	-7.71	1.16	1.34
1	1-A	30	MET	CG-SD	-7.69	1.61	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	70	ILE	CA-CB	7.64	1.72	1.54
1	1-A	78	TYR	CG-CD1	-7.57	1.29	1.39
1	1-A	90	TRP	NE1-CE2	7.54	1.47	1.37
1	2-A	71	SER	CA-CB	7.51	1.64	1.52
1	1-A	50	GLY	CA-C	-7.47	1.39	1.51
1	2-A	40	VAL	CB-CG2	-7.47	1.37	1.52
1	2-A	35	LYS	CG-CD	7.41	1.77	1.52
1	1-A	90	TRP	CB-CG	7.39	1.63	1.50
1	1-A	16	ARG	CZ-NH1	-7.36	1.23	1.33
1	1-A	76	CYS	N-CA	7.35	1.61	1.46
1	2-A	20	GLU	CD-OE1	7.35	1.33	1.25
1	1-A	36	VAL	N-CA	7.33	1.61	1.46
1	2-A	12	GLU	CA-CB	-7.31	1.37	1.53
1	1-A	43	TYR	CZ-OH	7.25	1.50	1.37
1	2-A	96	SER	CA-CB	7.24	1.63	1.52
1	2-A	7	LYS	CD-CE	7.23	1.69	1.51
1	1-A	38	ASP	C-N	7.15	1.50	1.34
1	1-A	35	LYS	CG-CD	7.12	1.76	1.52
1	2-A	28	TYR	CD1-CE1	-7.12	1.28	1.39
1	1-A	31	ARG	CZ-NH2	7.10	1.42	1.33
1	2-A	83	PHE	N-CA	-7.08	1.32	1.46
1	1-A	95	HIS	CA-C	-7.04	1.34	1.52
1	2-A	76	CYS	N-CA	-7.04	1.32	1.46
1	2-A	32	ASN	CA-C	-7.02	1.34	1.52
1	1-A	81	ASP	CG-OD1	-7.01	1.09	1.25
1	2-A	47	PHE	CE1-CZ	-6.94	1.24	1.37
1	1-A	35	LYS	C-O	-6.94	1.10	1.23
1	2-A	12	GLU	CG-CD	6.91	1.62	1.51
1	2-A	31	ARG	C-O	-6.86	1.10	1.23
1	2-A	79	VAL	CB-CG1	-6.77	1.38	1.52
1	2-A	52	GLY	C-O	-6.73	1.12	1.23
1	2-A	11	ASN	CA-C	-6.73	1.35	1.52
1	2-A	47	PHE	CD2-CE2	-6.71	1.25	1.39
1	1-A	95	HIS	CG-CD2	-6.68	1.24	1.35
1	2-A	73	ILE	CG1-CD1	-6.67	1.04	1.50
1	1-A	69	SER	C-O	6.66	1.36	1.23
1	2-A	43	TYR	CZ-OH	-6.66	1.26	1.37
1	2-A	35	LYS	C-O	6.65	1.35	1.23
1	1-A	35	LYS	CA-C	-6.64	1.35	1.52
1	2-A	98	VAL	CB-CG2	-6.64	1.39	1.52
1	2-A	81	ASP	CB-CG	-6.61	1.37	1.51
1	1-A	28	TYR	CE2-CZ	6.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	11	ASN	CB-CG	-6.53	1.36	1.51
1	2-A	44	VAL	C-N	-6.49	1.22	1.34
1	1-A	31	ARG	CB-CG	6.49	1.70	1.52
1	2-A	26	ILE	CA-C	-6.46	1.36	1.52
1	2-A	15	ARG	CG-CD	6.45	1.68	1.51
1	2-A	67	SER	CA-CB	-6.44	1.43	1.52
1	2-A	27	GLU	CG-CD	6.43	1.61	1.51
1	1-A	45	PRO	N-CA	6.42	1.58	1.47
1	2-A	28	TYR	CB-CG	-6.37	1.42	1.51
1	1-A	99	PHE	CE1-CZ	6.37	1.49	1.37
1	1-A	82	THR	C-N	6.34	1.48	1.34
1	2-A	98	VAL	CA-CB	6.34	1.68	1.54
1	2-A	99	PHE	CA-C	6.34	1.69	1.52
1	2-A	90	TRP	CD1-NE1	6.32	1.48	1.38
1	2-A	10	TRP	CD2-CE3	6.32	1.49	1.40
1	2-A	31	ARG	C-N	6.31	1.48	1.34
1	2-A	38	ASP	CB-CG	-6.30	1.38	1.51
1	1-A	78	TYR	CE1-CZ	-6.29	1.30	1.38
1	2-A	50	GLY	C-O	6.28	1.33	1.23
1	1-A	96	SER	C-O	6.26	1.35	1.23
1	2-A	78	TYR	CG-CD2	6.23	1.47	1.39
1	1-A	77	SER	CA-CB	6.16	1.62	1.52
1	1-A	5	PRO	CG-CD	6.13	1.70	1.50
1	1-A	47	PHE	CB-CG	-6.12	1.41	1.51
1	2-A	45	PRO	N-CD	-6.11	1.39	1.47
1	1-A	83	PHE	CD2-CE2	6.10	1.51	1.39
1	2-A	17	PHE	CE1-CZ	6.10	1.49	1.37
1	1-A	36	VAL	CB-CG2	6.09	1.65	1.52
1	2-A	55	SER	C-N	-6.09	1.20	1.34
1	2-A	30	MET	N-CA	-6.08	1.34	1.46
1	2-A	15	ARG	C-N	6.08	1.48	1.34
1	1-A	78	TYR	CZ-OH	6.07	1.48	1.37
1	1-A	81	ASP	CA-C	-6.07	1.37	1.52
1	2-A	28	TYR	C-N	6.06	1.48	1.34
1	1-A	91	LYS	CD-CE	6.05	1.66	1.51
1	2-A	45	PRO	CA-C	-6.04	1.40	1.52
1	1-A	13	GLY	CA-C	-6.02	1.42	1.51
1	1-A	10	TRP	CE3-CZ3	5.98	1.48	1.38
1	2-A	5	PRO	CG-CD	5.98	1.70	1.50
1	2-A	28	TYR	CE2-CZ	-5.96	1.30	1.38
1	1-A	90	TRP	CD1-NE1	-5.93	1.27	1.38
1	2-A	51	LEU	CB-CG	5.93	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	98	VAL	CB-CG2	5.92	1.65	1.52
1	1-A	86	ARG	CG-CD	-5.91	1.37	1.51
1	1-A	78	TYR	CB-CG	-5.88	1.42	1.51
1	1-A	43	TYR	CE1-CZ	-5.87	1.30	1.38
1	2-A	38	ASP	CG-OD2	5.85	1.38	1.25
1	1-A	10	TRP	C-N	-5.82	1.20	1.34
1	1-A	11	ASN	N-CA	-5.81	1.34	1.46
1	2-A	7	LYS	CB-CG	-5.77	1.36	1.52
1	1-A	47	PHE	CG-CD1	5.75	1.47	1.38
1	1-A	99	PHE	CE2-CZ	-5.75	1.26	1.37
1	1-A	51	LEU	C-O	5.72	1.34	1.23
1	2-A	96	SER	N-CA	5.69	1.57	1.46
1	1-A	25	PHE	CG-CD1	5.67	1.47	1.38
1	1-A	72	ILE	CB-CG1	-5.65	1.38	1.54
1	1-A	92	PRO	C-O	-5.64	1.11	1.23
1	2-A	12	GLU	N-CA	-5.64	1.35	1.46
1	1-A	8	ILE	C-O	5.61	1.34	1.23
1	2-A	84	LEU	CG-CD2	5.60	1.72	1.51
1	2-A	69	SER	CB-OG	-5.59	1.34	1.42
1	2-A	31	ARG	CD-NE	5.59	1.55	1.46
1	1-A	56	HIS	C-O	5.58	1.33	1.23
1	1-A	63	GLU	CG-CD	-5.57	1.43	1.51
1	2-A	47	PHE	CG-CD2	-5.56	1.30	1.38
1	2-A	23	GLU	C-N	-5.56	1.21	1.34
1	1-A	90	TRP	CE2-CZ2	5.55	1.49	1.39
1	1-A	85	PRO	C-N	5.54	1.46	1.34
1	2-A	90	TRP	CZ2-CH2	-5.54	1.26	1.37
1	1-A	9	VAL	CB-CG2	-5.51	1.41	1.52
1	1-A	47	PHE	CA-CB	5.50	1.66	1.53
1	2-A	76	CYS	CA-C	5.50	1.67	1.52
1	2-A	31	ARG	CZ-NH1	5.50	1.40	1.33
1	2-A	13	GLY	C-N	5.48	1.46	1.34
1	2-A	90	TRP	CE3-CZ3	5.47	1.47	1.38
1	2-A	17	PHE	CG-CD1	5.45	1.47	1.38
1	1-A	93	LEU	CA-CB	-5.43	1.41	1.53
1	1-A	23	GLU	CD-OE1	5.42	1.31	1.25
1	2-A	97	GLU	CG-CD	-5.40	1.43	1.51
1	1-A	13	GLY	C-O	5.38	1.32	1.23
1	2-A	31	ARG	CG-CD	5.38	1.65	1.51
1	2-A	66	SER	CA-CB	5.37	1.61	1.52
1	1-A	68	HIS	CB-CG	-5.37	1.40	1.50
1	2-A	14	LYS	CE-NZ	5.37	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	88	PRO	CB-CG	5.37	1.76	1.50
1	2-A	79	VAL	N-CA	5.35	1.57	1.46
1	2-A	21	ASP	CG-OD2	5.35	1.37	1.25
1	1-A	66	SER	CA-C	-5.32	1.39	1.52
1	2-A	31	ARG	CA-CB	5.32	1.65	1.53
1	2-A	77	SER	C-N	-5.31	1.21	1.34
1	1-A	97	GLU	CB-CG	5.31	1.62	1.52
1	1-A	12	GLU	CG-CD	5.30	1.59	1.51
1	1-A	95	HIS	C-N	5.30	1.46	1.34
1	1-A	20	GLU	C-O	5.30	1.33	1.23
1	1-A	64	HIS	CB-CG	-5.28	1.40	1.50
1	2-A	88	PRO	CG-CD	5.25	1.68	1.50
1	2-A	21	ASP	CA-C	5.25	1.66	1.52
1	2-A	86	ARG	CZ-NH2	5.25	1.39	1.33
1	1-A	25	PHE	CD1-CE1	5.22	1.49	1.39
1	1-A	28	TYR	CD1-CE1	-5.19	1.31	1.39
1	2-A	16	ARG	CA-C	-5.19	1.39	1.52
1	1-A	99	PHE	CG-CD1	5.19	1.46	1.38
1	1-A	47	PHE	CE1-CZ	-5.19	1.27	1.37
1	2-A	34	GLY	N-CA	5.17	1.53	1.46
1	1-A	84	LEU	C-O	-5.16	1.13	1.23
1	1-A	55	SER	CB-OG	5.14	1.49	1.42
1	1-A	51	LEU	CG-CD2	-5.13	1.32	1.51
1	2-A	14	LYS	CA-CB	-5.13	1.42	1.53
1	2-A	15	ARG	N-CA	5.12	1.56	1.46
1	1-A	15	ARG	C-N	-5.12	1.22	1.34
1	1-A	76	CYS	CA-CB	5.11	1.65	1.53
1	2-A	12	GLU	C-N	5.09	1.42	1.33
1	2-A	16	ARG	CZ-NH2	5.08	1.39	1.33
1	2-A	85	PRO	N-CD	-5.06	1.40	1.47
1	1-A	20	GLU	CD-OE1	5.05	1.31	1.25
1	1-A	58	CYS	C-O	5.05	1.32	1.23
1	1-A	80	SER	C-O	5.04	1.32	1.23
1	1-A	20	GLU	CB-CG	-5.02	1.42	1.52
1	2-A	28	TYR	CG-CD1	5.01	1.45	1.39

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	31	ARG	NE-CZ-NH2	27.75	134.17	120.30
1	2-A	38	ASP	CB-CG-OD2	-24.60	96.16	118.30
1	1-A	31	ARG	NH1-CZ-NH2	-15.58	102.27	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	81	ASP	CB-CG-OD1	-14.94	104.86	118.30
1	1-A	81	ASP	CB-CG-OD2	14.86	131.68	118.30
1	1-A	17	PHE	CB-CG-CD1	-14.84	110.41	120.80
1	2-A	83	PHE	CZ-CE2-CD2	-14.26	102.99	120.10
1	1-A	96	SER	CA-CB-OG	-14.16	72.96	111.20
1	2-A	81	ASP	CB-CG-OD2	14.05	130.95	118.30
1	1-A	23	GLU	OE1-CD-OE2	14.03	140.13	123.30
1	2-A	63	GLU	OE1-CD-OE2	-13.83	106.70	123.30
1	2-A	97	GLU	OE1-CD-OE2	13.00	138.90	123.30
1	2-A	17	PHE	CB-CG-CD2	-12.85	111.81	120.80
1	2-A	49	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	1-A	38	ASP	CB-CG-OD2	12.45	129.50	118.30
1	2-A	29	LYS	CD-CE-NZ	12.32	140.03	111.70
1	1-A	23	GLU	CG-CD-OE2	-11.31	95.67	118.30
1	2-A	18	GLU	OE1-CD-OE2	11.14	136.68	123.30
1	1-A	78	TYR	CB-CG-CD2	10.96	127.58	121.00
1	1-A	78	TYR	CG-CD1-CE1	10.88	130.01	121.30
1	1-A	83	PHE	CG-CD2-CE2	10.87	132.75	120.80
1	1-A	17	PHE	CG-CD2-CE2	-10.47	109.28	120.80
1	1-A	37	MET	CG-SD-CE	-10.44	83.50	100.20
1	2-A	62	PHE	CB-CG-CD1	10.41	128.09	120.80
1	2-A	31	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	1-A	63	GLU	OE1-CD-OE2	10.34	135.71	123.30
1	2-A	27	GLU	OE1-CD-OE2	-10.33	110.91	123.30
1	2-A	16	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	1-A	38	ASP	OD1-CG-OD2	-10.16	104.00	123.30
1	2-A	43	TYR	CB-CG-CD2	10.08	127.05	121.00
1	1-A	47	PHE	CB-CG-CD2	9.50	127.45	120.80
1	2-A	31	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	2-A	78	TYR	CG-CD1-CE1	-9.24	113.90	121.30
1	1-A	28	TYR	CG-CD2-CE2	-8.94	114.15	121.30
1	1-A	41	HIS	N-CA-CB	-8.81	94.74	110.60
1	2-A	78	TYR	CG-CD2-CE2	-8.77	114.29	121.30
1	1-A	16	ARG	CG-CD-NE	8.76	130.19	111.80
1	2-A	90	TRP	CB-CG-CD1	-8.70	115.69	127.00
1	2-A	9	VAL	CA-CB-CG1	-8.48	98.18	110.90
1	1-A	39	LEU	CA-C-O	-8.39	102.48	120.10
1	1-A	17	PHE	CD1-CE1-CZ	-8.33	110.10	120.10
1	1-A	99	PHE	CG-CD2-CE2	8.30	129.93	120.80
1	2-A	87	ASN	CB-CG-OD1	-8.29	105.02	121.60
1	2-A	7	LYS	CD-CE-NZ	-8.21	92.81	111.70
1	1-A	18	GLU	OE1-CD-OE2	-8.05	113.63	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	28	TYR	CZ-CE2-CD2	8.03	127.03	119.80
1	1-A	38	ASP	CB-CG-OD1	8.02	125.52	118.30
1	2-A	62	PHE	CB-CG-CD2	-8.00	115.20	120.80
1	2-A	38	ASP	CB-CG-OD1	7.96	125.47	118.30
1	2-A	8	ILE	CB-CG1-CD1	-7.92	91.71	113.90
1	1-A	73	ILE	CG1-CB-CG2	7.91	128.80	111.40
1	1-A	78	TYR	CG-CD2-CE2	-7.90	114.98	121.30
1	2-A	31	ARG	CD-NE-CZ	-7.67	112.86	123.60
1	1-A	28	TYR	CB-CG-CD2	-7.63	116.42	121.00
1	1-A	85	PRO	O-C-N	-7.61	110.52	122.70
1	2-A	27	GLU	CG-CD-OE2	7.58	133.47	118.30
1	1-A	84	LEU	CB-CG-CD1	-7.57	98.13	111.00
1	2-A	78	TYR	CB-CG-CD2	-7.56	116.46	121.00
1	2-A	10	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	1-A	47	PHE	CG-CD1-CE1	-7.29	112.78	120.80
1	1-A	98	VAL	CG1-CB-CG2	7.23	122.47	110.90
1	1-A	12	GLU	OE1-CD-OE2	7.19	131.93	123.30
1	2-A	90	TRP	CD1-NE1-CE2	-7.15	102.56	109.00
1	1-A	97	GLU	OE1-CD-OE2	7.15	131.88	123.30
1	1-A	99	PHE	CG-CD1-CE1	-7.15	112.93	120.80
1	2-A	82	THR	O-C-N	-7.09	111.36	122.70
1	1-A	88	PRO	N-CA-CB	-7.04	94.85	103.30
1	2-A	9	VAL	CG1-CB-CG2	7.03	122.15	110.90
1	2-A	49	ARG	CD-NE-CZ	7.02	133.43	123.60
1	1-A	22	HIS	N-CA-CB	7.00	123.20	110.60
1	2-A	30	MET	O-C-N	7.00	133.90	122.70
1	2-A	90	TRP	CB-CG-CD2	6.98	135.67	126.60
1	2-A	5	PRO	N-CA-CB	6.96	111.65	103.30
1	2-A	25	PHE	CB-CG-CD1	-6.89	115.97	120.80
1	1-A	78	TYR	CA-C-O	6.89	134.56	120.10
1	1-A	98	VAL	CA-CB-CG2	-6.86	100.61	110.90
1	2-A	66	SER	O-C-N	-6.81	111.81	122.70
1	1-A	95	HIS	CA-C-O	6.81	134.40	120.10
1	1-A	49	ARG	CA-CB-CG	-6.80	98.44	113.40
1	2-A	11	ASN	CB-CA-C	6.79	123.99	110.40
1	1-A	31	ARG	CD-NE-CZ	-6.76	114.14	123.60
1	1-A	80	SER	CA-C-O	-6.76	105.90	120.10
1	2-A	88	PRO	N-CD-CG	-6.73	93.10	103.20
1	2-A	86	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	1-A	92	PRO	N-CD-CG	-6.71	93.14	103.20
1	1-A	21	ASP	CB-CG-OD1	6.71	124.33	118.30
1	2-A	90	TRP	CA-CB-CG	-6.66	101.05	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	51	LEU	CA-CB-CG	-6.65	100.00	115.30
1	1-A	80	SER	CA-CB-OG	-6.62	93.32	111.20
1	1-A	50	GLY	O-C-N	-6.57	112.19	122.70
1	2-A	8	ILE	O-C-N	-6.53	112.26	122.70
1	1-A	14	LYS	CD-CE-NZ	-6.49	96.77	111.70
1	2-A	90	TRP	CH2-CZ2-CE2	-6.47	110.93	117.40
1	1-A	90	TRP	CZ3-CH2-CZ2	6.46	129.35	121.60
1	1-A	21	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	2-A	37	MET	CG-SD-CE	6.45	110.52	100.20
1	2-A	23	GLU	CG-CD-OE2	-6.45	105.40	118.30
1	2-A	99	PHE	N-CA-C	6.44	128.38	111.00
1	2-A	8	ILE	CG1-CB-CG2	-6.40	97.32	111.40
1	2-A	38	ASP	OD1-CG-OD2	6.33	135.33	123.30
1	2-A	90	TRP	O-C-N	-6.32	112.59	122.70
1	1-A	81	ASP	OD1-CG-OD2	-6.31	111.31	123.30
1	2-A	78	TYR	CE1-CZ-CE2	6.29	129.87	119.80
1	2-A	28	TYR	CG-CD2-CE2	6.26	126.31	121.30
1	1-A	39	LEU	O-C-N	6.24	132.68	122.70
1	1-A	16	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	2-A	25	PHE	CD1-CG-CD2	6.22	126.39	118.30
1	2-A	90	TRP	CZ3-CH2-CZ2	6.22	129.06	121.60
1	2-A	31	ARG	CA-C-O	6.21	133.15	120.10
1	1-A	10	TRP	CG-CD1-NE1	6.16	116.26	110.10
1	1-A	95	HIS	O-C-N	-6.15	112.85	122.70
1	2-A	36	VAL	O-C-N	-6.12	112.90	122.70
1	1-A	7	LYS	O-C-N	6.06	132.40	122.70
1	1-A	25	PHE	CZ-CE2-CD2	-6.05	112.83	120.10
1	1-A	47	PHE	CB-CG-CD1	-6.02	116.59	120.80
1	2-A	10	TRP	CB-CG-CD2	-5.95	118.86	126.60
1	2-A	75	SER	C-N-CA	5.95	136.58	121.70
1	2-A	87	ASN	CB-CG-ND2	5.94	130.96	116.70
1	2-A	30	MET	C-N-CA	-5.94	106.85	121.70
1	1-A	90	TRP	CE3-CZ3-CH2	-5.93	114.67	121.20
1	1-A	53	LEU	CB-CG-CD2	-5.93	100.92	111.00
1	2-A	23	GLU	CG-CD-OE1	5.92	130.13	118.30
1	1-A	98	VAL	C-N-CA	5.91	136.46	121.70
1	1-A	31	ARG	O-C-N	-5.90	113.25	122.70
1	1-A	84	LEU	CA-CB-CG	-5.86	101.81	115.30
1	2-A	39	LEU	CA-C-O	5.85	132.38	120.10
1	1-A	21	ASP	OD1-CG-OD2	-5.83	112.22	123.30
1	1-A	30	MET	CB-CA-C	-5.82	98.76	110.40
1	2-A	13	GLY	C-N-CA	5.82	136.24	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	25	PHE	CG-CD1-CE1	-5.79	114.44	120.80
1	2-A	20	GLU	CA-CB-CG	-5.78	100.69	113.40
1	2-A	20	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	1-A	95	HIS	N-CA-CB	-5.70	100.34	110.60
1	1-A	51	LEU	CA-CB-CG	5.69	128.38	115.30
1	2-A	17	PHE	CB-CG-CD1	5.68	124.78	120.80
1	2-A	12	GLU	OE1-CD-OE2	5.68	130.12	123.30
1	2-A	53	LEU	CB-CG-CD2	5.67	120.64	111.00
1	2-A	31	ARG	CA-C-N	-5.65	104.77	117.20
1	2-A	83	PHE	CE1-CZ-CE2	5.65	130.17	120.00
1	2-A	21	ASP	N-CA-CB	5.65	120.77	110.60
1	2-A	10	TRP	CD2-CE3-CZ3	-5.63	111.48	118.80
1	1-A	63	GLU	CG-CD-OE2	-5.59	107.12	118.30
1	1-A	10	TRP	CD1-CG-CD2	-5.59	101.83	106.30
1	1-A	45	PRO	CA-CB-CG	5.58	115.41	104.80
1	1-A	80	SER	N-CA-CB	-5.55	102.18	110.50
1	2-A	26	ILE	O-C-N	-5.55	113.82	122.70
1	2-A	18	GLU	CG-CD-OE2	-5.51	107.28	118.30
1	1-A	90	TRP	CB-CG-CD1	5.50	134.14	127.00
1	1-A	86	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	2-A	16	ARG	NH1-CZ-NH2	5.45	125.39	119.40
1	2-A	34	GLY	O-C-N	-5.45	113.99	122.70
1	1-A	78	TYR	CB-CG-CD1	-5.44	117.73	121.00
1	2-A	83	PHE	CB-CG-CD2	-5.42	117.00	120.80
1	2-A	66	SER	CA-C-N	5.41	129.11	117.20
1	2-A	88	PRO	O-C-N	5.41	131.36	122.70
1	2-A	31	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	2-A	14	LYS	CD-CE-NZ	-5.32	99.47	111.70
1	1-A	17	PHE	CD1-CG-CD2	5.31	125.20	118.30
1	2-A	10	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	1-A	90	TRP	CB-CG-CD2	-5.29	119.73	126.60
1	2-A	47	PHE	CB-CG-CD1	5.28	124.50	120.80
1	2-A	51	LEU	CB-CG-CD1	-5.26	102.05	111.00
1	2-A	6	PRO	O-C-N	5.24	131.09	122.70
1	2-A	51	LEU	CA-C-N	5.24	126.68	116.20
1	2-A	25	PHE	CZ-CE2-CD2	-5.23	113.82	120.10
1	2-A	55	SER	N-CA-CB	-5.23	102.66	110.50
1	2-A	92	PRO	O-C-N	5.21	131.04	122.70
1	2-A	76	CYS	N-CA-CB	5.18	119.92	110.60
1	1-A	21	ASP	O-C-N	5.17	130.97	122.70
1	1-A	83	PHE	CG-CD1-CE1	-5.16	115.12	120.80
1	2-A	75	SER	O-C-N	-5.16	114.45	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	76	CYS	CA-C-N	-5.15	105.87	117.20
1	1-A	18	GLU	CG-CD-OE1	5.14	128.59	118.30
1	2-A	66	SER	N-CA-CB	-5.14	102.79	110.50
1	2-A	80	SER	CB-CA-C	5.14	119.86	110.10
1	1-A	47	PHE	CG-CD2-CE2	5.13	126.45	120.80
1	2-A	44	VAL	O-C-N	5.13	130.85	121.10
1	1-A	29	LYS	CA-CB-CG	5.12	124.66	113.40
1	1-A	40	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	1-A	25	PHE	CE1-CZ-CE2	5.09	129.16	120.00
1	1-A	96	SER	N-CA-CB	5.08	118.12	110.50
1	1-A	84	LEU	N-CA-CB	5.07	120.54	110.40
1	1-A	76	CYS	O-C-N	5.05	130.77	122.70
1	2-A	50	GLY	O-C-N	-5.04	114.64	122.70
1	1-A	19	THR	CA-CB-CG2	-5.04	105.35	112.40
1	2-A	25	PHE	CE1-CZ-CE2	5.03	129.06	120.00
1	1-A	8	ILE	O-C-N	5.03	130.74	122.70
1	2-A	29	LYS	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	13	GLY	Mainchain
1	1-A	14	LYS	Mainchain
1	1-A	15	ARG	Mainchain
1	1-A	21	ASP	Sidechain
1	1-A	28	TYR	Mainchain
1	1-A	30	MET	Mainchain
1	1-A	31	ARG	Sidechain
1	1-A	79	VAL	Mainchain
1	1-A	97	GLU	Mainchain
1	2-A	15	ARG	Mainchain
1	2-A	28	TYR	Mainchain
1	2-A	30	MET	Mainchain
1	2-A	31	ARG	Sidechain
1	2-A	79	VAL	Mainchain
1	2-A	8	ILE	Mainchain
1	2-A	81	ASP	Sidechain
1	2-A	82	THR	Mainchain
1	2-A	93	LEU	Mainchain
1	2-A	98	VAL	Mainchain

## 5.2 Too-close contacts ⓘ

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	1-A	768	0	746	58	0
1	2-A	768	0	749	56	0
2	1-A	11	0	0	0	0
3	1-A	125	0	0	26	0
3	2-A	125	0	0	9	0
All	All	1797	0	1495	119	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 39.

All (119) 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:A:48:LYS:CB	1:A:48:LYS:CG	1.74	1.65
1:A:16:ARG:CD	1:A:16:ARG:CG	1.79	1.60
1:A:29:LYS:CD	1:A:29:LYS:CE	1.76	1.60
1:A:83:PHE:CB	1:A:83:PHE:CG	1.77	1.59
1:A:80:SER:CB	1:A:80:SER:CA	1.75	1.59
1:A:76:CYS:CB	1:A:76:CYS:CA	1.75	1.59
1:A:35:LYS:CD	1:A:35:LYS:CG	1.77	1.57
1:A:35:LYS:CG	1:A:35:LYS:CD	1.76	1.55
1:A:99:PHE:C	1:A:99:PHE:CA	1.78	1.52
1:A:91:LYS:NZ	1:A:91:LYS:CE	1.73	1.51
1:A:14:LYS:C	1:A:14:LYS:CA	1.77	1.51
1:A:74:PRO:CG	1:A:74:PRO:CD	1.84	1.50
1:A:96:SER:CB	1:A:96:SER:OG	1.65	1.45
1:A:91:LYS:CE	1:A:91:LYS:NZ	1.80	1.43
1:A:88:PRO:CB	1:A:88:PRO:CG	1.76	1.39
1:A:29:LYS:CG	1:A:29:LYS:CD	2.01	1.39
1:A:30:MET:CG	1:A:30:MET:SD	2.13	1.36
1:A:8:ILE:CB	1:A:8:ILE:CG1	2.02	1.35
1:A:31:ARG:CD	1:A:31:ARG:CG	2.05	1.35
1:A:55:SER:OG	3:A:205:BR:BR	2.03	1.30
1:A:31:ARG:HD3	3:A:317:HOH:O	1.31	1.24
3:A:205:BR:BR	3:A:278:HOH:O	2.01	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:HA	3:A:308:HOH:O	1.47	1.14
3:A:206:BR:BR	3:A:240:HOH:O	2.22	1.13
1:A:81:ASP:OD1	3:A:285:HOH:O	1.77	0.99
1:A:80:SER:OG	1:A:80:SER:CA	2.18	0.92
1:A:16:ARG:CD	1:A:16:ARG:CB	2.47	0.91
1:A:8:ILE:CD1	1:A:8:ILE:CB	2.56	0.83
1:A:15:ARG:HD3	3:A:210:BR:BR	2.35	0.82
1:A:37:MET:HB3	1:A:72:ILE:CD1	2.10	0.81
1:A:15:ARG:O	1:A:27:GLU:HG3	1.79	0.81
3:A:207:BR:BR	3:A:239:HOH:O	2.53	0.81
1:A:37:MET:HB3	1:A:72:ILE:HD11	1.62	0.81
1:A:10:TRP:CE2	1:A:12:GLU:HG2	2.20	0.76
1:A:31:ARG:HH11	1:A:31:ARG:HG3	1.50	0.75
1:A:83:PHE:CA	1:A:83:PHE:CG	2.70	0.75
1:A:76:CYS:SG	1:A:76:CYS:CA	2.72	0.75
1:A:31:ARG:HD3	3:A:210:HOH:O	1.87	0.75
1:A:35:LYS:CE	1:A:35:LYS:CG	2.66	0.74
1:A:98:VAL:O	1:A:99:PHE:HB3	1.87	0.74
1:A:7:LYS:O	3:A:136:HOH:O	2.07	0.73
1:A:83:PHE:CB	1:A:83:PHE:CD1	2.61	0.72
1:A:35:LYS:CB	1:A:35:LYS:CD	2.68	0.71
1:A:80:SER:CB	1:A:80:SER:N	2.54	0.71
1:A:29:LYS:CG	1:A:29:LYS:CE	2.70	0.69
1:A:35:LYS:CE	1:A:35:LYS:CG	2.70	0.69
1:A:14:LYS:HD2	3:A:242:HOH:O	1.92	0.69
1:A:31:ARG:CD	3:A:210:HOH:O	2.38	0.68
1:A:31:ARG:HH11	1:A:31:ARG:CG	2.05	0.67
1:A:14:LYS:HD2	3:A:135:HOH:O	1.94	0.67
3:A:201:BR:BR	3:A:202:BR:BR	3.23	0.66
1:A:47:PHE:CE2	1:A:48:LYS:HG3	2.33	0.64
1:A:31:ARG:HG3	1:A:31:ARG:NH1	2.13	0.64
1:A:29:LYS:CD	1:A:29:LYS:CB	2.77	0.63
1:A:91:LYS:HE2	3:A:221:HOH:O	1.98	0.62
1:A:8:ILE:HD11	1:A:56:HIS:HB3	1.82	0.62
1:A:8:ILE:CG2	1:A:8:ILE:CG1	2.77	0.62
1:A:35:LYS:CB	1:A:35:LYS:CD	2.73	0.62
1:A:93:LEU:HD22	1:A:93:LEU:N	2.15	0.61
1:A:71:SER:O	1:A:72:ILE:HD13	2.01	0.61
3:A:206:BR:BR	3:A:207:BR:BR	3.29	0.61
1:A:82:THR:O	1:A:85:PRO:HD2	2.01	0.61
1:A:98:VAL:O	1:A:99:PHE:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LYS:CA	1:A:14:LYS:O	2.44	0.60
1:A:21:ASP:N	3:A:202:BR:BR	2.85	0.59
1:A:99:PHE:HD2	1:A:99:PHE:C	2.06	0.59
1:A:31:ARG:NH1	1:A:31:ARG:CG	2.67	0.58
1:A:18:GLU:OE1	3:A:123:HOH:O	2.17	0.58
1:A:88:PRO:HB3	3:A:208:BR:BR	2.59	0.58
1:A:52:GLY:N	3:A:207:BR:BR	2.90	0.57
1:A:95:HIS:CE1	1:A:97:GLU:HB2	2.39	0.56
1:A:76:CYS:CB	1:A:76:CYS:HA	2.17	0.56
1:A:13:GLY:HA2	3:A:313:HOH:O	2.06	0.56
1:A:21:ASP:OD2	1:A:48:LYS:NZ	2.35	0.56
1:A:99:PHE:CD2	1:A:99:PHE:C	2.79	0.55
1:A:21:ASP:CG	3:A:202:BR:BR	3.00	0.55
1:A:37:MET:O	1:A:72:ILE:HD12	2.06	0.54
1:A:28:TYR:CD1	1:A:28:TYR:C	2.80	0.54
1:A:8:ILE:CG1	1:A:8:ILE:CA	2.82	0.54
1:A:96:SER:HG	1:A:96:SER:CB	2.08	0.53
1:A:37:MET:HB2	1:A:70:ILE:HG21	1.91	0.53
1:A:29:LYS:CD	1:A:29:LYS:NZ	2.69	0.53
1:A:6:PRO:HG2	1:A:56:HIS:CG	2.45	0.52
1:A:50:GLY:N	3:A:207:BR:BR	2.97	0.52
1:A:31:ARG:CB	1:A:31:ARG:CD	2.87	0.52
1:A:31:ARG:CG	3:A:210:HOH:O	2.59	0.51
1:A:93:LEU:CD2	1:A:93:LEU:N	2.74	0.50
1:A:91:LYS:N	1:A:92:PRO:HD3	2.28	0.49
1:A:82:THR:HG23	1:A:86:ARG:CZ	2.43	0.48
1:A:71:SER:C	1:A:72:ILE:HD13	2.33	0.48
1:A:91:LYS:NZ	1:A:91:LYS:CD	2.71	0.48
1:A:11:ASN:HB2	1:A:18:GLU:OE2	2.12	0.48
1:A:91:LYS:N	1:A:92:PRO:CD	2.76	0.48
1:A:10:TRP:CZ2	1:A:12:GLU:HG2	2.50	0.47
1:A:38:ASP:O	1:A:40:VAL:HG13	2.15	0.47
1:A:28:TYR:HB2	1:A:38:ASP:O	2.15	0.47
1:A:87:ASN:HA	3:A:204:BR:BR	2.70	0.46
1:A:50:GLY:CA	3:A:207:BR:BR	3.19	0.46
1:A:15:ARG:CD	3:A:210:BR:BR	3.12	0.46
1:A:9:VAL:O	1:A:17:PHE:HA	2.16	0.46
1:A:16:ARG:HB3	1:A:16:ARG:CD	2.41	0.46
1:A:13:GLY:CA	3:A:313:HOH:O	2.63	0.44
1:A:28:TYR:HB2	1:A:37:MET:HG3	1.99	0.44
1:A:15:ARG:CZ	3:A:210:BR:BR	3.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HG21	1:A:8:ILE:HD13	2.00	0.44
1:A:84:LEU:HA	1:A:84:LEU:HD23	1.69	0.44
1:A:15:ARG:NH1	3:A:210:BR:BR	3.06	0.43
1:A:31:ARG:HD2	1:A:31:ARG:HH11	1.52	0.42
1:A:30:MET:CB	1:A:30:MET:SD	3.03	0.42
1:A:90:TRP:O	1:A:93:LEU:HD23	2.19	0.42
1:A:13:GLY:HA3	3:A:206:HOH:O	2.19	0.42
1:A:76:CYS:C	1:A:76:CYS:CB	2.78	0.41
1:A:55:SER:HB2	3:A:128:HOH:O	2.19	0.41
1:A:31:ARG:HG2	3:A:210:HOH:O	2.20	0.41
1:A:77:SER:O	1:A:81:ASP:HB2	2.20	0.41
1:A:74:PRO:O	1:A:80:SER:HB3	2.21	0.41
1:A:41:HIS:HA	3:A:226:HOH:O	2.21	0.41
1:A:82:THR:O	1:A:83:PHE:C	2.60	0.40
1:A:31:ARG:CD	3:A:317:HOH:O	2.16	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	1-A	93/103 (90%)	88 (95%)	4 (4%)	1 (1%)	17	1
1	2-A	93/103 (90%)	88 (95%)	5 (5%)	0	100	100
All	All	186/206 (90%)	176 (95%)	9 (5%)	1 (0%)	34	7

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	79	VAL

### 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	1-A	86/93 (92%)	83 (96%)	3 (4%)	43 7
1	2-A	86/93 (92%)	84 (98%)	2 (2%)	58 17
All	All	172/186 (92%)	167 (97%)	5 (3%)	50 10

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	31	ARG
1	1-A	74	PRO
1	1-A	99	PHE
1	2-A	77	SER
1	2-A	99	PHE

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

Mol	Chain	Res	Type
1	1-A	56	HIS
1	1-A	64	HIS
1	2-A	56	HIS
1	2-A	64	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1-A	95/103 (92%)	0.72	7 (7%) 17 17	6, 11, 24, 35	95 (100%)
1	2-A	95/103 (92%)	0.72	7 (7%) 17 17	6, 11, 24, 35	95 (100%)
All	All	190/206 (92%)	0.72	14 (7%) 17 17	6, 11, 24, 35	190 (100%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	99	PHE	6.9
1	2-A	99	PHE	6.9
1	1-A	5	PRO	4.3
1	2-A	5	PRO	4.3
1	1-A	17	PHE	2.6
1	2-A	17	PHE	2.6
1	1-A	26	ILE	2.5
1	2-A	26	ILE	2.5
1	1-A	15	ARG	2.4
1	2-A	15	ARG	2.4
1	1-A	33	ASN	2.3
1	2-A	33	ASN	2.3
1	1-A	13	GLY	2.2
1	2-A	13	GLY	2.2

### 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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	BR	1-A	205	1/1	0.91	0.52	23.08	20,20,20,20	1
3	BR	1-A	207	1/1	0.98	0.21	3.57	19,19,19,19	1
3	BR	1-A	206	1/1	0.99	0.08	-0.80	11,11,11,11	1
3	BR	1-A	204	1/1	0.97	0.17	-	22,22,22,22	1
3	BR	1-A	208	1/1	0.97	0.37	-	20,20,20,20	1
3	BR	1-A	201	1/1	0.95	0.30	-	22,22,22,22	1
3	BR	1-A	203	1/1	0.97	0.32	-	21,21,21,21	1
3	BR	1-A	200	1/1	0.83	0.20	-	44,44,44,44	1
3	BR	1-A	202	1/1	0.96	0.34	-	21,21,21,21	1
3	BR	1-A	209	1/1	0.86	0.12	-	49,49,49,49	1
3	BR	1-A	210	1/1	0.91	0.10	-	27,27,27,27	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.