Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2016 – 07:39 PM EDT

PDB ID	:	5CU1
Title	:	Crystal structure of DMSP lyase DddQ from Ruegeria pomeroyi DSS-3
Authors	:	Chong, S.Y.; Moran, M.A.; Lanzilotta, W.N.; Whitman, W.B.
Deposited on	:	2015-07-24
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

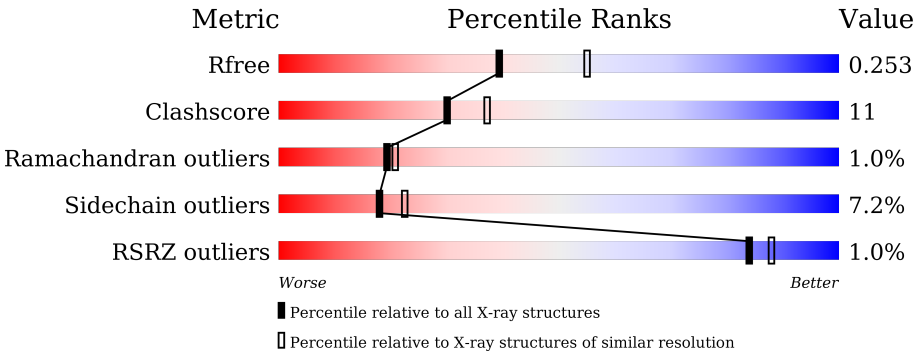
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	212	% 18% 55% 17% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1590 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 DMSP lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1527	988	255	277	7			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q5LT18
A	-9	SER	-	expression tag	UNP Q5LT18
A	-8	HIS	-	expression tag	UNP Q5LT18
A	-7	HIS	-	expression tag	UNP Q5LT18
A	-6	HIS	-	expression tag	UNP Q5LT18
A	-5	HIS	-	expression tag	UNP Q5LT18
A	-4	HIS	-	expression tag	UNP Q5LT18
A	-3	HIS	-	expression tag	UNP Q5LT18
A	-2	SER	-	expression tag	UNP Q5LT18
A	-1	GLY	-	expression tag	UNP Q5LT18
A	0	SER	-	expression tag	UNP Q5LT18

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

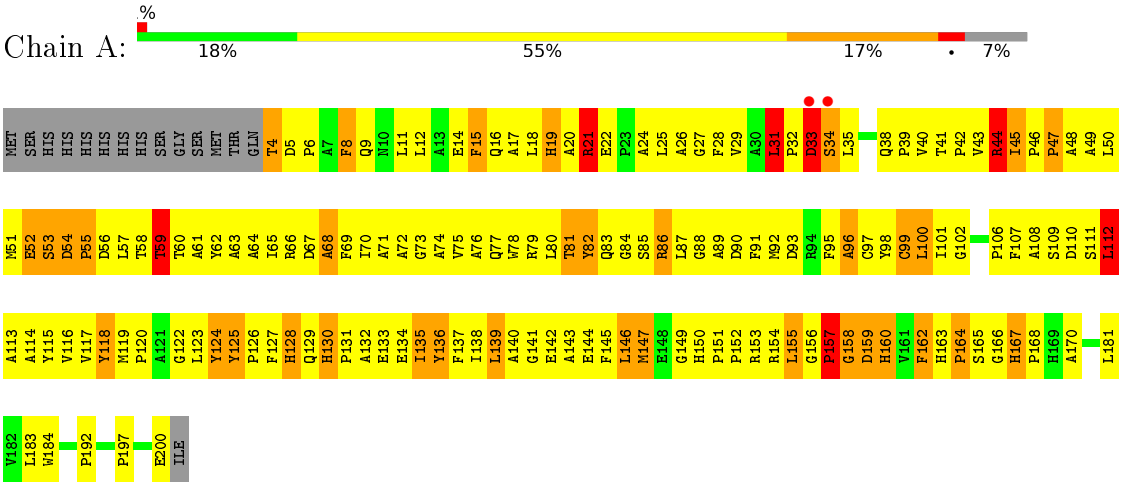
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		

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: DMSP lyase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	62.58Å 69.88Å 49.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.62 – 2.30 46.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.62-2.30) 99.6 (46.62-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	1.07	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.216 , 0.267 0.233 , 0.253	Depositor DCC
R_{free} test set	479 reflections (4.72%)	DCC
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	1590	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	3.89	264/1581 (16.7%)	2.22	72/2167 (3.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (264) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	GLU	CD-OE2	-21.14	1.02	1.25
1	A	22	GLU	CD-OE1	-20.31	1.03	1.25
1	A	66	ARG	CZ-NH2	-17.19	1.10	1.33
1	A	79	ARG	CZ-NH1	-16.70	1.11	1.33
1	A	153	ARG	CZ-NH2	-16.07	1.12	1.33
1	A	122	GLY	C-O	-15.33	0.99	1.23
1	A	79	ARG	CZ-NH2	-14.95	1.13	1.33
1	A	134	GLU	CD-OE1	-14.51	1.09	1.25
1	A	82	TYR	C-O	-14.46	0.95	1.23
1	A	134	GLU	CD-OE2	-14.30	1.09	1.25
1	A	133	GLU	CD-OE1	-13.60	1.10	1.25
1	A	156	GLY	C-O	-13.49	1.02	1.23
1	A	14	GLU	CD-OE1	-12.86	1.11	1.25
1	A	144	GLU	CD-OE1	-12.75	1.11	1.25
1	A	98	TYR	CE1-CZ	-12.72	1.22	1.38
1	A	14	GLU	CD-OE2	-12.72	1.11	1.25
1	A	28	PHE	C-O	-12.33	0.99	1.23
1	A	88	GLY	C-O	-12.01	1.04	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ARG	CZ-NH2	-11.99	1.17	1.33
1	A	45	ILE	C-O	-11.57	1.01	1.23
1	A	66	ARG	CZ-NH1	-11.45	1.18	1.33
1	A	82	TYR	CZ-OH	-11.31	1.18	1.37
1	A	145	PHE	C-O	-11.23	1.02	1.23
1	A	141	GLY	C-O	-11.07	1.05	1.23
1	A	52	GLU	CD-OE1	-11.01	1.13	1.25
1	A	134	GLU	C-O	-10.95	1.02	1.23
1	A	165	SER	CB-OG	-10.78	1.28	1.42
1	A	127	PHE	CG-CD1	-10.75	1.22	1.38
1	A	153	ARG	C-O	-10.75	1.02	1.23
1	A	162	PHE	CG-CD1	-10.58	1.22	1.38
1	A	90	ASP	CB-CG	-10.57	1.29	1.51
1	A	109	SER	CB-OG	-10.55	1.28	1.42
1	A	101	ILE	C-O	-10.45	1.03	1.23
1	A	48	ALA	C-O	-10.24	1.03	1.23
1	A	62	TYR	CZ-OH	-10.09	1.20	1.37
1	A	78	TRP	C-O	-10.07	1.04	1.23
1	A	47	PRO	C-O	-9.99	1.03	1.23
1	A	17	ALA	C-O	-9.90	1.04	1.23
1	A	68	ALA	C-O	-9.90	1.04	1.23
1	A	153	ARG	CZ-NH1	-9.89	1.20	1.33
1	A	82	TYR	CE1-CZ	-9.86	1.25	1.38
1	A	21	ARG	CZ-NH2	-9.83	1.20	1.33
1	A	125	TYR	CZ-OH	-9.74	1.21	1.37
1	A	140	ALA	C-O	-9.74	1.04	1.23
1	A	4	THR	C-O	-9.72	1.04	1.23
1	A	133	GLU	CD-OE2	-9.59	1.15	1.25
1	A	142	GLU	C-O	-9.58	1.05	1.23
1	A	92	MET	C-O	-9.48	1.05	1.23
1	A	84	GLY	C-O	-9.38	1.08	1.23
1	A	98	TYR	CD2-CE2	-9.37	1.25	1.39
1	A	120	PRO	C-O	-9.35	1.04	1.23
1	A	21	ARG	CZ-NH1	-9.30	1.21	1.33
1	A	159	ASP	CG-OD2	-9.29	1.03	1.25
1	A	150	HIS	C-O	-9.27	1.05	1.23
1	A	93	ASP	C-O	-9.19	1.05	1.23
1	A	56	ASP	C-O	-9.18	1.05	1.23
1	A	154	ARG	C-O	-9.12	1.06	1.23
1	A	142	GLU	CD-OE2	-9.07	1.15	1.25
1	A	163	HIS	C-O	-9.02	1.06	1.23
1	A	118	TYR	C-O	-9.01	1.06	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	ALA	C-O	-9.01	1.06	1.23
1	A	98	TYR	CZ-OH	-8.98	1.22	1.37
1	A	166	GLY	C-O	-8.98	1.09	1.23
1	A	90	ASP	CG-OD1	-8.96	1.04	1.25
1	A	162	PHE	C-O	-8.91	1.06	1.23
1	A	147	MET	C-O	-8.89	1.06	1.23
1	A	65	ILE	C-O	-8.83	1.06	1.23
1	A	93	ASP	CG-OD2	-8.82	1.05	1.25
1	A	118	TYR	CZ-OH	-8.82	1.22	1.37
1	A	118	TYR	CE2-CZ	-8.81	1.27	1.38
1	A	118	TYR	CD2-CE2	-8.73	1.26	1.39
1	A	137	PHE	C-O	-8.70	1.06	1.23
1	A	160	HIS	C-O	-8.65	1.06	1.23
1	A	79	ARG	NE-CZ	-8.63	1.21	1.33
1	A	113	ALA	C-O	-8.59	1.07	1.23
1	A	87	LEU	C-O	-8.53	1.07	1.23
1	A	124	TYR	CG-CD1	-8.52	1.28	1.39
1	A	53	SER	C-O	-8.52	1.07	1.23
1	A	82	TYR	CE2-CZ	-8.52	1.27	1.38
1	A	70	ILE	C-O	-8.47	1.07	1.23
1	A	50	LEU	C-O	-8.45	1.07	1.23
1	A	115	TYR	CE1-CZ	-8.29	1.27	1.38
1	A	111	SER	C-O	-8.27	1.07	1.23
1	A	59	THR	CB-CG2	-8.21	1.25	1.52
1	A	76	ALA	C-O	-8.15	1.07	1.23
1	A	125	TYR	C-O	-8.11	1.07	1.23
1	A	90	ASP	CG-OD2	-8.02	1.06	1.25
1	A	66	ARG	C-O	-7.97	1.08	1.23
1	A	108	ALA	C-O	-7.94	1.08	1.23
1	A	29	VAL	C-O	-7.93	1.08	1.23
1	A	40	VAL	C-O	-7.92	1.08	1.23
1	A	51	MET	C-O	-7.90	1.08	1.23
1	A	143	ALA	C-O	-7.87	1.08	1.23
1	A	24	ALA	C-O	-7.87	1.08	1.23
1	A	156	GLY	N-CA	-7.83	1.34	1.46
1	A	135	ILE	C-O	-7.83	1.08	1.23
1	A	102	GLY	C-O	-7.82	1.11	1.23
1	A	58	THR	CB-CG2	-7.81	1.26	1.52
1	A	85	SER	C-O	-7.80	1.08	1.23
1	A	86	ARG	C-O	-7.76	1.08	1.23
1	A	117	VAL	C-O	-7.70	1.08	1.23
1	A	53	SER	CB-OG	-7.63	1.32	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ALA	C-O	-7.62	1.08	1.23
1	A	67	ASP	CG-OD1	-7.60	1.07	1.25
1	A	77	GLN	CD-NE2	-7.60	1.13	1.32
1	A	74	ALA	C-O	-7.58	1.08	1.23
1	A	99	CYS	C-O	-7.49	1.09	1.23
1	A	22	GLU	C-O	-7.45	1.09	1.23
1	A	162	PHE	CG-CD2	-7.44	1.27	1.38
1	A	149	GLY	C-O	-7.39	1.11	1.23
1	A	61	ALA	C-O	-7.38	1.09	1.23
1	A	27	GLY	C-O	-7.37	1.11	1.23
1	A	18	LEU	C-O	-7.37	1.09	1.23
1	A	124	TYR	CD2-CE2	-7.37	1.28	1.39
1	A	9	GLN	C-O	-7.35	1.09	1.23
1	A	118	TYR	CG-CD1	-7.34	1.29	1.39
1	A	78	TRP	CD1-NE1	-7.34	1.25	1.38
1	A	98	TYR	CG-CD2	-7.30	1.29	1.39
1	A	124	TYR	CZ-OH	-7.30	1.25	1.37
1	A	73	GLY	C-O	-7.27	1.12	1.23
1	A	159	ASP	CG-OD1	-7.25	1.08	1.25
1	A	127	PHE	C-O	-7.25	1.09	1.23
1	A	145	PHE	CE2-CZ	-7.25	1.23	1.37
1	A	11	LEU	C-O	-7.23	1.09	1.23
1	A	157	PRO	C-O	-7.19	1.08	1.23
1	A	129	GLN	CD-NE2	-7.19	1.14	1.32
1	A	72	ALA	C-O	-7.18	1.09	1.23
1	A	64	ALA	C-O	-7.15	1.09	1.23
1	A	123	LEU	C-O	-7.12	1.09	1.23
1	A	73	GLY	N-CA	-7.09	1.35	1.46
1	A	146	LEU	C-O	-7.07	1.09	1.23
1	A	93	ASP	CG-OD1	-7.07	1.09	1.25
1	A	129	GLN	C-O	-7.00	1.10	1.23
1	A	90	ASP	C-O	-7.00	1.10	1.23
1	A	71	ALA	C-O	-6.98	1.10	1.23
1	A	8	PHE	CG-CD1	-6.97	1.28	1.38
1	A	60	THR	C-O	-6.97	1.10	1.23
1	A	33	ASP	CA-C	6.97	1.71	1.52
1	A	96	ALA	CA-CB	-6.97	1.37	1.52
1	A	20	ALA	N-CA	-6.96	1.32	1.46
1	A	132	ALA	N-CA	-6.94	1.32	1.46
1	A	168	PRO	C-O	-6.87	1.09	1.23
1	A	32	PRO	CA-C	-6.82	1.39	1.52
1	A	165	SER	CA-CB	-6.82	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ASP	C-O	-6.81	1.10	1.23
1	A	126	PRO	CG-CD	-6.81	1.28	1.50
1	A	62	TYR	C-O	-6.79	1.10	1.23
1	A	26	ALA	C-O	-6.78	1.10	1.23
1	A	98	TYR	CE2-CZ	-6.74	1.29	1.38
1	A	139	LEU	C-O	-6.72	1.10	1.23
1	A	54	ASP	C-O	-6.72	1.10	1.23
1	A	86	ARG	CZ-NH2	-6.71	1.24	1.33
1	A	57	LEU	C-O	-6.68	1.10	1.23
1	A	46	PRO	C-O	-6.68	1.09	1.23
1	A	119	MET	C-O	-6.60	1.10	1.23
1	A	118	TYR	CD1-CE1	-6.57	1.29	1.39
1	A	88	GLY	CA-C	-6.55	1.41	1.51
1	A	91	PHE	CD1-CE1	-6.48	1.26	1.39
1	A	98	TYR	C-O	-6.44	1.11	1.23
1	A	154	ARG	CZ-NH2	-6.43	1.24	1.33
1	A	154	ARG	CD-NE	-6.42	1.35	1.46
1	A	79	ARG	CA-CB	-6.40	1.39	1.53
1	A	82	TYR	CG-CD2	-6.37	1.30	1.39
1	A	6	PRO	C-O	-6.34	1.10	1.23
1	A	144	GLU	C-O	-6.34	1.11	1.23
1	A	115	TYR	CD1-CE1	-6.33	1.29	1.39
1	A	49	ALA	C-O	-6.32	1.11	1.23
1	A	43	VAL	C-O	-6.32	1.11	1.23
1	A	38	GLN	N-CA	-6.31	1.33	1.46
1	A	58	THR	C-O	-6.31	1.11	1.23
1	A	109	SER	CA-CB	-6.29	1.43	1.52
1	A	67	ASP	CG-OD2	-6.27	1.10	1.25
1	A	153	ARG	NE-CZ	-6.24	1.25	1.33
1	A	21	ARG	CD-NE	-6.17	1.35	1.46
1	A	111	SER	N-CA	-6.17	1.34	1.46
1	A	110	ASP	C-O	-6.17	1.11	1.23
1	A	116	VAL	C-O	-6.16	1.11	1.23
1	A	142	GLU	CD-OE1	-6.13	1.19	1.25
1	A	98	TYR	CG-CD1	-6.12	1.31	1.39
1	A	159	ASP	C-O	-6.11	1.11	1.23
1	A	97	CYS	C-O	-6.10	1.11	1.23
1	A	145	PHE	CG-CD2	-6.09	1.29	1.38
1	A	25	LEU	C-O	-6.06	1.11	1.23
1	A	44	ARG	CZ-NH1	-6.01	1.25	1.33
1	A	156	GLY	CA-C	-5.97	1.42	1.51
1	A	126	PRO	CA-CB	-5.97	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	LEU	C-O	-5.97	1.12	1.23
1	A	167	HIS	C-O	-5.97	1.12	1.23
1	A	41	THR	C-O	-5.95	1.12	1.23
1	A	75	VAL	C-O	-5.94	1.12	1.23
1	A	92	MET	N-CA	-5.93	1.34	1.46
1	A	5	ASP	CG-OD1	-5.93	1.11	1.25
1	A	124	TYR	CG-CD2	-5.92	1.31	1.39
1	A	137	PHE	CD1-CE1	-5.90	1.27	1.39
1	A	38	GLN	C-O	-5.90	1.12	1.23
1	A	14	GLU	C-O	-5.89	1.12	1.23
1	A	82	TYR	CG-CD1	-5.87	1.31	1.39
1	A	52	GLU	CD-OE2	-5.87	1.19	1.25
1	A	115	TYR	CD2-CE2	-5.85	1.30	1.39
1	A	8	PHE	CA-CB	-5.84	1.41	1.53
1	A	136	TYR	C-O	-5.84	1.12	1.23
1	A	128	HIS	C-O	-5.80	1.12	1.23
1	A	52	GLU	C-O	-5.79	1.12	1.23
1	A	124	TYR	CE1-CZ	-5.78	1.31	1.38
1	A	162	PHE	CE1-CZ	-5.77	1.26	1.37
1	A	119	MET	CG-SD	-5.76	1.66	1.81
1	A	15	PHE	CG-CD1	-5.73	1.30	1.38
1	A	20	ALA	C-O	-5.73	1.12	1.23
1	A	107	PHE	C-O	-5.70	1.12	1.23
1	A	115	TYR	CG-CD1	-5.69	1.31	1.39
1	A	151	PRO	CA-CB	-5.68	1.42	1.53
1	A	70	ILE	N-CA	-5.68	1.34	1.46
1	A	19	HIS	CA-CB	-5.67	1.41	1.53
1	A	28	PHE	CG-CD2	-5.66	1.30	1.38
1	A	159	ASP	CB-CG	-5.66	1.39	1.51
1	A	145	PHE	CG-CD1	-5.62	1.30	1.38
1	A	79	ARG	C-O	-5.62	1.12	1.23
1	A	131	PRO	C-O	-5.62	1.12	1.23
1	A	53	SER	N-CA	-5.61	1.35	1.46
1	A	137	PHE	CG-CD2	-5.61	1.30	1.38
1	A	96	ALA	C-O	-5.59	1.12	1.23
1	A	145	PHE	CD2-CE2	-5.59	1.28	1.39
1	A	109	SER	C-O	-5.57	1.12	1.23
1	A	112	LEU	C-O	-5.57	1.12	1.23
1	A	66	ARG	N-CA	-5.56	1.35	1.46
1	A	8	PHE	CE1-CZ	-5.55	1.26	1.37
1	A	5	ASP	CG-OD2	-5.54	1.12	1.25
1	A	5	ASP	CB-CG	-5.53	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	MET	SD-CE	-5.52	1.47	1.77
1	A	162	PHE	CB-CG	-5.49	1.42	1.51
1	A	63	ALA	C-O	-5.49	1.12	1.23
1	A	19	HIS	N-CA	-5.42	1.35	1.46
1	A	124	TYR	C-O	-5.39	1.13	1.23
1	A	17	ALA	CA-C	-5.38	1.39	1.52
1	A	56	ASP	CG-OD2	-5.38	1.12	1.25
1	A	136	TYR	CD2-CE2	-5.36	1.31	1.39
1	A	54	ASP	CB-CG	-5.36	1.40	1.51
1	A	130	HIS	C-O	-5.34	1.13	1.23
1	A	12	LEU	C-O	-5.32	1.13	1.23
1	A	8	PHE	CE2-CZ	-5.29	1.27	1.37
1	A	85	SER	CB-OG	-5.27	1.35	1.42
1	A	69	PHE	C-O	-5.27	1.13	1.23
1	A	38	GLN	CD-OE1	-5.27	1.12	1.24
1	A	5	ASP	CA-C	-5.26	1.39	1.52
1	A	95	PHE	C-O	-5.26	1.13	1.23
1	A	78	TRP	CA-C	-5.24	1.39	1.52
1	A	66	ARG	CA-CB	-5.23	1.42	1.53
1	A	43	VAL	N-CA	-5.22	1.35	1.46
1	A	136	TYR	CZ-OH	-5.19	1.29	1.37
1	A	114	ALA	C-O	-5.17	1.13	1.23
1	A	117	VAL	CB-CG1	-5.17	1.42	1.52
1	A	100	LEU	C-O	-5.16	1.13	1.23
1	A	81	THR	N-CA	-5.14	1.36	1.46
1	A	75	VAL	N-CA	-5.13	1.36	1.46
1	A	78	TRP	CD2-CE2	-5.12	1.35	1.41
1	A	62	TYR	CD2-CE2	-5.12	1.31	1.39
1	A	16	GLN	CD-OE1	-5.09	1.12	1.24
1	A	164	PRO	CA-C	5.09	1.63	1.52
1	A	86	ARG	CZ-NH1	-5.08	1.26	1.33
1	A	141	GLY	CA-C	-5.05	1.43	1.51
1	A	15	PHE	C-O	-5.04	1.13	1.23
1	A	14	GLU	CG-CD	-5.03	1.44	1.51
1	A	127	PHE	CB-CG	-5.02	1.42	1.51
1	A	62	TYR	CG-CD1	-5.01	1.32	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	ARG	NE-CZ-NH1	32.52	136.56	120.30
1	A	44	ARG	NE-CZ-NH1	15.64	128.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	ASP	CB-CG-OD1	13.93	130.84	118.30
1	A	21	ARG	NE-CZ-NH1	13.43	127.01	120.30
1	A	66	ARG	NH1-CZ-NH2	-10.31	108.06	119.40
1	A	56	ASP	CB-CG-OD2	-10.22	109.10	118.30
1	A	66	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	A	67	ASP	CB-CG-OD1	10.07	127.36	118.30
1	A	21	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	A	22	GLU	OE1-CD-OE2	-9.21	112.25	123.30
1	A	153	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	A	67	ASP	OD1-CG-OD2	-8.89	106.41	123.30
1	A	67	ASP	CB-CG-OD2	8.72	126.15	118.30
1	A	8	PHE	CB-CG-CD1	8.59	126.81	120.80
1	A	123	LEU	CB-CG-CD2	8.00	124.59	111.00
1	A	164	PRO	CA-N-CD	-7.95	100.37	111.50
1	A	93	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	139	LEU	CB-CG-CD1	7.41	123.59	111.00
1	A	35	LEU	CB-CG-CD1	-7.29	98.61	111.00
1	A	153	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	133	GLU	OE1-CD-OE2	-7.27	114.58	123.30
1	A	112	LEU	CA-CB-CG	7.23	131.94	115.30
1	A	136	TYR	CA-CB-CG	7.23	127.13	113.40
1	A	157	PRO	CA-N-CD	-7.00	101.70	111.50
1	A	86	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	A	163	HIS	C-N-CD	6.92	142.93	128.40
1	A	86	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	44	ARG	CG-CD-NE	6.83	126.14	111.80
1	A	44	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	147	MET	CG-SD-CE	-6.67	89.54	100.20
1	A	42	PRO	CA-N-CD	-6.63	102.21	111.50
1	A	38	GLN	C-N-CD	6.58	142.22	128.40
1	A	134	GLU	OE1-CD-OE2	-6.56	115.42	123.30
1	A	151	PRO	CA-N-CD	-6.49	102.41	111.50
1	A	57	LEU	C-N-CA	6.32	137.49	121.70
1	A	41	THR	C-N-CD	6.25	141.52	128.40
1	A	8	PHE	CB-CG-CD2	-6.18	116.47	120.80
1	A	55	PRO	CA-N-CD	-6.17	102.86	111.50
1	A	119	MET	CA-CB-CG	6.09	123.66	113.30
1	A	152	PRO	CA-N-CD	-6.09	102.98	111.50
1	A	90	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	5	ASP	C-N-CD	5.98	140.97	128.40
1	A	79	ARG	CD-NE-CZ	5.92	131.89	123.60
1	A	156	GLY	C-N-CD	5.92	140.83	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	PRO	C-N-CD	5.86	140.71	128.40
1	A	95	PHE	C-N-CA	5.83	136.27	121.70
1	A	33	ASP	N-CA-C	5.78	126.59	111.00
1	A	54	ASP	C-N-CD	5.69	140.35	128.40
1	A	159	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	167	HIS	C-N-CD	5.66	140.29	128.40
1	A	127	PHE	CB-CG-CD2	5.66	124.76	120.80
1	A	39	PRO	CA-N-CD	-5.66	103.58	111.50
1	A	12	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	A	151	PRO	C-N-CD	5.60	140.17	128.40
1	A	4	THR	N-CA-C	5.54	125.95	111.00
1	A	162	PHE	CB-CG-CD2	5.53	124.67	120.80
1	A	158	GLY	N-CA-C	5.41	126.63	113.10
1	A	157	PRO	C-N-CA	5.40	133.64	122.30
1	A	5	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	A	119	MET	C-N-CD	5.35	139.64	128.40
1	A	127	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	A	144	GLU	OE1-CD-OE2	-5.34	116.90	123.30
1	A	66	ARG	CD-NE-CZ	5.33	131.07	123.60
1	A	154	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	31	LEU	C-N-CD	5.17	139.25	128.40
1	A	150	HIS	C-N-CD	5.15	139.22	128.40
1	A	168	PRO	CA-N-CD	-5.15	104.29	111.50
1	A	159	ASP	OD1-CG-OD2	-5.11	113.59	123.30
1	A	144	GLU	CG-CD-OE2	5.10	128.50	118.30
1	A	159	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	57	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	114	ALA	C-N-CA	5.04	134.30	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	LEU	Peptide
1	A	157	PRO	Peptide
1	A	33	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1527	0	1452	33	0
2	A	1	0	0	0	0
3	A	62	0	0	6	0
All	All	1590	0	1452	33	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 11.

All (33) 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:4:THR:N	3:A:401:HOH:O	1.63	1.31
1:A:45:ILE:HG13	1:A:47:PRO:HD2	1.47	0.94
1:A:54:ASP:OD2	1:A:118:TYR:OH	1.99	0.80
1:A:83:GLN:O	3:A:403:HOH:O	2.05	0.74
1:A:21:ARG:NH2	3:A:404:HOH:O	2.15	0.73
1:A:45:ILE:CG1	1:A:47:PRO:HD2	2.21	0.70
1:A:8:PHE:CD1	1:A:106:PRO:HG3	2.35	0.62
1:A:44:ARG:NH2	1:A:52:GLU:OE1	2.33	0.62
1:A:19:HIS:NE2	1:A:31:LEU:HD13	2.20	0.57
1:A:184:TRP:HH2	1:A:192:PRO:HD3	1.71	0.56
1:A:130:HIS:HD2	1:A:192:PRO:HB3	1.72	0.54
1:A:47:PRO:HB3	1:A:96:ALA:HB2	1.92	0.52
1:A:86:ARG:HD3	1:A:197:PRO:O	2.11	0.50
1:A:4:THR:HG22	3:A:462:HOH:O	2.11	0.50
1:A:59:THR:CG2	1:A:139:LEU:O	2.61	0.49
1:A:125:TYR:CZ	1:A:128:HIS:CE1	3.01	0.48
1:A:33:ASP:C	1:A:34:SER:OG	2.49	0.48
1:A:45:ILE:HG21	1:A:80:LEU:HD11	1.96	0.47
1:A:59:THR:HG23	1:A:139:LEU:O	2.15	0.47
1:A:146:LEU:HB2	1:A:170:ALA:HB3	1.98	0.46
1:A:81:THR:O	1:A:82:TYR:HB2	2.16	0.46
1:A:15:PHE:HE1	1:A:181:LEU:HD21	1.81	0.45
1:A:124:TYR:OH	1:A:200:GLU:OE1	2.22	0.45
1:A:162:PHE:CE2	1:A:164:PRO:HG3	2.52	0.45
1:A:167:HIS:ND1	3:A:402:HOH:O	1.94	0.44
1:A:19:HIS:CD2	1:A:31:LEU:HD13	2.53	0.44
1:A:136:TYR:O	1:A:160:HIS:HA	2.17	0.43
1:A:68:ALA:HB2	3:A:410:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TYR:CE2	1:A:128:HIS:CE1	3.06	0.43
1:A:155:LEU:HD22	1:A:159:ASP:HB3	2.00	0.43
1:A:19:HIS:CE1	1:A:31:LEU:HD13	2.54	0.43
1:A:138:ILE:HG22	1:A:157:PRO:HA	2.01	0.42
1:A:135:ILE:HG22	1:A:183:LEU:HB2	2.03	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	195/212 (92%)	178 (91%)	15 (8%)	2 (1%)	19 21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	158	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	153/167 (92%)	142 (93%)	11 (7%)	18 22

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	31	LEU
1	A	33	ASP
1	A	44	ARG
1	A	53	SER
1	A	55	PRO
1	A	59	THR
1	A	99	CYS
1	A	100	LEU
1	A	112	LEU
1	A	147	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 1 ligands modelled in this entry, 1 is 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

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	197/212 (92%)	-0.11	2 (1%) 84 88	16, 23, 37, 60	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	SER	4.2
1	A	33	ASP	2.7

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	FE	A	301	1/1	0.90	0.13	0.62	35,35,35,35	1

6.5 Other polymers (i)

There are no such residues in this entry.