



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:15 PM UTC

PDB ID : 5CU1 / pdb_00005cu1
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

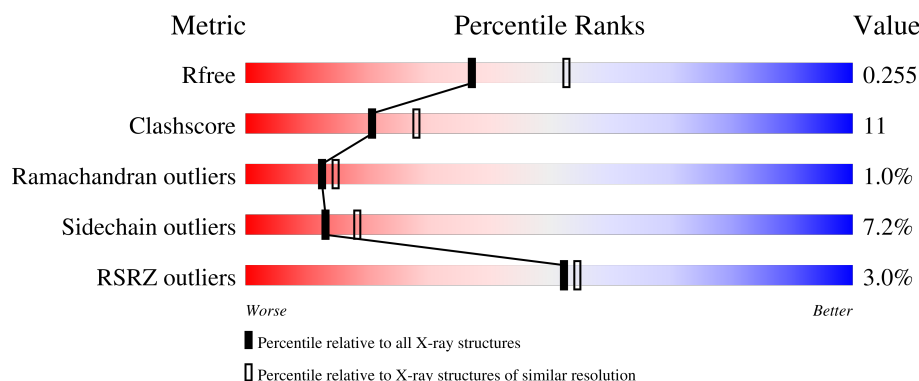
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	A	212	

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 (CCD ID: FE) (formula: Fe).

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

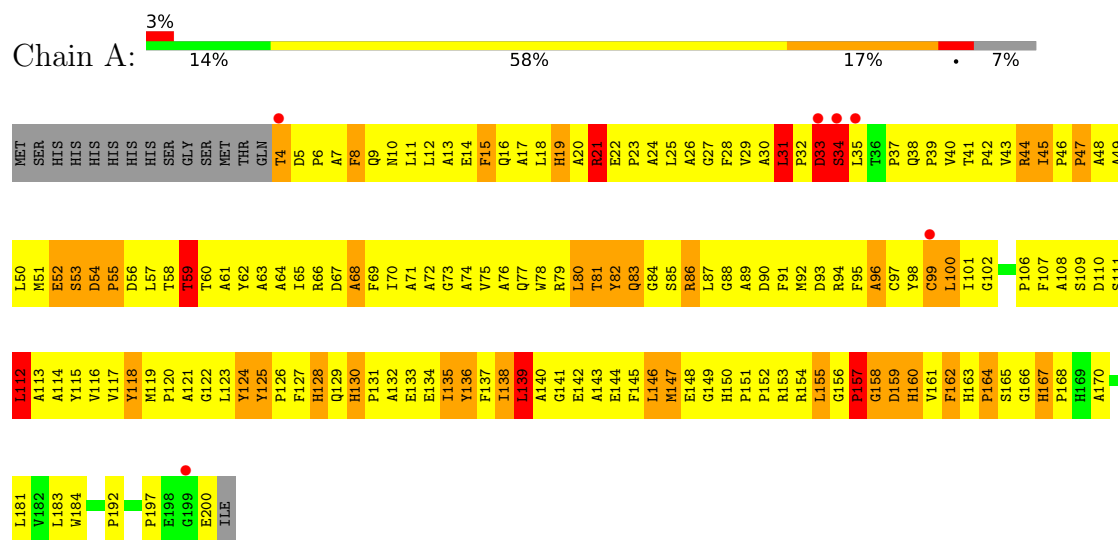
- Molecule 3 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

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 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.62-2.30) 100.0 (46.62-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	1.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.216 , 0.267 0.235 , 0.255	Depositor DCC
R_{free} test set	552 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	5.00	355/1581 (22.5%)	2.62	146/2167 (6.7%)

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 (355) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	PHE	C-O	-19.78	0.99	1.24
1	A	101	ILE	C-O	-18.86	1.03	1.24
1	A	153	ARG	C-O	-18.80	1.02	1.24
1	A	134	GLU	C-O	-18.79	1.02	1.24
1	A	122	GLY	C-O	-18.37	0.99	1.23
1	A	45	ILE	C-O	-18.29	1.01	1.24
1	A	145	PHE	C-O	-18.06	1.02	1.24
1	A	48	ALA	C-O	-17.57	1.03	1.24
1	A	66	ARG	CZ-NH2	-17.50	1.10	1.33
1	A	22	GLU	C-O	-17.24	1.09	1.25
1	A	68	ALA	C-O	-16.73	1.04	1.24
1	A	78	TRP	C-O	-16.43	1.04	1.23
1	A	153	ARG	CZ-NH2	-16.38	1.12	1.33
1	A	156	GLY	C-O	-16.21	1.02	1.24
1	A	163	HIS	C-O	-16.10	1.06	1.24
1	A	47	PRO	C-O	-15.77	1.03	1.24
1	A	17	ALA	C-O	-15.51	1.04	1.24
1	A	154	ARG	C-O	-15.38	1.06	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	ARG	CZ-NH1	-15.30	1.11	1.32
1	A	79	ARG	CZ-NH2	-15.26	1.13	1.33
1	A	92	MET	C-O	-15.12	1.05	1.24
1	A	120	PRO	C-O	-15.07	1.04	1.23
1	A	142	GLU	C-O	-14.95	1.05	1.24
1	A	70	ILE	C-O	-14.93	1.07	1.24
1	A	118	TYR	C-O	-14.71	1.06	1.24
1	A	50	LEU	C-O	-14.58	1.07	1.24
1	A	162	PHE	C-O	-14.53	1.06	1.24
1	A	40	VAL	C-O	-14.46	1.08	1.24
1	A	137	PHE	C-O	-14.43	1.06	1.24
1	A	135	ILE	C-O	-14.42	1.08	1.24
1	A	89	ALA	C-O	-14.40	1.06	1.24
1	A	53	SER	C-O	-14.24	1.07	1.24
1	A	65	ILE	C-O	-14.20	1.06	1.24
1	A	150	HIS	C-O	-14.14	1.05	1.24
1	A	117	VAL	C-O	-14.08	1.08	1.24
1	A	140	ALA	C-O	-14.03	1.04	1.23
1	A	87	LEU	C-O	-13.90	1.07	1.24
1	A	160	HIS	C-O	-13.88	1.06	1.23
1	A	147	MET	C-O	-13.86	1.06	1.23
1	A	66	ARG	C-O	-13.79	1.08	1.24
1	A	51	MET	C-O	-13.70	1.08	1.24
1	A	33	ASP	CA-C	13.66	1.71	1.52
1	A	93	ASP	C-O	-13.60	1.05	1.24
1	A	29	VAL	C-O	-13.42	1.08	1.23
1	A	141	GLY	C-O	-13.32	1.05	1.23
1	A	113	ALA	C-O	-13.32	1.07	1.23
1	A	85	SER	C-O	-13.20	1.08	1.23
1	A	157	PRO	C-O	-13.09	1.08	1.23
1	A	51	MET	SD-CE	-13.05	1.47	1.79
1	A	46	PRO	C-O	-13.04	1.09	1.24
1	A	76	ALA	C-O	-12.89	1.07	1.23
1	A	143	ALA	C-O	-12.86	1.08	1.23
1	A	108	ALA	C-O	-12.80	1.08	1.23
1	A	125	TYR	C-O	-12.73	1.07	1.24
1	A	102	GLY	C-O	-12.68	1.11	1.24
1	A	9	GLN	C-O	-12.63	1.09	1.24
1	A	11	LEU	C-O	-12.60	1.09	1.24
1	A	132	ALA	C-O	-12.60	1.08	1.23
1	A	64	ALA	C-O	-12.46	1.09	1.24
1	A	24	ALA	C-O	-12.44	1.08	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ARG	CZ-NH2	-12.30	1.17	1.33
1	A	56	ASP	C-O	-12.21	1.05	1.24
1	A	88	GLY	C-O	-12.08	1.04	1.23
1	A	22	GLU	CD-OE2	-12.08	1.02	1.25
1	A	74	ALA	C-O	-12.01	1.08	1.24
1	A	86	ARG	C-O	-11.94	1.08	1.24
1	A	71	ALA	C-O	-11.87	1.10	1.24
1	A	96	ALA	CA-CB	-11.82	1.37	1.53
1	A	82	TYR	C-O	-11.80	0.95	1.24
1	A	43	VAL	C-O	-11.74	1.11	1.24
1	A	99	CYS	C-O	-11.74	1.09	1.23
1	A	67	ASP	C-O	-11.71	1.10	1.24
1	A	116	VAL	C-O	-11.65	1.11	1.24
1	A	111	SER	C-O	-11.64	1.07	1.23
1	A	22	GLU	CD-OE1	-11.60	1.03	1.25
1	A	123	LEU	C-O	-11.56	1.09	1.23
1	A	26	ALA	C-O	-11.47	1.10	1.24
1	A	127	PHE	C-O	-11.43	1.09	1.24
1	A	146	LEU	C-O	-11.43	1.09	1.24
1	A	20	ALA	N-CA	-11.32	1.32	1.46
1	A	84	GLY	C-O	-11.32	1.08	1.23
1	A	159	ASP	CG-OD2	-11.25	1.03	1.25
1	A	18	LEU	C-O	-11.12	1.09	1.24
1	A	129	GLN	C-O	-11.12	1.10	1.23
1	A	49	ALA	C-O	-11.07	1.11	1.24
1	A	90	ASP	C-O	-11.05	1.10	1.24
1	A	132	ALA	N-CA	-11.04	1.32	1.46
1	A	60	THR	C-O	-11.02	1.10	1.24
1	A	72	ALA	C-O	-10.86	1.09	1.24
1	A	90	ASP	CG-OD1	-10.85	1.04	1.25
1	A	166	GLY	C-O	-10.83	1.09	1.23
1	A	93	ASP	CG-OD2	-10.68	1.05	1.25
1	A	168	PRO	C-O	-10.65	1.09	1.23
1	A	61	ALA	C-O	-10.63	1.09	1.24
1	A	5	ASP	CA-C	-10.59	1.39	1.52
1	A	25	LEU	C-O	-10.57	1.11	1.24
1	A	97	CYS	C-O	-10.56	1.11	1.23
1	A	155	LEU	C-O	-10.55	1.12	1.24
1	A	66	ARG	CZ-NH1	-10.42	1.18	1.32
1	A	144	GLU	C-O	-10.38	1.11	1.24
1	A	54	ASP	C-O	-10.38	1.10	1.24
1	A	139	LEU	C-O	-10.33	1.10	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	PRO	C-O	-10.31	1.10	1.24
1	A	75	VAL	C-O	-10.27	1.12	1.24
1	A	17	ALA	CA-C	-10.21	1.39	1.52
1	A	79	ARG	NE-CZ	-10.20	1.21	1.33
1	A	145	PHE	CA-C	-10.19	1.40	1.52
1	A	78	TRP	CA-C	-10.15	1.39	1.52
1	A	21	ARG	CZ-NH2	-10.13	1.20	1.33
1	A	41	THR	C-O	-10.12	1.12	1.24
1	A	98	TYR	C-O	-10.12	1.11	1.23
1	A	58	THR	C-O	-10.12	1.11	1.23
1	A	52	GLU	C-O	-10.07	1.12	1.24
1	A	151	PRO	C-O	-9.97	1.13	1.24
1	A	62	TYR	C-O	-9.94	1.10	1.24
1	A	119	MET	C-O	-9.93	1.10	1.24
1	A	38	GLN	C-O	-9.91	1.12	1.24
1	A	70	ILE	N-CA	-9.90	1.34	1.46
1	A	167	HIS	C-O	-9.89	1.12	1.24
1	A	20	ALA	C-O	-9.86	1.12	1.24
1	A	161	VAL	C-O	-9.82	1.13	1.24
1	A	149	GLY	C-O	-9.72	1.11	1.24
1	A	136	TYR	C-O	-9.71	1.12	1.23
1	A	90	ASP	CG-OD2	-9.71	1.06	1.25
1	A	75	VAL	N-CA	-9.47	1.36	1.46
1	A	96	ALA	C-O	-9.47	1.12	1.24
1	A	111	SER	N-CA	-9.43	1.34	1.46
1	A	131	PRO	C-O	-9.43	1.12	1.24
1	A	12	LEU	C-O	-9.41	1.13	1.24
1	A	107	PHE	C-O	-9.35	1.12	1.23
1	A	4	THR	C-O	-9.34	1.04	1.23
1	A	124	TYR	C-O	-9.34	1.13	1.24
1	A	69	PHE	C-O	-9.34	1.13	1.24
1	A	92	MET	N-CA	-9.30	1.34	1.46
1	A	27	GLY	C-O	-9.30	1.11	1.23
1	A	110	ASP	C-O	-9.29	1.11	1.24
1	A	66	ARG	N-CA	-9.28	1.35	1.46
1	A	82	TYR	CZ-OH	-9.25	1.18	1.38
1	A	128	HIS	C-O	-9.25	1.12	1.23
1	A	77	GLN	CD-NE2	-9.24	1.13	1.33
1	A	14	GLU	C-O	-9.23	1.12	1.24
1	A	95	PHE	C-O	-9.22	1.13	1.24
1	A	67	ASP	CG-OD1	-9.20	1.07	1.25
1	A	19	HIS	N-CA	-9.14	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	SER	N-CA	-9.14	1.35	1.46
1	A	63	ALA	CA-C	-9.12	1.40	1.52
1	A	159	ASP	C-O	-9.12	1.11	1.23
1	A	79	ARG	C-O	-9.09	1.12	1.23
1	A	90	ASP	CB-CG	-9.00	1.29	1.52
1	A	15	PHE	C-O	-8.98	1.13	1.24
1	A	153	ARG	CZ-NH1	-8.97	1.20	1.32
1	A	63	ALA	C-O	-8.94	1.12	1.24
1	A	18	LEU	CA-C	-8.90	1.40	1.52
1	A	112	LEU	C-O	-8.89	1.12	1.23
1	A	56	ASP	N-CA	-8.87	1.36	1.46
1	A	159	ASP	CG-OD1	-8.78	1.08	1.25
1	A	114	ALA	C-O	-8.77	1.13	1.23
1	A	129	GLN	CD-NE2	-8.74	1.14	1.33
1	A	79	ARG	CA-CB	-8.74	1.39	1.53
1	A	38	GLN	CA-C	-8.68	1.42	1.52
1	A	119	MET	SD-CE	-8.66	1.57	1.79
1	A	151	PRO	CA-CB	-8.64	1.42	1.54
1	A	115	TYR	CA-C	8.63	1.63	1.52
1	A	130	HIS	C-O	-8.61	1.13	1.24
1	A	126	PRO	CA-CB	-8.59	1.41	1.53
1	A	35	LEU	C-O	-8.57	1.14	1.24
1	A	93	ASP	CG-OD1	-8.55	1.09	1.25
1	A	69	PHE	CA-C	8.53	1.64	1.52
1	A	72	ALA	CA-C	-8.43	1.41	1.52
1	A	21	ARG	CZ-NH1	-8.42	1.21	1.32
1	A	73	GLY	C-O	-8.41	1.12	1.23
1	A	32	PRO	CA-C	-8.40	1.39	1.52
1	A	28	PHE	C-N	-8.39	1.24	1.33
1	A	137	PHE	C-N	-8.36	1.23	1.33
1	A	83	GLN	CA-C	-8.35	1.41	1.52
1	A	8	PHE	C-O	-8.31	1.14	1.24
1	A	88	GLY	C-N	-8.28	1.23	1.34
1	A	59	THR	CB-CG2	-8.27	1.25	1.52
1	A	62	TYR	CZ-OH	-8.26	1.20	1.38
1	A	39	PRO	C-O	-8.25	1.14	1.23
1	A	134	GLU	CD-OE1	-8.24	1.09	1.25
1	A	7	ALA	C-O	-8.22	1.14	1.24
1	A	109	SER	C-O	-8.16	1.12	1.23
1	A	43	VAL	N-CA	-8.16	1.35	1.46
1	A	91	PHE	C-O	-8.15	1.14	1.24
1	A	134	GLU	CD-OE2	-8.12	1.09	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	THR	N-CA	-8.12	1.36	1.46
1	A	39	PRO	CA-C	8.10	1.62	1.52
1	A	133	GLU	C-O	-7.99	1.14	1.23
1	A	125	TYR	CZ-OH	-7.98	1.21	1.38
1	A	57	LEU	C-O	-7.94	1.10	1.23
1	A	19	HIS	C-O	-7.92	1.15	1.24
1	A	10	ASN	C-O	-7.91	1.14	1.24
1	A	58	THR	CB-CG2	-7.87	1.26	1.52
1	A	8	PHE	CA-CB	-7.82	1.41	1.53
1	A	127	PHE	CG-CD1	-7.73	1.22	1.38
1	A	13	ALA	N-CA	-7.72	1.36	1.46
1	A	133	GLU	CD-OE1	-7.72	1.10	1.25
1	A	129	GLN	N-CA	-7.70	1.36	1.46
1	A	148	GLU	C-O	-7.69	1.14	1.24
1	A	37	PRO	C-O	-7.67	1.15	1.23
1	A	19	HIS	CA-CB	-7.67	1.41	1.53
1	A	100	LEU	C-O	-7.66	1.13	1.23
1	A	154	ARG	CD-NE	-7.65	1.35	1.46
1	A	30	ALA	CA-C	-7.64	1.42	1.52
1	A	162	PHE	CG-CD1	-7.60	1.22	1.38
1	A	156	GLY	N-CA	-7.60	1.34	1.44
1	A	67	ASP	CG-OD2	-7.59	1.10	1.25
1	A	147	MET	SD-CE	-7.55	1.60	1.79
1	A	118	TYR	CA-C	-7.54	1.43	1.52
1	A	165	SER	C-O	-7.54	1.14	1.23
1	A	164	PRO	CA-C	7.49	1.63	1.52
1	A	125	TYR	C-N	7.41	1.42	1.33
1	A	153	ARG	NE-CZ	-7.38	1.25	1.33
1	A	98	TYR	CZ-OH	-7.37	1.22	1.38
1	A	21	ARG	CD-NE	-7.35	1.35	1.46
1	A	65	ILE	CA-C	-7.29	1.42	1.52
1	A	14	GLU	CD-OE1	-7.29	1.11	1.25
1	A	124	TYR	N-CA	-7.27	1.37	1.46
1	A	118	TYR	CZ-OH	-7.24	1.22	1.38
1	A	144	GLU	CD-OE1	-7.22	1.11	1.25
1	A	117	VAL	CA-C	-7.21	1.43	1.52
1	A	14	GLU	CD-OE2	-7.21	1.11	1.25
1	A	5	ASP	CG-OD1	-7.18	1.11	1.25
1	A	23	PRO	C-O	-7.06	1.15	1.24
1	A	66	ARG	CA-CB	-7.03	1.42	1.53
1	A	73	GLY	N-CA	-7.02	1.35	1.45
1	A	138	ILE	C-O	-7.02	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	ARG	CZ-NH2	-7.01	1.24	1.33
1	A	77	GLN	C-O	-6.98	1.14	1.23
1	A	13	ALA	C-O	-6.98	1.15	1.24
1	A	75	VAL	CA-CB	-6.96	1.47	1.54
1	A	165	SER	CB-OG	-6.96	1.28	1.42
1	A	18	LEU	C-N	-6.95	1.25	1.33
1	A	110	ASP	C-N	-6.90	1.24	1.33
1	A	126	PRO	C-O	-6.89	1.15	1.23
1	A	157	PRO	CA-CB	-6.85	1.44	1.53
1	A	165	SER	CA-CB	-6.84	1.42	1.53
1	A	41	THR	C-N	6.82	1.42	1.33
1	A	109	SER	CB-OG	-6.81	1.28	1.42
1	A	98	TYR	CE1-CZ	-6.77	1.22	1.38
1	A	154	ARG	CZ-NH2	-6.74	1.24	1.33
1	A	150	HIS	CA-C	-6.73	1.45	1.52
1	A	156	GLY	CA-C	-6.73	1.42	1.51
1	A	5	ASP	CG-OD2	-6.70	1.12	1.25
1	A	30	ALA	C-O	-6.66	1.15	1.23
1	A	126	PRO	CG-CD	-6.64	1.28	1.50
1	A	89	ALA	CA-C	-6.62	1.43	1.52
1	A	52	GLU	N-CA	-6.60	1.38	1.46
1	A	109	SER	CA-CB	-6.60	1.43	1.53
1	A	93	ASP	N-CA	-6.59	1.37	1.46
1	A	164	PRO	CA-CB	-6.53	1.44	1.53
1	A	111	SER	CA-C	6.53	1.60	1.52
1	A	56	ASP	CG-OD2	-6.51	1.12	1.25
1	A	81	THR	C-O	-6.49	1.16	1.23
1	A	86	ARG	N-CA	-6.47	1.37	1.46
1	A	7	ALA	CA-C	6.47	1.61	1.52
1	A	68	ALA	N-CA	-6.45	1.38	1.46
1	A	22	GLU	N-CA	-6.43	1.38	1.46
1	A	10	ASN	N-CA	-6.42	1.38	1.46
1	A	46	PRO	C-N	6.40	1.43	1.33
1	A	114	ALA	N-CA	-6.39	1.38	1.46
1	A	118	TYR	C-N	-6.34	1.24	1.33
1	A	164	PRO	C-O	-6.34	1.15	1.24
1	A	52	GLU	CD-OE1	-6.21	1.13	1.25
1	A	74	ALA	C-N	-6.21	1.26	1.33
1	A	91	PHE	CA-C	-6.19	1.45	1.52
1	A	31	LEU	C-N	6.13	1.41	1.34
1	A	92	MET	SD-CE	-6.11	1.64	1.79
1	A	138	ILE	CA-C	6.10	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ASP	N-CA	-6.04	1.38	1.46
1	A	158	GLY	C-O	-6.02	1.15	1.23
1	A	121	ALA	CA-CB	-6.01	1.43	1.53
1	A	124	TYR	CZ-OH	-6.00	1.25	1.38
1	A	82	TYR	CA-C	-5.96	1.45	1.52
1	A	165	SER	CA-C	-5.96	1.45	1.52
1	A	153	ARG	CD-NE	-5.91	1.38	1.46
1	A	34	SER	C-O	-5.91	1.16	1.24
1	A	162	PHE	C-N	-5.90	1.24	1.33
1	A	34	SER	N-CA	-5.89	1.38	1.46
1	A	78	TRP	CD1-NE1	-5.89	1.25	1.37
1	A	38	GLN	CD-OE1	-5.89	1.12	1.23
1	A	89	ALA	N-CA	-5.88	1.38	1.46
1	A	40	VAL	CA-C	-5.87	1.45	1.52
1	A	119	MET	N-CA	-5.87	1.36	1.45
1	A	65	ILE	C-N	-5.86	1.26	1.33
1	A	68	ALA	CA-CB	-5.86	1.44	1.53
1	A	107	PHE	CA-C	-5.86	1.45	1.52
1	A	31	LEU	CA-C	-5.85	1.46	1.52
1	A	119	MET	CG-SD	-5.83	1.66	1.80
1	A	150	HIS	N-CA	-5.82	1.38	1.45
1	A	94	ARG	C-O	-5.81	1.15	1.23
1	A	46	PRO	CA-CB	-5.80	1.46	1.54
1	A	116	VAL	CA-C	-5.79	1.45	1.52
1	A	94	ARG	NE-CZ	-5.79	1.26	1.33
1	A	57	LEU	CA-C	5.79	1.60	1.53
1	A	146	LEU	C-N	-5.78	1.25	1.33
1	A	45	ILE	CA-C	-5.77	1.46	1.52
1	A	91	PHE	N-CA	-5.77	1.39	1.46
1	A	141	GLY	CA-C	-5.76	1.43	1.51
1	A	58	THR	C-N	-5.75	1.25	1.33
1	A	19	HIS	C-N	-5.69	1.26	1.33
1	A	16	GLN	CD-OE1	-5.68	1.12	1.23
1	A	52	GLU	C-N	-5.65	1.26	1.33
1	A	66	ARG	CD-NE	-5.65	1.38	1.46
1	A	5	ASP	C-O	-5.65	1.17	1.24
1	A	44	ARG	CA-C	-5.60	1.45	1.52
1	A	29	VAL	C-N	-5.56	1.25	1.33
1	A	127	PHE	C-N	-5.56	1.26	1.33
1	A	42	PRO	CA-CB	-5.55	1.46	1.53
1	A	61	ALA	N-CA	-5.53	1.39	1.46
1	A	87	LEU	N-CA	-5.53	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	LEU	N-CA	-5.51	1.39	1.46
1	A	97	CYS	N-CA	-5.42	1.39	1.46
1	A	133	GLU	CD-OE2	-5.39	1.15	1.25
1	A	168	PRO	CA-C	5.39	1.58	1.52
1	A	38	GLN	N-CA	-5.39	1.33	1.45
1	A	83	GLN	C-N	-5.38	1.25	1.33
1	A	70	ILE	CB-CG1	-5.38	1.42	1.53
1	A	124	TYR	CG-CD1	-5.37	1.28	1.39
1	A	54	ASP	C-N	5.37	1.39	1.33
1	A	162	PHE	CG-CD2	-5.37	1.27	1.38
1	A	44	ARG	CZ-NH1	-5.36	1.25	1.32
1	A	21	ARG	NE-CZ	-5.36	1.27	1.33
1	A	34	SER	CA-C	-5.35	1.45	1.52
1	A	32	PRO	C-O	-5.34	1.17	1.24
1	A	155	LEU	CB-CG	-5.34	1.42	1.53
1	A	60	THR	C-N	-5.33	1.26	1.33
1	A	163	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	16	GLN	C-O	-5.29	1.18	1.24
1	A	113	ALA	C-N	-5.27	1.26	1.33
1	A	55	PRO	C-O	-5.25	1.17	1.24
1	A	133	GLU	N-CA	-5.24	1.39	1.46
1	A	11	LEU	C-N	-5.23	1.27	1.33
1	A	5	ASP	C-N	5.22	1.40	1.33
1	A	24	ALA	C-N	-5.22	1.26	1.33
1	A	82	TYR	CE1-CZ	-5.21	1.25	1.38
1	A	160	HIS	ND1-CE1	-5.18	1.27	1.32
1	A	111	SER	C-N	-5.18	1.26	1.33
1	A	29	VAL	CA-C	5.18	1.58	1.52
1	A	79	ARG	N-CA	-5.16	1.39	1.45
1	A	24	ALA	CA-CB	-5.16	1.44	1.53
1	A	88	GLY	CA-C	-5.11	1.41	1.52
1	A	136	TYR	C-N	-5.10	1.25	1.33
1	A	142	GLU	CD-OE2	-5.09	1.15	1.25
1	A	83	GLN	C-O	-5.06	1.17	1.24
1	A	142	GLU	CA-C	-5.06	1.46	1.52
1	A	49	ALA	CA-C	-5.04	1.46	1.52
1	A	8	PHE	CG-CD1	-5.03	1.28	1.38
1	A	81	THR	CB-CG2	-5.03	1.35	1.52
1	A	40	VAL	N-CA	-5.03	1.39	1.46
1	A	160	HIS	C-N	-5.02	1.26	1.33
1	A	145	PHE	CE2-CZ	-5.02	1.23	1.38
1	A	77	GLN	CD-OE1	-5.01	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	GLU	N-CA	-5.01	1.39	1.46

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ARG	NE-CZ-NH1	15.06	136.56	121.50
1	A	53	SER	N-CA-C	11.84	124.27	111.36
1	A	95	PHE	CA-C-N	10.33	136.27	122.84
1	A	95	PHE	C-N-CA	10.33	136.27	122.84
1	A	57	LEU	CA-C-N	10.21	137.49	121.56
1	A	57	LEU	C-N-CA	10.21	137.49	121.56
1	A	37	PRO	CA-C-O	-9.63	109.92	121.67
1	A	135	ILE	N-CA-C	9.39	121.42	107.80
1	A	66	ARG	NH1-CZ-NH2	-8.65	108.06	119.30
1	A	157	PRO	N-CA-C	8.32	124.61	111.38
1	A	164	PRO	CA-N-CD	-8.31	100.37	112.00
1	A	76	ALA	N-CA-C	8.27	121.60	110.35
1	A	134	GLU	N-CA-C	8.27	122.73	108.76
1	A	151	PRO	CB-CA-C	-8.21	100.91	110.92
1	A	20	ALA	N-CA-C	7.98	120.99	111.33
1	A	12	LEU	N-CA-C	7.98	120.69	111.11
1	A	52	GLU	N-CA-C	7.97	119.97	111.28
1	A	98	TYR	CA-C-N	7.90	133.83	121.26
1	A	98	TYR	C-N-CA	7.90	133.83	121.26
1	A	89	ALA	N-CA-C	7.72	121.64	111.75
1	A	70	ILE	N-CA-C	7.67	117.78	110.42
1	A	27	GLY	N-CA-C	7.57	123.15	113.24
1	A	130	HIS	CA-C-N	7.53	127.90	119.32
1	A	130	HIS	C-N-CA	7.53	127.90	119.32
1	A	92	MET	N-CA-C	7.51	121.37	111.75
1	A	96	ALA	N-CA-C	7.50	121.03	108.20
1	A	144	GLU	N-CA-C	7.50	121.91	109.46
1	A	114	ALA	CA-C-N	7.46	134.30	122.21
1	A	114	ALA	C-N-CA	7.46	134.30	122.21
1	A	58	THR	N-CA-C	7.46	121.32	110.42
1	A	47	PRO	CA-C-N	7.43	130.10	120.44
1	A	47	PRO	C-N-CA	7.43	130.10	120.44
1	A	71	ALA	N-CA-C	7.42	120.31	111.33
1	A	33	ASP	N-CA-C	7.41	126.59	110.80
1	A	157	PRO	CA-N-CD	-7.36	101.70	112.00
1	A	136	TYR	CA-CB-CG	7.35	127.13	113.90
1	A	64	ALA	N-CA-C	7.34	118.92	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PRO	N-CA-C	7.32	119.63	110.70
1	A	68	ALA	N-CA-C	7.26	119.20	111.28
1	A	13	ALA	N-CA-C	7.15	119.93	111.71
1	A	42	PRO	CA-N-CD	-6.99	102.21	112.00
1	A	67	ASP	OD1-CG-OD2	-6.87	106.41	122.90
1	A	151	PRO	CA-N-CD	-6.85	102.41	112.00
1	A	15	PHE	CA-C-N	6.74	129.31	120.28
1	A	15	PHE	C-N-CA	6.74	129.31	120.28
1	A	131	PRO	N-CA-C	6.66	123.67	113.75
1	A	115	TYR	CA-C-N	6.63	131.82	123.14
1	A	115	TYR	C-N-CA	6.63	131.82	123.14
1	A	44	ARG	NE-CZ-NH1	6.62	128.12	121.50
1	A	129	GLN	CB-CG-CD	6.61	123.83	112.60
1	A	59	THR	N-CA-C	6.58	118.95	109.14
1	A	5	ASP	CA-C-N	-6.57	112.86	119.56
1	A	5	ASP	C-N-CA	-6.57	112.86	119.56
1	A	55	PRO	CA-N-CD	-6.53	102.86	112.00
1	A	152	PRO	CA-N-CD	-6.44	102.98	112.00
1	A	44	ARG	CG-CD-NE	6.42	126.14	112.00
1	A	140	ALA	N-CA-C	6.38	118.09	108.46
1	A	153	ARG	CA-C-N	6.38	130.42	121.24
1	A	153	ARG	C-N-CA	6.38	130.42	121.24
1	A	116	VAL	CA-C-N	6.35	131.54	123.10
1	A	116	VAL	C-N-CA	6.35	131.54	123.10
1	A	38	GLN	CB-CA-C	6.31	118.60	109.45
1	A	9	GLN	CA-C-O	-6.26	114.18	121.07
1	A	99	CYS	N-CA-C	6.26	119.70	110.30
1	A	61	ALA	N-CA-C	6.26	120.95	112.88
1	A	157	PRO	CA-C-N	6.24	133.64	121.41
1	A	157	PRO	C-N-CA	6.24	133.64	121.41
1	A	85	SER	CA-C-N	6.17	131.02	120.72
1	A	85	SER	C-N-CA	6.17	131.02	120.72
1	A	66	ARG	CA-C-N	6.14	128.51	120.28
1	A	66	ARG	C-N-CA	6.14	128.51	120.28
1	A	63	ALA	N-CA-C	6.06	118.68	111.71
1	A	18	LEU	CA-C-N	6.02	128.27	120.44
1	A	18	LEU	C-N-CA	6.02	128.27	120.44
1	A	50	LEU	N-CA-C	6.01	118.33	111.11
1	A	82	TYR	CA-C-N	6.01	133.03	121.54
1	A	82	TYR	C-N-CA	6.01	133.03	121.54
1	A	39	PRO	CA-N-CD	-6.01	103.58	112.00
1	A	21	ARG	N-CA-C	5.99	120.43	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	LEU	CD1-CG-CD2	-5.98	97.65	110.80
1	A	152	PRO	N-CA-C	5.97	120.70	111.21
1	A	31	LEU	CA-C-N	-5.94	113.64	119.64
1	A	31	LEU	C-N-CA	-5.94	113.64	119.64
1	A	39	PRO	N-CA-C	5.93	120.64	111.21
1	A	97	CYS	N-CA-C	5.93	119.16	108.48
1	A	4	THR	CA-C-O	-5.92	110.74	120.80
1	A	72	ALA	CA-C-N	5.90	127.56	120.13
1	A	72	ALA	C-N-CA	5.90	127.56	120.13
1	A	10	ASN	N-CA-C	5.83	118.39	111.33
1	A	42	PRO	N-CA-C	5.80	120.19	111.14
1	A	12	LEU	CA-C-N	5.78	128.60	120.28
1	A	12	LEU	C-N-CA	5.78	128.60	120.28
1	A	10	ASN	CA-C-N	5.76	127.92	120.44
1	A	10	ASN	C-N-CA	5.76	127.92	120.44
1	A	92	MET	CA-C-N	5.71	132.39	122.56
1	A	92	MET	C-N-CA	5.71	132.39	122.56
1	A	139	LEU	CA-C-N	5.71	134.15	121.81
1	A	139	LEU	C-N-CA	5.71	134.15	121.81
1	A	149	GLY	CA-C-O	-5.70	112.23	119.19
1	A	80	LEU	CA-C-N	5.70	128.80	120.71
1	A	80	LEU	C-N-CA	5.70	128.80	120.71
1	A	69	PHE	CA-C-N	5.68	127.72	120.56
1	A	69	PHE	C-N-CA	5.68	127.72	120.56
1	A	158	GLY	N-CA-C	5.68	126.63	113.18
1	A	168	PRO	N-CA-C	5.62	120.06	110.95
1	A	155	LEU	N-CA-C	5.58	117.78	108.02
1	A	131	PRO	CA-C-O	-5.57	110.43	119.84
1	A	21	ARG	NE-CZ-NH1	5.51	127.01	121.50
1	A	168	PRO	CA-N-CD	-5.51	104.29	112.00
1	A	78	TRP	CB-CA-C	5.50	118.70	109.89
1	A	38	GLN	CA-C-N	-5.43	114.19	119.78
1	A	38	GLN	C-N-CA	-5.43	114.19	119.78
1	A	124	TYR	N-CA-C	5.43	117.60	107.99
1	A	161	VAL	N-CA-C	5.42	115.92	108.12
1	A	56	ASP	CB-CG-OD1	5.41	130.84	118.40
1	A	111	SER	CB-CA-C	5.40	117.78	109.03
1	A	59	THR	CB-CA-C	-5.40	98.63	110.67
1	A	110	ASP	N-CA-C	5.39	119.84	113.16
1	A	50	LEU	CA-C-N	5.37	127.42	120.44
1	A	50	LEU	C-N-CA	5.37	127.42	120.44
1	A	79	ARG	CD-NE-CZ	5.35	131.89	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	LEU	CA-C-N	5.35	127.88	120.29
1	A	25	LEU	C-N-CA	5.35	127.88	120.29
1	A	4	THR	N-CA-C	5.34	125.95	111.00
1	A	136	TYR	CA-C-N	5.29	129.72	122.84
1	A	136	TYR	C-N-CA	5.29	129.72	122.84
1	A	108	ALA	CA-C-O	-5.28	115.20	121.16
1	A	120	PRO	CA-N-CD	-5.23	104.68	112.00
1	A	87	LEU	N-CA-C	5.21	118.04	109.76
1	A	147	MET	CG-SD-CE	-5.17	89.54	100.90
1	A	75	VAL	N-CA-C	5.16	119.06	113.43
1	A	61	ALA	CA-C-N	5.13	130.65	121.15
1	A	61	ALA	C-N-CA	5.13	130.65	121.15
1	A	28	PHE	CA-C-N	5.13	129.79	121.95
1	A	28	PHE	C-N-CA	5.13	129.79	121.95
1	A	28	PHE	N-CA-C	5.12	117.99	111.69
1	A	56	ASP	N-CA-CB	-5.12	102.99	111.49
1	A	85	SER	N-CA-C	5.11	117.78	109.86
1	A	125	TYR	CB-CA-C	5.10	120.22	110.17
1	A	44	ARG	CA-CB-CG	5.08	124.26	114.10
1	A	93	ASP	N-CA-C	5.06	119.10	113.02
1	A	15	PHE	N-CA-C	5.06	116.48	111.07
1	A	52	GLU	CA-C-N	5.04	127.44	120.29
1	A	52	GLU	C-N-CA	5.04	127.44	120.29
1	A	15	PHE	O-C-N	5.03	127.25	122.07
1	A	167	HIS	O-C-N	5.00	125.56	121.31

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 ⓘ

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:33:ASP:C	1:A:34:SER:OG	2.49	0.53
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	12 15

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%)	13 18

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	53	SER
1	A	55	PRO
1	A	59	THR
1	A	99	CYS
1	A	100	LEU
1	A	112	LEU
1	A	139	LEU
1	A	147	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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%)	0.47	6 (3%) 52 54	16, 23, 37, 60	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	ASP	3.7
1	A	34	SER	3.3
1	A	4	THR	2.5
1	A	35	LEU	2.4
1	A	199	GLY	2.3
1	A	99	CYS	2.0

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	FE	A	301	1/1	0.94	0.09	35,35,35,35	1

6.5 Other polymers [i](#)

There are no such residues in this entry.