



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:04 AM GMT

PDB ID : 2ZDS
Title : Crystal Structure of SCO6571 from Streptomyces coelicolor A3(2)
Authors : Begum, P.; Gao, Y.G.; Sakai, N.; Yao, M.; Watanabe, N.; Tanaka, I.
Deposited on : 2007-11-27
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 ⓘ symbol.

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

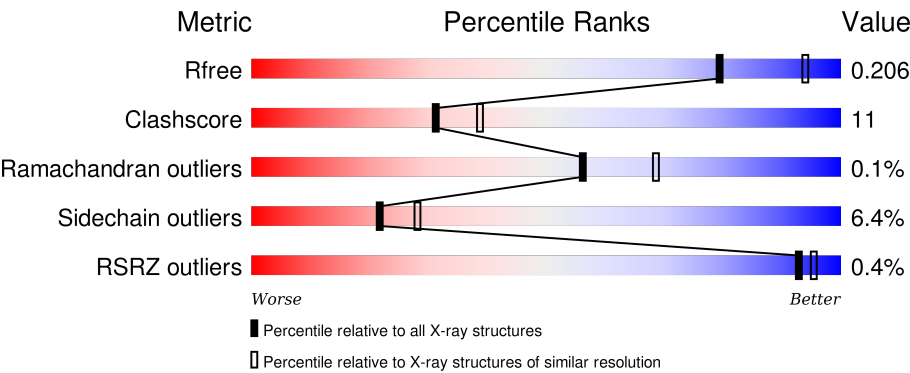
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance 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 $\leq 5\%$. 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	340	<div><div></div><div>72%18%•6%</div></div>
1	B	340	<div><div>%</div><div>77%12%••5%</div></div>
1	C	340	<div><div></div><div>75%15%•5%</div></div>
1	D	340	<div><div>%</div><div>77%14%••5%</div></div>
1	E	340	<div><div></div><div>76%14%••6%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	340	<div><div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>75%15%• • 5%</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16757 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 Putative DNA-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	Se	0	0	0
			2584	1645	461	469	5	4			
1	B	322	Total	C	N	O	S	Se	0	0	0
			2590	1648	462	471	5	4			
1	C	322	Total	C	N	O	S	Se	0	0	0
			2590	1648	462	471	5	4			
1	D	322	Total	C	N	O	S	Se	0	0	0
			2590	1648	462	471	5	4			
1	E	321	Total	C	N	O	S	Se	0	0	0
			2584	1645	461	469	5	4			
1	F	322	Total	C	N	O	S	Se	0	0	0
			2590	1648	462	471	5	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	LEU	-	EXPRESSION TAG	UNP O69946
A	333	GLU	-	EXPRESSION TAG	UNP O69946
A	334	HIS	-	EXPRESSION TAG	UNP O69946
A	335	HIS	-	EXPRESSION TAG	UNP O69946
A	336	HIS	-	EXPRESSION TAG	UNP O69946
A	337	HIS	-	EXPRESSION TAG	UNP O69946
A	338	HIS	-	EXPRESSION TAG	UNP O69946
A	339	HIS	-	EXPRESSION TAG	UNP O69946
B	332	LEU	-	EXPRESSION TAG	UNP O69946
B	333	GLU	-	EXPRESSION TAG	UNP O69946
B	334	HIS	-	EXPRESSION TAG	UNP O69946
B	335	HIS	-	EXPRESSION TAG	UNP O69946
B	336	HIS	-	EXPRESSION TAG	UNP O69946
B	337	HIS	-	EXPRESSION TAG	UNP O69946
B	338	HIS	-	EXPRESSION TAG	UNP O69946
B	339	HIS	-	EXPRESSION TAG	UNP O69946
C	332	LEU	-	EXPRESSION TAG	UNP O69946

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Chain	Residue	Modelled	Actual	Comment	Reference
C	333	GLU	-	EXPRESSION TAG	UNP O69946
C	334	HIS	-	EXPRESSION TAG	UNP O69946
C	335	HIS	-	EXPRESSION TAG	UNP O69946
C	336	HIS	-	EXPRESSION TAG	UNP O69946
C	337	HIS	-	EXPRESSION TAG	UNP O69946
C	338	HIS	-	EXPRESSION TAG	UNP O69946
C	339	HIS	-	EXPRESSION TAG	UNP O69946
D	332	LEU	-	EXPRESSION TAG	UNP O69946
D	333	GLU	-	EXPRESSION TAG	UNP O69946
D	334	HIS	-	EXPRESSION TAG	UNP O69946
D	335	HIS	-	EXPRESSION TAG	UNP O69946
D	336	HIS	-	EXPRESSION TAG	UNP O69946
D	337	HIS	-	EXPRESSION TAG	UNP O69946
D	338	HIS	-	EXPRESSION TAG	UNP O69946
D	339	HIS	-	EXPRESSION TAG	UNP O69946
E	332	LEU	-	EXPRESSION TAG	UNP O69946
E	333	GLU	-	EXPRESSION TAG	UNP O69946
E	334	HIS	-	EXPRESSION TAG	UNP O69946
E	335	HIS	-	EXPRESSION TAG	UNP O69946
E	336	HIS	-	EXPRESSION TAG	UNP O69946
E	337	HIS	-	EXPRESSION TAG	UNP O69946
E	338	HIS	-	EXPRESSION TAG	UNP O69946
E	339	HIS	-	EXPRESSION TAG	UNP O69946
F	332	LEU	-	EXPRESSION TAG	UNP O69946
F	333	GLU	-	EXPRESSION TAG	UNP O69946
F	334	HIS	-	EXPRESSION TAG	UNP O69946
F	335	HIS	-	EXPRESSION TAG	UNP O69946
F	336	HIS	-	EXPRESSION TAG	UNP O69946
F	337	HIS	-	EXPRESSION TAG	UNP O69946
F	338	HIS	-	EXPRESSION TAG	UNP O69946
F	339	HIS	-	EXPRESSION TAG	UNP O69946

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	153	Total O 153 153	0	0
2	B	205	Total O 205 205	0	0
2	C	206	Total O 206 206	0	0
2	D	217	Total O 217 217	0	0

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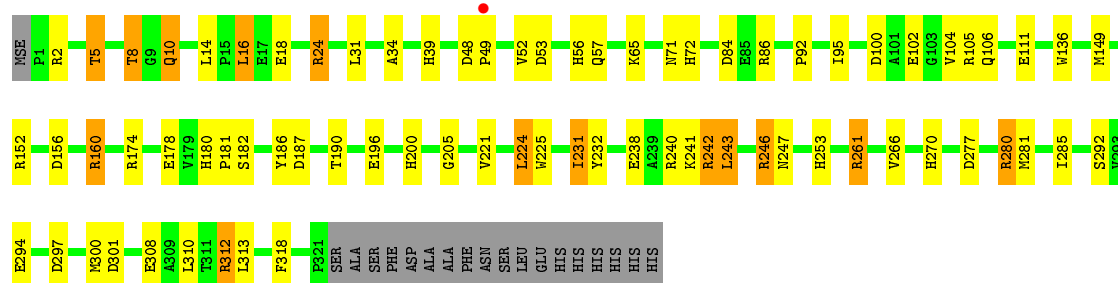
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	229	Total	O	0	0
			229	229		
2	F	219	Total	O	0	0
			219	219		

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: Putative DNA-binding protein

Chain A: 



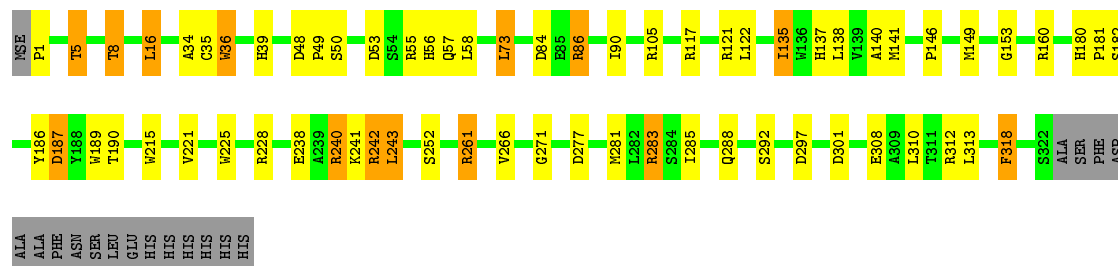
• Molecule 1: Putative DNA-binding protein

Chain B: 

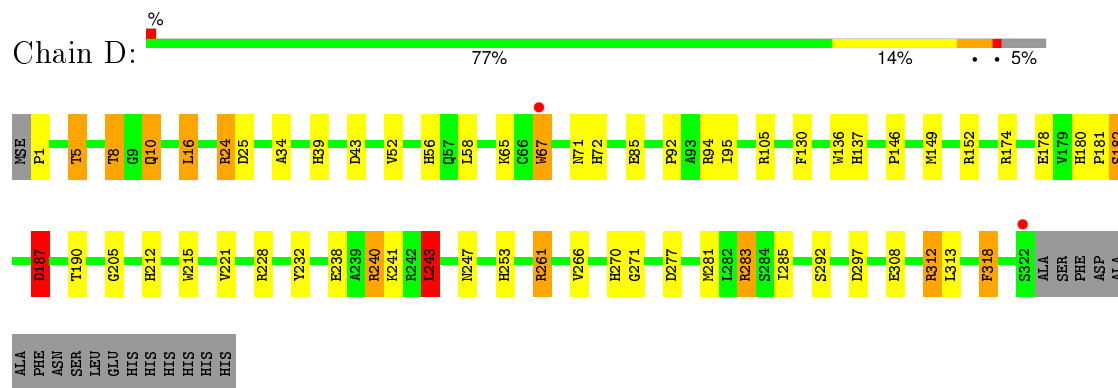


• Molecule 1: Putative DNA-binding protein

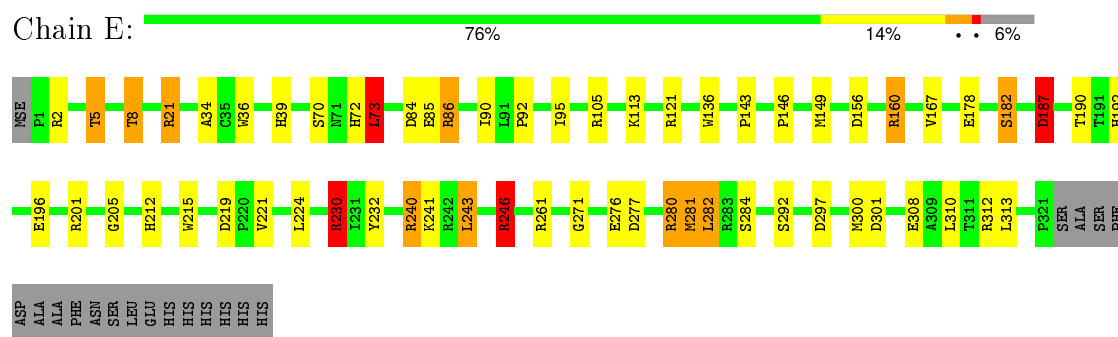
Chain C: 



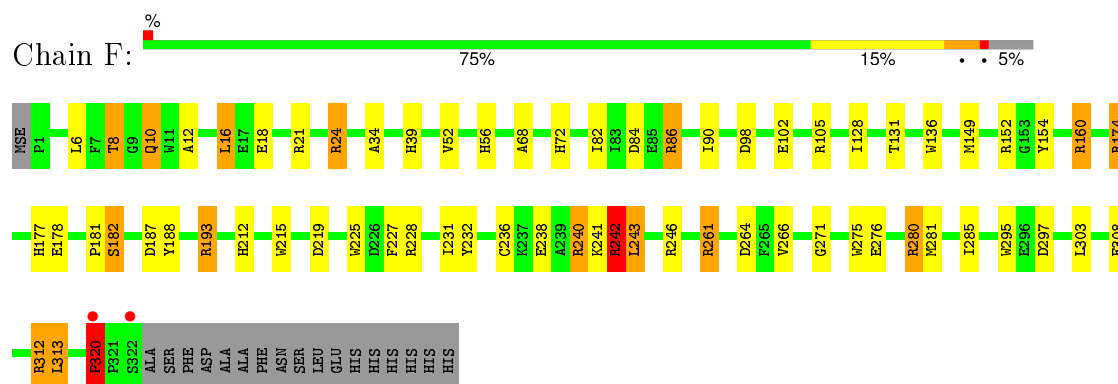
- Molecule 1: Putative DNA-binding protein



- Molecule 1: Putative DNA-binding protein



- Molecule 1: Putative DNA-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.48Å 171.59Å 184.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 41.91 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.30) 99.6 (41.91-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.63 (at 2.29Å)	Xtriage
Refinement program	REFMAC5.2.0019	Depositor
R, R_{free}	0.167 , 0.210 0.164 , 0.206	Depositor DCC
R_{free} test set	5997 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 120306 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16757	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.90	1/2663 (0.0%)	1.13	20/3618 (0.6%)
1	B	0.97	5/2669 (0.2%)	1.13	29/3626 (0.8%)
1	C	0.94	1/2669 (0.0%)	1.12	24/3626 (0.7%)
1	D	0.96	1/2669 (0.0%)	1.03	15/3626 (0.4%)
1	E	0.99	1/2663 (0.0%)	1.15	26/3618 (0.7%)
1	F	0.98	3/2669 (0.1%)	1.25	35/3626 (1.0%)
All	All	0.96	12/16002 (0.1%)	1.14	149/21740 (0.7%)

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	B	0	1
1	F	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	GLN	CB-CG	9.44	1.78	1.52
1	F	187	ASP	CG-OD1	8.98	1.46	1.25
1	D	187	ASP	CB-CG	-7.95	1.35	1.51
1	C	187	ASP	CG-OD1	7.62	1.42	1.25
1	A	187	ASP	CG-OD1	7.00	1.41	1.25
1	B	187	ASP	CB-CG	-6.37	1.38	1.51
1	B	76	GLN	CG-CD	-5.60	1.38	1.51
1	F	295	TRP	CE3-CZ3	5.51	1.47	1.38
1	B	241	LYS	CE-NZ	-5.36	1.35	1.49
1	E	187	ASP	CB-CG	-5.32	1.40	1.51
1	F	82	ILE	C-N	-5.30	1.21	1.34
1	B	85	GLU	CB-CG	5.20	1.62	1.52

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	ARG	NE-CZ-NH2	-17.40	111.60	120.30
1	A	280	ARG	NE-CZ-NH2	-17.39	111.60	120.30
1	E	240	ARG	NE-CZ-NH2	-17.13	111.73	120.30
1	F	240	ARG	NE-CZ-NH2	-17.05	111.77	120.30
1	F	187	ASP	CB-CG-OD2	-16.47	103.47	118.30
1	F	280	ARG	NE-CZ-NH2	-16.41	112.09	120.30
1	E	160	ARG	NE-CZ-NH2	-15.47	112.56	120.30
1	F	160	ARG	NE-CZ-NH2	-15.24	112.68	120.30
1	C	240	ARG	NE-CZ-NH2	-15.03	112.78	120.30
1	A	240	ARG	NE-CZ-NH2	-15.01	112.79	120.30
1	B	160	ARG	NE-CZ-NH2	-14.81	112.89	120.30
1	D	240	ARG	NE-CZ-NH2	-14.78	112.91	120.30
1	A	187	ASP	CB-CG-OD2	-14.06	105.65	118.30
1	D	187	ASP	CB-CG-OD1	-13.91	105.78	118.30
1	C	160	ARG	NE-CZ-NH1	13.84	127.22	120.30
1	B	160	ARG	NE-CZ-NH1	13.80	127.20	120.30
1	A	280	ARG	NE-CZ-NH1	13.48	127.04	120.30
1	E	187	ASP	CB-CG-OD1	-13.48	106.17	118.30
1	C	187	ASP	CB-CG-OD2	-13.34	106.29	118.30
1	F	280	ARG	NE-CZ-NH1	13.13	126.87	120.30
1	B	240	ARG	NE-CZ-NH2	-12.53	114.04	120.30
1	B	249	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	E	230	ARG	NE-CZ-NH1	-12.07	114.27	120.30
1	A	242	ARG	NE-CZ-NH1	-11.94	114.33	120.30
1	B	249	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	F	240	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	E	240	ARG	NE-CZ-NH1	11.79	126.20	120.30
1	D	261	ARG	NE-CZ-NH2	-11.70	114.45	120.30
1	F	187	ASP	CB-CG-OD1	11.69	128.82	118.30
1	A	240	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	B	280	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	F	242	ARG	NE-CZ-NH1	-11.22	114.69	120.30
1	F	261	ARG	NE-CZ-NH2	-11.18	114.71	120.30
1	D	105	ARG	NE-CZ-NH2	-10.75	114.92	120.30
1	E	160	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	C	240	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	F	160	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	A	187	ASP	CB-CG-OD1	10.10	127.39	118.30
1	B	242	ARG	NE-CZ-NH1	-10.02	115.29	120.30
1	E	246	ARG	NE-CZ-NH2	9.73	125.17	120.30
1	D	240	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	E	187	ASP	CB-CG-OD2	9.23	126.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	86	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	D	187	ASP	CB-CG-OD2	9.19	126.58	118.30
1	B	261	ARG	NE-CZ-NH2	-9.17	115.71	120.30
1	F	312	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	C	261	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	160	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	C	242	ARG	NE-CZ-NH1	-8.93	115.83	120.30
1	B	187	ASP	CB-CG-OD1	-8.63	110.53	118.30
1	F	320	PRO	C-N-CD	-8.27	102.41	120.60
1	E	86	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	E	261	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	F	105	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	C	187	ASP	CB-CG-OD1	8.21	125.69	118.30
1	E	280	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	A	160	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	D	94	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	A	105	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	E	230	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	B	187	ASP	CB-CG-OD2	7.70	125.23	118.30
1	B	2	ARG	N-CA-C	7.61	131.55	111.00
1	E	246	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	D	312	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	A	261	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	231	ILE	CG1-CB-CG2	7.37	127.61	111.40
1	C	86	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	F	193	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	249	ARG	CD-NE-CZ	7.30	133.82	123.60
1	E	201	ARG	NE-CZ-NH1	-7.27	116.66	120.30
1	A	242	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	F	261	ARG	CG-CD-NE	-7.06	96.97	111.80
1	B	249	ARG	CG-CD-NE	-6.92	97.28	111.80
1	F	21	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	240	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	242	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	D	243	LEU	CB-CG-CD1	6.73	122.45	111.00
1	F	261	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	C	241	LYS	CD-CE-NZ	-6.64	96.42	111.70
1	F	193	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	246	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	246	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	D	261	ARG	CG-CD-NE	-6.52	98.11	111.80
1	E	160	ARG	CG-CD-NE	-6.51	98.13	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	86	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	160	ARG	CD-NE-CZ	6.44	132.61	123.60
1	E	280	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	E	86	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	E	240	ARG	CD-NE-CZ	6.29	132.41	123.60
1	E	301	ASP	CB-CG-OD1	6.29	123.96	118.30
1	F	242	ARG	CG-CD-NE	-6.24	98.69	111.80
1	B	280	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	F	98	ASP	CB-CG-OD1	6.16	123.84	118.30
1	F	320	PRO	C-N-CA	6.11	147.67	122.00
1	C	242	ARG	CG-CD-NE	-6.09	99.02	111.80
1	B	243	LEU	CA-CB-CG	6.07	129.27	115.30
1	E	240	ARG	CG-CD-NE	-6.03	99.13	111.80
1	E	105	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	105	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	249	ARG	CB-CG-CD	5.99	127.16	111.60
1	F	280	ARG	CD-NE-CZ	5.95	131.93	123.60
1	B	160	ARG	CG-CD-NE	-5.92	99.37	111.80
1	F	240	ARG	CG-CD-NE	-5.87	99.47	111.80
1	F	240	ARG	CD-NE-CZ	5.87	131.81	123.60
1	E	261	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	76	GLN	CB-CG-CD	-5.86	96.37	111.60
1	F	21	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	301	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	301	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	240	ARG	CD-NE-CZ	5.80	131.72	123.60
1	C	228	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	261	ARG	CG-CD-NE	-5.73	99.76	111.80
1	E	160	ARG	CD-NE-CZ	5.70	131.58	123.60
1	F	160	ARG	CG-CD-NE	-5.65	99.94	111.80
1	A	280	ARG	CD-NE-CZ	5.62	131.47	123.60
1	C	55	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	261	ARG	CG-CD-NE	-5.59	100.05	111.80
1	B	224	LEU	CA-CB-CG	5.59	128.16	115.30
1	D	240	ARG	CG-CD-NE	-5.56	100.12	111.80
1	E	219	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C	283	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	187	ASP	CB-CA-C	-5.48	99.45	110.40
1	E	282	LEU	CB-CG-CD1	5.44	120.25	111.00
1	C	240	ARG	CD-NE-CZ	5.44	131.21	123.60
1	F	280	ARG	CG-CD-NE	-5.43	100.39	111.80
1	C	243	LEU	CA-CB-CG	5.43	127.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	105	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	283	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	F	264	ASP	CB-CG-OD1	5.32	123.08	118.30
1	C	55	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	D	105	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	160	ARG	CD-NE-CZ	5.29	131.01	123.60
1	E	73	LEU	CB-CG-CD1	5.29	120.00	111.00
1	C	86	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	F	313	LEU	CA-CB-CG	5.25	127.37	115.30
1	D	187	ASP	CB-CA-C	-5.21	99.97	110.40
1	F	228	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	280	ARG	CG-CD-NE	-5.21	100.86	111.80
1	B	105	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	D	312	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	86	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	246	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	F	312	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	F	242	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	A	312	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	43	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	160	ARG	CG-CD-NE	-5.03	101.23	111.80
1	F	219	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	PRO	Peptide
1	F	320	PRO	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	2584	0	2423	69	0
1	B	2590	0	2428	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2590	0	2428	51	0
1	D	2590	0	2428	58	0
1	E	2584	0	2423	61	0
1	F	2590	0	2427	58	0
2	A	153	0	0	4	0
2	B	205	0	0	6	0
2	C	206	0	0	7	0
2	D	217	0	0	8	0
2	E	229	0	0	8	0
2	F	219	0	0	7	0
All	All	16757	0	14557	326	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 (326) 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:E:281:MSE:CE	1:E:284:SER:HB2	1.29	1.60
1:B:76:GLN:CG	1:B:76:GLN:CB	1.78	1.59
1:A:281:MSE:CE	1:A:285:ILE:HG23	1.46	1.44
1:B:281:MSE:HE2	1:B:285:ILE:CG2	1.49	1.43
1:F:281:MSE:CE	1:F:285:ILE:HG23	1.49	1.42
1:C:281:MSE:CE	1:C:285:ILE:HG23	1.56	1.32
1:B:281:MSE:CE	1:B:285:ILE:HG23	1.59	1.30
1:A:281:MSE:HE2	1:A:285:ILE:CG2	1.64	1.26
1:A:8:THR:HG23	1:A:39:HIS:CD2	1.70	1.24
1:F:281:MSE:HE2	1:F:285:ILE:CG2	1.67	1.23
1:A:246:ARG:NH2	1:F:246:ARG:HH22	1.37	1.22
1:E:281:MSE:CE	1:E:284:SER:CB	2.18	1.20
1:C:281:MSE:HE3	1:C:285:ILE:CG2	1.73	1.19
1:C:281:MSE:CE	1:C:285:ILE:CG2	2.25	1.15
1:A:8:THR:CG2	1:A:39:HIS:HD2	1.64	1.09
1:C:8:THR:HG23	1:C:39:HIS:ND1	1.67	1.09
1:E:276:GLU:OE1	1:E:280:ARG:NH1	1.86	1.08
1:F:8:THR:HG23	1:F:39:HIS:ND1	1.70	1.07
1:C:225:TRP:HE3	1:C:281:MSE:HE1	1.14	1.06
1:E:281:MSE:HE2	1:E:284:SER:HB2	1.19	1.06
1:A:281:MSE:HE2	1:A:285:ILE:HG23	1.12	1.06
1:A:281:MSE:HE3	1:A:285:ILE:HG23	1.33	1.05
1:D:24:ARG:HH11	1:D:24:ARG:HG2	1.19	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:MSE:CE	1:A:285:ILE:CG2	2.26	1.03
1:E:8:THR:HG23	1:E:39:HIS:ND1	1.74	1.02
1:A:8:THR:HG23	1:A:39:HIS:HD2	0.88	1.02
1:C:225:TRP:CE3	1:C:281:MSE:HE1	1.95	1.02
1:B:8:THR:HG23	1:B:39:HIS:ND1	1.77	0.99
1:E:281:MSE:HE3	1:E:284:SER:HB2	1.39	0.99
1:E:281:MSE:HE1	1:E:284:SER:HB2	1.41	0.98
1:D:8:THR:HG23	1:D:39:HIS:ND1	1.79	0.98
1:F:281:MSE:HE2	1:F:285:ILE:HG23	0.99	0.97
1:F:24:ARG:HG2	1:F:24:ARG:HH11	1.28	0.96
1:F:212:HIS:HD2	1:F:215:TRP:HE1	1.08	0.94
1:F:281:MSE:HE3	1:F:285:ILE:HG23	1.49	0.92
1:B:76:GLN:CD	1:B:76:GLN:CB	2.36	0.92
1:A:246:ARG:NH2	1:F:246:ARG:NH2	2.17	0.92
1:B:76:GLN:OE1	1:B:76:GLN:HB3	1.70	0.91
1:E:212:HIS:HD2	1:E:215:TRP:HE1	1.13	0.91
1:A:5:THR:HG21	2:A:360:HOH:O	1.71	0.90
1:C:146:PRO:HD2	1:C:149:MSE:HE3	1.55	0.89
1:B:76:GLN:OE1	1:B:76:GLN:CB	2.23	0.87
1:E:2:ARG:HD2	2:E:369:HOH:O	1.72	0.87
1:E:146:PRO:HD2	1:E:149:MSE:HE3	1.54	0.87
1:E:281:MSE:HE1	1:E:284:SER:CB	1.98	0.86
1:A:231:ILE:HD12	1:A:285:ILE:HD12	1.57	0.86
1:C:225:TRP:HE3	1:C:281:MSE:CE	1.87	0.86
1:E:149:MSE:HE2	2:E:561:HOH:O	1.75	0.85
1:B:84:ASP:OD1	1:B:86:ARG:HD3	1.77	0.85
1:D:24:ARG:NH2	2:D:403:HOH:O	2.06	0.85
1:B:146:PRO:HD2	1:B:149:MSE:HE3	1.59	0.85
1:D:212:HIS:HD2	1:D:215:TRP:HE1	1.25	0.84
1:F:149:MSE:SE	1:F:152:ARG:HH21	2.10	0.84
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.43	0.83
1:A:8:THR:CG2	1:A:39:HIS:CD2	2.49	0.82
1:F:281:MSE:CE	1:F:285:ILE:CG2	2.37	0.81
1:B:281:MSE:HE2	1:B:285:ILE:HG23	0.84	0.81
1:F:8:THR:HG22	1:F:34:ALA:H	1.45	0.81
1:C:8:THR:CG2	1:C:39:HIS:ND1	2.44	0.80
1:E:84:ASP:OD1	1:E:86:ARG:HD3	1.82	0.79
1:C:281:MSE:HE3	1:C:285:ILE:HG23	0.80	0.79
1:A:84:ASP:OD2	1:A:86:ARG:HD3	1.82	0.78
1:E:5:THR:HG21	2:E:346:HOH:O	1.82	0.78
1:C:5:THR:HG21	2:C:343:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:HIS:HE1	1:D:308:GLU:OE1	1.66	0.78
1:E:297:ASP:OD2	1:E:300:MSE:HE3	1.85	0.76
1:B:281:MSE:CE	1:B:285:ILE:CG2	2.38	0.76
1:A:180:HIS:HD2	1:A:181:PRO:O	1.68	0.76
1:C:84:ASP:OD1	1:C:86:ARG:HD3	1.85	0.76
1:D:24:ARG:NH1	2:D:403:HOH:O	2.11	0.75
1:F:24:ARG:HH11	1:F:24:ARG:CG	1.99	0.75
1:D:146:PRO:HD2	1:D:149:MSE:HE3	1.68	0.75
1:D:24:ARG:HG2	1:D:24:ARG:NH1	1.96	0.74
1:C:135:ILE:HG13	1:C:138:LEU:HD12	1.67	0.74
1:F:212:HIS:CD2	1:F:215:TRP:HE1	1.99	0.74
1:E:281:MSE:HA	1:E:281:MSE:HE3	1.69	0.74
1:C:283:ARG:NH2	1:C:318:PHE:O	2.19	0.74
1:B:2:ARG:HG2	2:B:481:HOH:O	1.87	0.74
1:A:270:HIS:HE1	1:A:308:GLU:OE1	1.71	0.73
1:D:8:THR:HG22	1:D:34:ALA:H	1.54	0.73
1:B:8:THR:CG2	1:B:39:HIS:ND1	2.52	0.73
1:C:5:THR:HG22	1:C:292:SER:OG	1.89	0.71
1:C:281:MSE:HE2	1:C:285:ILE:CG2	2.20	0.71
1:D:5:THR:HG21	2:D:350:HOH:O	1.90	0.71
1:C:8:THR:HG22	1:C:34:ALA:H	1.55	0.71
1:C:135:ILE:HD13	1:C:153:GLY:HA3	1.72	0.70
1:B:281:MSE:HE3	1:B:284:SER:HB2	1.72	0.69
1:A:156:ASP:O	1:A:160:ARG:HG3	1.93	0.69
1:E:8:THR:CG2	1:E:39:HIS:ND1	2.54	0.69
1:B:16:LEU:HD13	1:B:58:LEU:HD23	1.75	0.68
1:C:181:PRO:O	1:C:182:SER:HB2	1.92	0.68
1:F:242:ARG:NH1	2:F:344:HOH:O	2.26	0.68
1:D:180:HIS:HD2	1:D:181:PRO:O	1.77	0.68
1:D:5:THR:HG22	1:D:292:SER:OG	1.93	0.67
1:A:247:ASN:HD22	1:B:189:TRP:HE1	1.42	0.67
1:F:24:ARG:NH1	2:F:541:HOH:O	1.93	0.66
1:B:281:MSE:HE2	1:B:285:ILE:HG22	1.67	0.66
1:D:8:THR:CG2	1:D:39:HIS:ND1	2.57	0.66
1:D:281:MSE:SE	1:D:285:ILE:HD13	2.45	0.66
1:C:180:HIS:HD2	1:C:181:PRO:O	1.78	0.66
1:E:8:THR:HG22	1:E:34:ALA:H	1.60	0.65
1:E:192:HIS:O	1:E:196:GLU:HG3	1.96	0.65
1:F:193:ARG:HD2	2:F:488:HOH:O	1.96	0.65
1:B:146:PRO:HD2	1:B:149:MSE:CE	2.28	0.64
1:D:228:ARG:HB2	1:D:285:ILE:HG13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ILE:HD12	1:B:285:ILE:HD11	1.78	0.64
1:A:5:THR:HG22	1:A:292:SER:CB	2.28	0.64
1:A:253:HIS:HD2	1:B:186:TYR:OH	1.81	0.64
1:F:227:PHE:O	1:F:231:ILE:HD12	1.97	0.64
1:F:24:ARG:HG2	1:F:24:ARG:NH1	2.08	0.63
1:E:281:MSE:HE3	1:E:284:SER:CB	2.12	0.63
1:F:8:THR:CG2	1:F:34:ALA:H	2.11	0.63
1:D:228:ARG:CB	1:D:285:ILE:HG13	2.29	0.63
1:A:149:MSE:HG3	1:A:152:ARG:NH2	2.14	0.63
1:C:86:ARG:HG3	1:D:149:MSE:HE1	1.82	0.62
1:F:8:THR:CG2	1:F:39:HIS:ND1	2.56	0.62
1:A:231:ILE:HD12	1:A:285:ILE:CD1	2.29	0.62
1:F:238:GLU:HB3	1:F:266:VAL:O	1.98	0.62
1:A:246:ARG:HH21	1:F:246:ARG:HH22	1.41	0.61
1:D:24:ARG:HH11	1:D:24:ARG:CG	2.03	0.61
1:F:84:ASP:OD2	1:F:86:ARG:HD3	2.00	0.61
1:A:8:THR:HG22	1:A:34:ALA:H	1.66	0.60
1:C:73:LEU:HG	1:C:90:ILE:HB	1.81	0.60
2:A:398:HOH:O	1:B:246:ARG:HD3	2.01	0.60
1:B:174:ARG:HG3	1:B:232:TYR:CD2	2.35	0.60
1:A:5:THR:HG22	1:A:292:SER:OG	2.00	0.60
1:C:56:HIS:HE1	2:C:406:HOH:O	1.84	0.60
1:C:189:TRP:HE1	1:D:247:ASN:HD22	1.49	0.60
1:A:5:THR:HG22	1:A:292:SER:HA	1.84	0.59
1:A:136:TRP:CG	1:A:182:SER:HA	2.38	0.59
1:F:56:HIS:HE1	2:F:414:HOH:O	1.84	0.59
1:E:281:MSE:HE1	1:E:284:SER:HB3	1.85	0.59
1:A:8:THR:CG2	1:A:34:ALA:H	2.16	0.58
1:E:5:THR:HG22	1:E:292:SER:CB	2.33	0.58
1:C:135:ILE:O	1:D:253:HIS:HE1	1.87	0.58
1:C:186:TYR:OH	1:D:253:HIS:HD2	1.87	0.58
1:E:136:TRP:CG	1:E:182:SER:HA	2.39	0.57
1:D:212:HIS:CD2	1:D:215:TRP:HE1	2.14	0.57
1:D:270:HIS:HD2	1:F:276:GLU:OE1	1.87	0.57
1:D:5:THR:HG22	1:D:292:SER:CB	2.34	0.57
1:F:174:ARG:HG3	1:F:232:TYR:CD2	2.40	0.57
1:B:281:MSE:HE3	1:B:285:ILE:HG23	1.76	0.57
1:E:212:HIS:CD2	1:E:215:TRP:HE1	2.06	0.56
1:E:8:THR:CG2	1:E:34:ALA:H	2.18	0.56
1:D:136:TRP:CG	1:D:182:SER:HA	2.41	0.56
1:B:297:ASP:OD2	1:B:300:MSE:HE3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:ARG:NH2	2:E:517:HOH:O	2.33	0.56
1:F:149:MSE:SE	1:F:152:ARG:NH2	2.85	0.55
1:B:240:ARG:HB2	1:B:271:GLY:HA2	1.88	0.55
1:D:92:PRO:HG2	1:D:95:ILE:HD12	1.88	0.55
1:C:135:ILE:HD13	1:C:153:GLY:CA	2.35	0.55
1:D:240:ARG:HB2	1:D:271:GLY:HA2	1.87	0.55
1:A:280:ARG:NH2	1:C:297:ASP:OD1	2.36	0.55
1:B:76:GLN:CG	1:B:76:GLN:CA	2.80	0.55
1:E:212:HIS:HD2	1:E:215:TRP:NE1	1.93	0.54
1:E:72:HIS:HE1	1:E:178:GLU:OE1	1.90	0.54
1:D:283:ARG:NH2	1:D:318:PHE:O	2.38	0.54
1:C:8:THR:CG2	1:C:34:ALA:H	2.18	0.54
1:E:36:TRP:CD2	1:E:73:LEU:HD22	2.43	0.54
1:D:85:GLU:CD	1:D:85:GLU:H	2.11	0.54
1:D:221:VAL:HG21	1:D:277:ASP:HB3	1.89	0.54
1:D:149:MSE:HG3	1:D:152:ARG:NH2	2.22	0.54
1:F:308:GLU:O	1:F:312:ARG:HG2	2.07	0.54
1:B:1:PRO:HB3	2:B:369:HOH:O	2.06	0.54
1:D:8:THR:CG2	1:D:34:ALA:H	2.20	0.54
2:C:491:HOH:O	1:D:137:HIS:HE1	1.91	0.54
1:C:8:THR:HG23	1:C:39:HIS:CE1	2.40	0.53
1:D:181:PRO:HG2	1:D:212:HIS:CD2	2.43	0.53
1:E:21:ARG:HD2	1:E:21:ARG:C	2.29	0.53
1:D:16:LEU:HG	1:D:39:HIS:HA	1.90	0.53
1:E:205:GLY:HA3	1:E:232:TYR:CE2	2.44	0.53
1:C:36:TRP:CD2	1:C:73:LEU:HD22	2.44	0.53
1:D:24:ARG:CZ	2:D:403:HOH:O	2.39	0.52
1:A:102:GLU:OE2	1:A:160:ARG:NH2	2.41	0.52
1:E:5:THR:HG22	1:E:292:SER:HA	1.90	0.52
1:E:312:ARG:NE	2:E:517:HOH:O	2.26	0.52
1:B:79:CYS:HB2	1:B:131:THR:O	2.09	0.52
1:A:16:LEU:HG	1:A:39:HIS:HA	1.91	0.52
1:F:154:TYR:CE1	1:F:193:ARG:HG2	2.44	0.52
1:A:312:ARG:NE	2:A:452:HOH:O	2.43	0.52
1:E:205:GLY:HA3	1:E:232:TYR:CD2	2.45	0.52
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.17	0.52
1:E:281:MSE:HE2	1:E:284:SER:CB	2.12	0.52
1:B:8:THR:HG23	1:B:39:HIS:CE1	2.43	0.52
1:C:283:ARG:HH11	1:C:283:ARG:HG3	1.75	0.52
1:E:73:LEU:HG	1:E:90:ILE:HB	1.92	0.52
1:A:53:ASP:O	1:A:57:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:O	1:A:106:GLN:HG2	2.10	0.51
1:E:308:GLU:O	1:E:312:ARG:HG2	2.10	0.51
1:E:8:THR:HG22	1:E:34:ALA:CB	2.40	0.51
1:A:86:ARG:HG3	1:B:149:MSE:HE1	1.92	0.51
1:D:238:GLU:HB3	1:D:266:VAL:O	2.11	0.51
1:C:240:ARG:HB2	1:C:271:GLY:HA2	1.92	0.51
1:A:238:GLU:HB3	1:A:266:VAL:O	2.11	0.51
1:D:136:TRP:CD2	1:D:182:SER:HA	2.46	0.51
1:C:149:MSE:HE2	2:C:537:HOH:O	2.10	0.50
1:A:231:ILE:CD1	1:A:285:ILE:HD12	2.35	0.50
1:A:8:THR:HG22	1:A:34:ALA:CB	2.42	0.50
1:F:131:THR:HG23	1:F:177:HIS:CD2	2.47	0.50
1:A:281:MSE:HE2	1:A:285:ILE:HG21	1.81	0.50
1:E:246:ARG:NH2	2:E:354:HOH:O	2.45	0.50
1:D:241:LYS:HB3	1:D:243:LEU:HD22	1.93	0.50
1:D:205:GLY:HA3	1:D:232:TYR:CD2	2.45	0.50
1:F:149:MSE:SE	1:F:152:ARG:HE	2.45	0.49
1:A:5:THR:HG22	1:A:292:SER:CA	2.43	0.49
1:B:281:MSE:CE	1:B:284:SER:HB2	2.39	0.49
1:E:241:LYS:HB3	1:E:243:LEU:HD22	1.94	0.49
1:F:18:GLU:HG2	2:F:516:HOH:O	2.12	0.49
1:F:24:ARG:CG	1:F:24:ARG:NH1	2.69	0.48
1:F:225:TRP:CE3	1:F:281:MSE:HE1	2.48	0.48
1:B:2:ARG:HH11	1:B:2:ARG:HG2	1.78	0.48
1:E:205:GLY:HA2	1:E:230:ARG:HG3	1.94	0.48
1:F:10:GLN:NE2	1:F:10:GLN:H	2.11	0.48
1:E:92:PRO:HG2	1:E:95:ILE:HG12	1.94	0.48
1:F:16:LEU:HG	1:F:39:HIS:HA	1.96	0.48
1:A:136:TRP:CD2	1:A:182:SER:HA	2.48	0.48
1:F:72:HIS:HE1	1:F:178:GLU:OE1	1.96	0.48
1:E:121:ARG:NH2	2:E:568:HOH:O	2.44	0.48
1:D:16:LEU:HD13	1:D:58:LEU:HD23	1.94	0.48
1:E:5:THR:HG22	1:E:292:SER:OG	2.13	0.48
1:C:35:CYS:C	1:C:36:TRP:CD1	2.87	0.48
1:A:196:GLU:HG3	1:A:200:HIS:HE1	1.78	0.48
1:C:187:ASP:HB3	1:C:190:THR:H	1.79	0.48
1:B:136:TRP:CG	1:B:182:SER:HA	2.49	0.47
1:A:297:ASP:OD1	1:E:280:ARG:NH2	2.46	0.47
1:D:187:ASP:HB2	1:D:190:THR:OG1	2.14	0.47
1:A:102:GLU:CD	1:A:160:ARG:HH22	2.18	0.47
1:B:280:ARG:NH2	1:F:297:ASP:OD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:MSE:HE2	1:C:285:ILE:HG21	1.96	0.47
1:D:24:ARG:NH1	1:D:25:ASP:OD1	2.48	0.47
1:B:187:ASP:HB2	1:B:190:THR:OG1	2.15	0.47
1:B:56:HIS:HE1	2:B:501:HOH:O	1.96	0.47
1:D:67:TRP:HD1	2:D:346:HOH:O	1.97	0.47
1:E:230:ARG:HD3	2:E:343:HOH:O	2.15	0.47
1:D:5:THR:HG22	1:D:292:SER:HA	1.97	0.46
1:B:241:LYS:HE3	1:B:272:ASP:OD2	2.15	0.46
1:F:240:ARG:HB2	1:F:271:GLY:HA2	1.97	0.46
1:F:225:TRP:HE3	1:F:281:MSE:HE1	1.79	0.46
1:B:221:VAL:HG21	1:B:277:ASP:HB3	1.97	0.46
1:D:205:GLY:HA3	1:D:232:TYR:CE2	2.51	0.46
1:E:136:TRP:CD2	1:E:182:SER:HA	2.51	0.46
1:E:146:PRO:HD2	1:E:149:MSE:CE	2.38	0.45
1:B:81:ALA:HB2	1:B:134:ALA:HA	1.98	0.45
1:F:181:PRO:HG2	1:F:212:HIS:CD2	2.51	0.45
1:B:100:ASP:HB3	2:B:460:HOH:O	2.16	0.45
1:D:174:ARG:HD3	2:D:551:HOH:O	2.15	0.45
1:A:300:MSE:HE3	1:E:280:ARG:NH2	2.32	0.45
1:F:136:TRP:CG	1:F:182:SER:HA	2.50	0.45
1:F:241:LYS:HB3	1:F:243:LEU:HD22	1.99	0.45
1:F:225:TRP:HE3	1:F:281:MSE:CE	2.30	0.45
1:F:8:THR:HG22	1:F:34:ALA:CB	2.47	0.45
1:E:5:THR:HG22	1:E:292:SER:CA	2.47	0.45
1:A:224:LEU:HD12	1:A:231:ILE:HG21	1.98	0.45
1:C:16:LEU:HG	1:C:39:HIS:HA	1.98	0.45
1:E:281:MSE:CE	1:E:281:MSE:HA	2.40	0.45
1:B:4:PHE:HA	1:B:291:VAL:O	2.17	0.44
1:A:56:HIS:HE1	2:A:437:HOH:O	1.99	0.44
1:D:56:HIS:HE1	2:D:461:HOH:O	1.99	0.44
1:E:246:ARG:HB3	1:F:188:TYR:CD1	2.52	0.44
1:A:48:ASP:HA	1:A:49:PRO:HD2	1.85	0.44
1:E:240:ARG:HB2	1:E:271:GLY:HA2	1.98	0.44
1:A:95:ILE:HD11	1:A:111:GLU:HG2	1.99	0.44
1:D:228:ARG:HB3	1:D:285:ILE:HG13	1.98	0.44
1:E:221:VAL:HG21	1:E:277:ASP:HB3	1.99	0.44
1:C:252:SER:OG	1:D:187:ASP:OD2	2.28	0.44
1:A:72:HIS:HE1	1:A:178:GLU:OE2	2.00	0.44
1:D:297:ASP:OD1	1:F:280:ARG:NH2	2.45	0.44
1:A:14:LEU:O	1:A:39:HIS:HE1	2.00	0.43
1:F:212:HIS:HB2	2:F:457:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:THR:HG22	1:C:292:SER:CB	2.47	0.43
1:E:156:ASP:OD1	1:E:160:ARG:HD2	2.18	0.43
1:D:270:HIS:CE1	1:D:308:GLU:OE1	2.58	0.43
1:C:137:HIS:HD2	2:C:418:HOH:O	2.01	0.43
1:E:246:ARG:HD3	2:F:355:HOH:O	2.18	0.43
1:A:205:GLY:HA3	1:A:232:TYR:CD2	2.53	0.43
1:C:135:ILE:HD11	2:C:444:HOH:O	2.18	0.43
1:B:1:PRO:O	1:B:291:VAL:CG2	2.66	0.43
1:A:231:ILE:O	1:A:231:ILE:HD13	2.18	0.43
1:A:225:TRP:HE3	1:A:281:MSE:HE1	1.84	0.43
1:F:236:CYS:HB3	1:F:275:TRP:CH2	2.53	0.43
1:E:143:PRO:HB3	1:F:90:ILE:HD13	2.01	0.43
1:A:24:ARG:NH1	1:A:24:ARG:HG2	2.18	0.43
1:A:8:THR:HG22	1:A:34:ALA:HB3	2.01	0.42
1:B:16:LEU:HG	1:B:39:HIS:HA	2.00	0.42
1:E:187:ASP:HB2	1:E:190:THR:OG1	2.18	0.42
1:B:310:LEU:O	1:B:314:LYS:HG3	2.19	0.42
1:B:242:ARG:HD3	2:D:418:HOH:O	2.17	0.42
1:E:5:THR:CG2	1:E:292:SER:OG	2.66	0.42
1:C:215:TRP:HD1	2:C:351:HOH:O	2.01	0.42
1:F:154:TYR:CZ	1:F:193:ARG:HG2	2.54	0.42
1:B:308:GLU:O	1:B:312:ARG:HG2	2.20	0.42
1:C:117:ARG:O	1:C:121:ARG:HG2	2.20	0.42
1:A:241:LYS:HB3	1:A:243:LEU:HD22	2.01	0.42
1:E:8:THR:HG22	1:E:34:ALA:HB3	2.00	0.42
1:C:140:ALA:O	1:C:141:MSE:HB2	2.19	0.42
1:D:308:GLU:O	1:D:312:ARG:HG2	2.19	0.42
1:A:221:VAL:HG21	1:A:277:ASP:HB3	2.02	0.42
1:A:246:ARG:HH22	1:F:246:ARG:HH22	1.51	0.42
1:A:92:PRO:HD2	1:A:95:ILE:HD12	2.02	0.42
1:D:72:HIS:CD2	1:D:72:HIS:H	2.37	0.41
1:C:181:PRO:O	1:C:182:SER:CB	2.63	0.41
1:A:205:GLY:HA3	1:A:232:TYR:CE2	2.54	0.41
1:C:238:GLU:HB3	1:C:266:VAL:O	2.19	0.41
1:B:180:HIS:H	1:B:186:TYR:HA	1.86	0.41
1:D:10:GLN:H	1:D:10:GLN:NE2	2.18	0.41
1:F:102:GLU:OE2	1:F:160:ARG:NH2	2.33	0.41
1:A:231:ILE:CD1	1:A:285:ILE:CD1	2.97	0.41
1:A:253:HIS:CD2	1:B:186:TYR:OH	2.69	0.41
1:E:113:LYS:HG2	1:E:167:VAL:HG21	2.01	0.41
1:A:10:GLN:HE22	1:A:294:GLU:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:VAL:HG21	1:C:277:ASP:HB3	2.02	0.41
1:D:8:THR:HG22	1:D:34:ALA:CB	2.51	0.41
1:F:68:ALA:HB1	1:F:128:ILE:CD1	2.51	0.41
1:B:212:HIS:HB2	2:B:510:HOH:O	2.21	0.41
1:B:77:ALA:O	1:B:105:ARG:HG2	2.21	0.41
1:A:246:ARG:CZ	1:F:246:ARG:NH2	2.80	0.41
1:F:10:GLN:HE21	1:F:10:GLN:H	1.69	0.41
1:A:186:TYR:CE2	1:A:190:THR:HG21	2.56	0.41
1:A:100:ASP:O	1:A:104:VAL:HG13	2.20	0.41
1:D:72:HIS:HE1	1:D:178:GLU:OE2	2.04	0.40
1:D:72:HIS:HB3	1:D:130:PHE:CD2	2.56	0.40
1:C:53:ASP:O	1:C:57:GLN:HG3	2.21	0.40
1:C:308:GLU:O	1:C:312:ARG:HG2	2.22	0.40
1:F:12:ALA:HA	1:F:39:HIS:CE1	2.56	0.40
1:B:312:ARG:NH2	2:B:512:HOH:O	2.55	0.40
1:C:48:ASP:HA	1:C:49:PRO:HD3	1.87	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	319/340 (94%)	310 (97%)	9 (3%)	0	100	100
1	B	320/340 (94%)	314 (98%)	6 (2%)	0	100	100
1	C	320/340 (94%)	310 (97%)	10 (3%)	0	100	100
1	D	320/340 (94%)	310 (97%)	10 (3%)	0	100	100
1	E	319/340 (94%)	314 (98%)	5 (2%)	0	100	100
1	F	320/340 (94%)	311 (97%)	8 (2%)	1 (0%)	46	57
All	All	1918/2040 (94%)	1869 (97%)	48 (2%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	320	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/271 (96%)	241 (93%)	19 (7%)	17	22
1	B	261/271 (96%)	244 (94%)	17 (6%)	21	27
1	C	261/271 (96%)	244 (94%)	17 (6%)	21	27
1	D	261/271 (96%)	244 (94%)	17 (6%)	21	27
1	E	260/271 (96%)	244 (94%)	16 (6%)	23	30
1	F	261/271 (96%)	247 (95%)	14 (5%)	27	36
All	All	1564/1626 (96%)	1464 (94%)	100 (6%)	22	28

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	8	THR
1	A	10	GLN
1	A	16	LEU
1	A	18	GLU
1	A	24	ARG
1	A	31	LEU
1	A	52	VAL
1	A	65	LYS
1	A	71	ASN
1	A	174	ARG
1	A	224	LEU
1	A	231	ILE
1	A	242	ARG
1	A	243	LEU
1	A	261	ARG

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Mol	Chain	Res	Type
1	A	310	LEU
1	A	313	LEU
1	A	318	PHE
1	B	2	ARG
1	B	8	THR
1	B	16	LEU
1	B	52	VAL
1	B	76	GLN
1	B	78	VAL
1	B	85	GLU
1	B	174	ARG
1	B	182	SER
1	B	187	ASP
1	B	195	LEU
1	B	224	LEU
1	B	231	ILE
1	B	242	ARG
1	B	243	LEU
1	B	249	ARG
1	B	313	LEU
1	C	1	PRO
1	C	5	THR
1	C	8	THR
1	C	16	LEU
1	C	36	TRP
1	C	50	SER
1	C	58	LEU
1	C	73	LEU
1	C	122	LEU
1	C	135	ILE
1	C	242	ARG
1	C	243	LEU
1	C	261	ARG
1	C	288	GLN
1	C	310	LEU
1	C	313	LEU
1	C	318	PHE
1	D	1	PRO
1	D	5	THR
1	D	8	THR
1	D	10	GLN
1	D	16	LEU

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Mol	Chain	Res	Type
1	D	24	ARG
1	D	52	VAL
1	D	65	LYS
1	D	67	TRP
1	D	71	ASN
1	D	182	SER
1	D	187	ASP
1	D	243	LEU
1	D	261	ARG
1	D	283	ARG
1	D	313	LEU
1	D	318	PHE
1	E	5	THR
1	E	8	THR
1	E	21	ARG
1	E	70	SER
1	E	73	LEU
1	E	85	GLU
1	E	182	SER
1	E	187	ASP
1	E	224	LEU
1	E	230	ARG
1	E	243	LEU
1	E	246	ARG
1	E	281	MSE
1	E	282	LEU
1	E	310	LEU
1	E	313	LEU
1	F	6	LEU
1	F	8	THR
1	F	10	GLN
1	F	16	LEU
1	F	24	ARG
1	F	52	VAL
1	F	174	ARG
1	F	182	SER
1	F	242	ARG
1	F	243	LEU
1	F	261	ARG
1	F	303	LEU
1	F	313	LEU
1	F	320	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	39	HIS
1	A	56	HIS
1	A	71	ASN
1	A	72	HIS
1	A	177	HIS
1	A	180	HIS
1	A	192	HIS
1	A	200	HIS
1	A	247	ASN
1	A	253	HIS
1	A	270	HIS
1	A	288	GLN
1	B	56	HIS
1	B	72	HIS
1	B	137	HIS
1	C	3	ASN
1	C	56	HIS
1	C	76	GLN
1	C	137	HIS
1	C	180	HIS
1	C	200	HIS
1	C	288	GLN
1	D	10	GLN
1	D	56	HIS
1	D	71	ASN
1	D	72	HIS
1	D	76	GLN
1	D	106	GLN
1	D	137	HIS
1	D	180	HIS
1	D	192	HIS
1	D	212	HIS
1	D	216	GLN
1	D	247	ASN
1	D	253	HIS
1	D	270	HIS
1	D	288	GLN
1	D	304	GLN
1	E	72	HIS
1	E	76	GLN

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Mol	Chain	Res	Type
1	E	137	HIS
1	E	212	HIS
1	F	10	GLN
1	F	56	HIS
1	F	72	HIS
1	F	76	GLN
1	F	177	HIS
1	F	200	HIS
1	F	212	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](#)

There are no ligands in this entry.

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, 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	317/340 (93%)	-0.55	1 (0%) 94 96	6, 16, 29, 38	0
1	B	318/340 (93%)	-0.62	2 (0%) 90 93	6, 12, 24, 41	0
1	C	318/340 (93%)	-0.73	0 100 100	5, 12, 24, 42	0
1	D	318/340 (93%)	-0.72	2 (0%) 90 93	5, 11, 22, 46	0
1	E	317/340 (93%)	-0.75	0 100 100	4, 10, 20, 32	0
1	F	318/340 (93%)	-0.67	2 (0%) 90 93	5, 10, 22, 50	0
All	All	1906/2040 (93%)	-0.67	7 (0%) 93 95	4, 11, 24, 50	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	322	SER	3.6
1	B	1	PRO	3.5
1	A	49	PRO	3.0
1	F	320	PRO	2.9
1	F	322	SER	2.4
1	D	322	SER	2.4
1	D	67	TRP	2.2

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.