



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:03 PM UTC

PDB ID : 5GS5 / pdb_00005gs5
Title : Crystal structure of apo rat STING
Authors : Zhang, H.; Han, M.J.; Tao, J.L.; Ye, Z.Y.; Du, X.X.; Deng, M.J.; Zhang, X.Y.;
Li, L.F.; Jiang, Z.F.; Su, X.D.
Deposited on : 2016-08-13
Resolution : 1.84 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
Mogul : 2022.3.0, CSD as543be (2022)
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

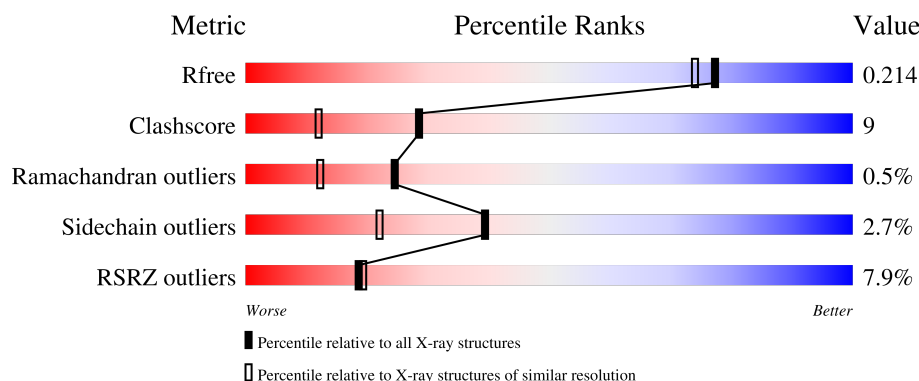
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	225	4% 51% 35% • 11%
1	B	225	6% 41% 43% 7% 9%
1	C	225	11% 59% 33% • •
1	D	225	8% 50% 41% • • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7224 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 Stimulator of interferon genes protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1582	990	284	298	10			
1	B	205	Total	C	N	O	S	0	0	0
			1616	1010	289	307	10			
1	C	216	Total	C	N	O	S	0	0	0
			1698	1061	302	325	10			
1	D	213	Total	C	N	O	S	0	0	0
			1683	1052	299	322	10			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	MET	-	expression tag	UNP F1M391
A	118	GLY	-	expression tag	UNP F1M391
A	119	SER	-	expression tag	UNP F1M391
A	120	SER	-	expression tag	UNP F1M391
A	121	HIS	-	expression tag	UNP F1M391
A	122	HIS	-	expression tag	UNP F1M391
A	123	HIS	-	expression tag	UNP F1M391
A	124	HIS	-	expression tag	UNP F1M391
A	125	HIS	-	expression tag	UNP F1M391
A	126	HIS	-	expression tag	UNP F1M391
A	127	SER	-	expression tag	UNP F1M391
A	128	SER	-	expression tag	UNP F1M391
A	129	GLY	-	expression tag	UNP F1M391
A	130	GLU	-	expression tag	UNP F1M391
A	131	ASN	-	expression tag	UNP F1M391
A	132	LEU	-	expression tag	UNP F1M391
A	133	TYR	-	expression tag	UNP F1M391
A	134	PHE	-	expression tag	UNP F1M391
A	135	GLN	-	expression tag	UNP F1M391
A	136	GLY	-	expression tag	UNP F1M391
A	137	SER	-	expression tag	UNP F1M391

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Chain	Residue	Modelled	Actual	Comment	Reference
A	138	HIS	-	expression tag	UNP F1M391
A	139	MET	-	expression tag	UNP F1M391
A	338	ALA	-	expression tag	UNP F1M391
A	339	ALA	-	expression tag	UNP F1M391
A	340	ALA	-	expression tag	UNP F1M391
A	341	ALA	-	expression tag	UNP F1M391
B	117	MET	-	expression tag	UNP F1M391
B	118	GLY	-	expression tag	UNP F1M391
B	119	SER	-	expression tag	UNP F1M391
B	120	SER	-	expression tag	UNP F1M391
B	121	HIS	-	expression tag	UNP F1M391
B	122	HIS	-	expression tag	UNP F1M391
B	123	HIS	-	expression tag	UNP F1M391
B	124	HIS	-	expression tag	UNP F1M391
B	125	HIS	-	expression tag	UNP F1M391
B	126	HIS	-	expression tag	UNP F1M391
B	127	SER	-	expression tag	UNP F1M391
B	128	SER	-	expression tag	UNP F1M391
B	129	GLY	-	expression tag	UNP F1M391
B	130	GLU	-	expression tag	UNP F1M391
B	131	ASN	-	expression tag	UNP F1M391
B	132	LEU	-	expression tag	UNP F1M391
B	133	TYR	-	expression tag	UNP F1M391
B	134	PHE	-	expression tag	UNP F1M391
B	135	GLN	-	expression tag	UNP F1M391
B	136	GLY	-	expression tag	UNP F1M391
B	137	SER	-	expression tag	UNP F1M391
B	138	HIS	-	expression tag	UNP F1M391
B	139	MET	-	expression tag	UNP F1M391
B	338	ALA	-	expression tag	UNP F1M391
B	339	ALA	-	expression tag	UNP F1M391
B	340	ALA	-	expression tag	UNP F1M391
B	341	ALA	-	expression tag	UNP F1M391
C	117	MET	-	expression tag	UNP F1M391
C	118	GLY	-	expression tag	UNP F1M391
C	119	SER	-	expression tag	UNP F1M391
C	120	SER	-	expression tag	UNP F1M391
C	121	HIS	-	expression tag	UNP F1M391
C	122	HIS	-	expression tag	UNP F1M391
C	123	HIS	-	expression tag	UNP F1M391
C	124	HIS	-	expression tag	UNP F1M391
C	125	HIS	-	expression tag	UNP F1M391

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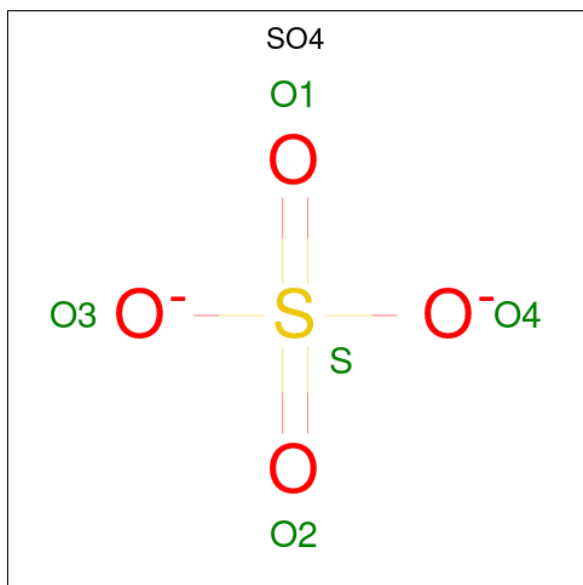
Chain	Residue	Modelled	Actual	Comment	Reference
C	126	HIS	-	expression tag	UNP F1M391
C	127	SER	-	expression tag	UNP F1M391
C	128	SER	-	expression tag	UNP F1M391
C	129	GLY	-	expression tag	UNP F1M391
C	130	GLU	-	expression tag	UNP F1M391
C	131	ASN	-	expression tag	UNP F1M391
C	132	LEU	-	expression tag	UNP F1M391
C	133	TYR	-	expression tag	UNP F1M391
C	134	PHE	-	expression tag	UNP F1M391
C	135	GLN	-	expression tag	UNP F1M391
C	136	GLY	-	expression tag	UNP F1M391
C	137	SER	-	expression tag	UNP F1M391
C	138	HIS	-	expression tag	UNP F1M391
C	139	MET	-	expression tag	UNP F1M391
C	338	ALA	-	expression tag	UNP F1M391
C	339	ALA	-	expression tag	UNP F1M391
C	340	ALA	-	expression tag	UNP F1M391
C	341	ALA	-	expression tag	UNP F1M391
D	117	MET	-	expression tag	UNP F1M391
D	118	GLY	-	expression tag	UNP F1M391
D	119	SER	-	expression tag	UNP F1M391
D	120	SER	-	expression tag	UNP F1M391
D	121	HIS	-	expression tag	UNP F1M391
D	122	HIS	-	expression tag	UNP F1M391
D	123	HIS	-	expression tag	UNP F1M391
D	124	HIS	-	expression tag	UNP F1M391
D	125	HIS	-	expression tag	UNP F1M391
D	126	HIS	-	expression tag	UNP F1M391
D	127	SER	-	expression tag	UNP F1M391
D	128	SER	-	expression tag	UNP F1M391
D	129	GLY	-	expression tag	UNP F1M391
D	130	GLU	-	expression tag	UNP F1M391
D	131	ASN	-	expression tag	UNP F1M391
D	132	LEU	-	expression tag	UNP F1M391
D	133	TYR	-	expression tag	UNP F1M391
D	134	PHE	-	expression tag	UNP F1M391
D	135	GLN	-	expression tag	UNP F1M391
D	136	GLY	-	expression tag	UNP F1M391
D	137	SER	-	expression tag	UNP F1M391
D	138	HIS	-	expression tag	UNP F1M391
D	139	MET	-	expression tag	UNP F1M391
D	338	ALA	-	expression tag	UNP F1M391

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Chain	Residue	Modelled	Actual	Comment	Reference
D	339	ALA	-	expression tag	UNP F1M391
D	340	ALA	-	expression tag	UNP F1M391
D	341	ALA	-	expression tag	UNP F1M391

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

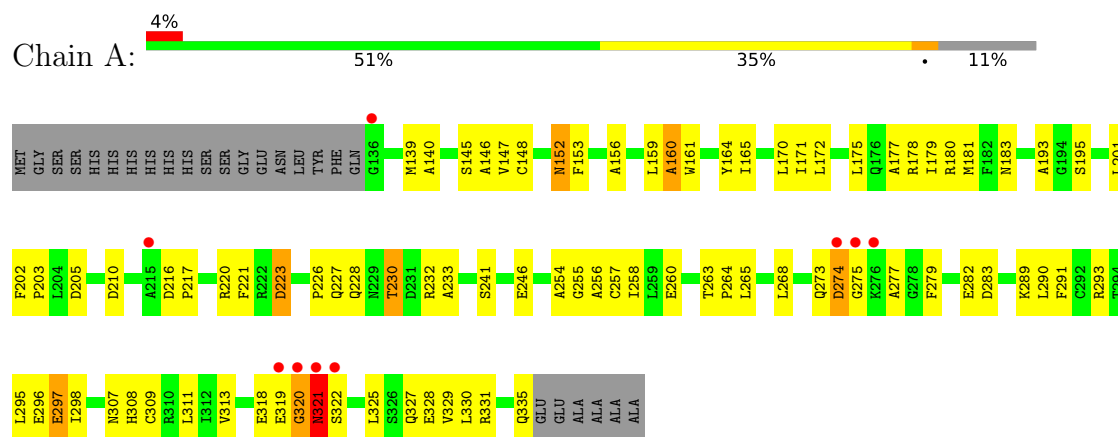
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total 139	O 139	0	0
3	B	152	Total 152	O 152	0	0
3	C	147	Total 147	O 147	0	0
3	D	162	Total 162	O 162	0	0

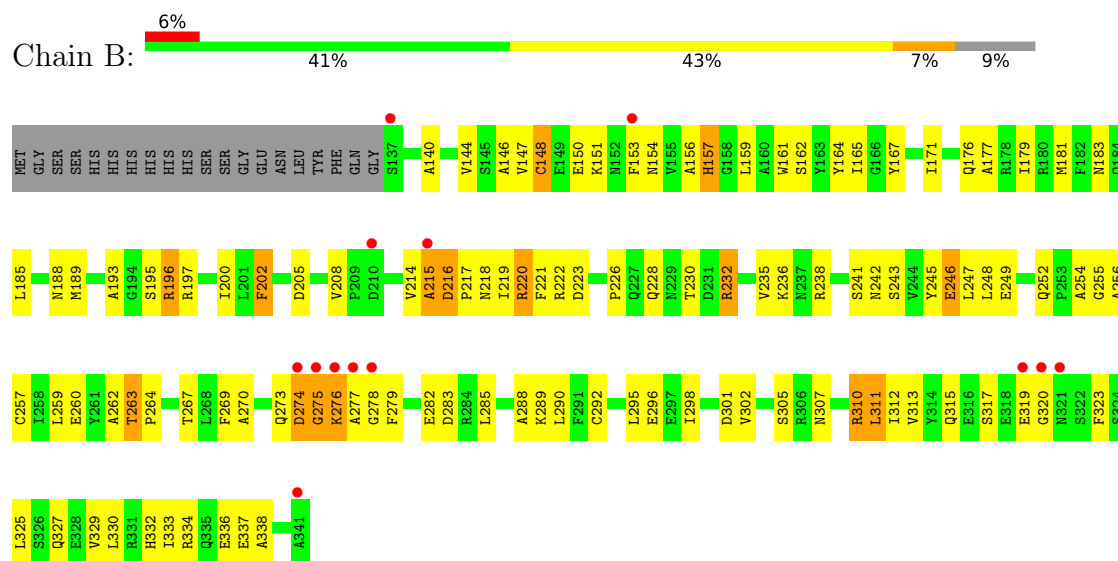
3 Residue-property plots

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: Stimulator of interferon genes protein

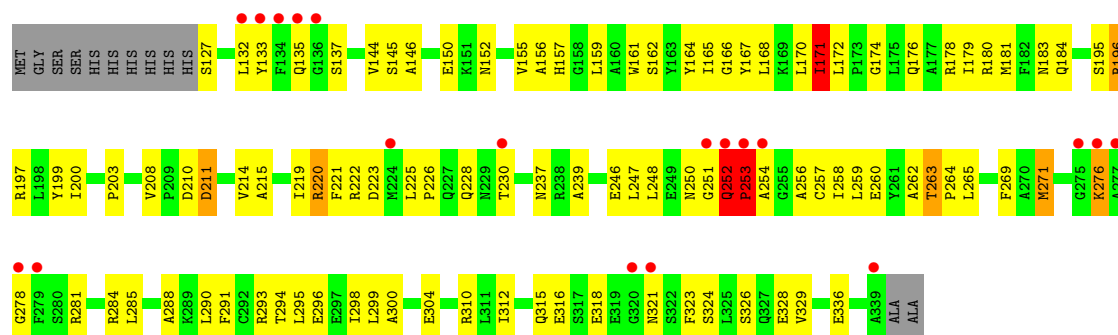


- Molecule 1: Stimulator of interferon genes protein



- Molecule 1: Stimulator of interferon genes protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.29Å 75.51Å 87.64Å 90.00° 115.35° 90.00°	Depositor
Resolution (Å)	42.73 – 1.84 42.73 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.73-1.84) 99.0 (42.73-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.181 , 0.222 0.190 , 0.214	Depositor DCC
R_{free} test set	3531 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7224	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.98% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	2.10	58/1613 (3.6%)	1.10	6/2180 (0.3%)
1	B	2.27	88/1647 (5.3%)	1.15	7/2227 (0.3%)
1	C	2.09	49/1731 (2.8%)	1.20	10/2340 (0.4%)
1	D	2.26	76/1716 (4.4%)	1.27	14/2319 (0.6%)
All	All	2.18	271/6707 (4.0%)	1.19	37/9066 (0.4%)

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	C	0	1
1	D	0	1
All	All	0	3

All (271) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	253	PRO	N-CD	30.10	1.89	1.47
1	B	167	TYR	N-CA	-16.63	1.24	1.46
1	D	161	TRP	C-O	-9.48	1.13	1.24
1	C	263	THR	C-O	-9.43	1.15	1.24
1	D	165	ILE	C-O	-9.13	1.13	1.24
1	C	146	ALA	CA-CB	-8.50	1.39	1.53
1	A	296	GLU	C-O	-8.08	1.14	1.24
1	C	307	ASN	C-O	-7.97	1.14	1.23
1	B	226	PRO	C-O	-7.94	1.14	1.23
1	A	181	MET	C-O	-7.86	1.15	1.24
1	D	263	THR	C-O	-7.83	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	219	ILE	C-O	-7.72	1.15	1.24
1	C	302	VAL	C-O	-7.69	1.15	1.24
1	A	159	LEU	C-O	-7.50	1.15	1.24
1	A	179	ILE	C-O	-7.49	1.15	1.24
1	D	164	TYR	C-O	-7.49	1.15	1.24
1	B	260	GLU	C-O	-7.40	1.15	1.23
1	A	172	LEU	C-O	-7.38	1.17	1.24
1	B	298	ILE	C-O	-7.37	1.15	1.24
1	B	313	VAL	C-O	-7.35	1.16	1.24
1	D	152	ASN	C-O	-7.22	1.15	1.24
1	D	176	GLN	C-O	-7.20	1.15	1.24
1	B	288	ALA	CA-CB	-7.19	1.42	1.53
1	B	183	ASN	C-O	-7.16	1.15	1.24
1	C	200	ILE	C-O	-7.10	1.16	1.24
1	B	161	TRP	C-O	-7.07	1.15	1.24
1	C	166	GLY	C-O	-7.04	1.15	1.23
1	D	211	ASP	C-O	-7.00	1.16	1.24
1	D	260	GLU	C-O	-6.99	1.15	1.23
1	D	200	ILE	C-O	-6.98	1.16	1.24
1	B	333	ILE	C-O	-6.96	1.16	1.24
1	D	291	PHE	C-O	-6.96	1.16	1.24
1	C	288	ALA	CA-CB	-6.94	1.42	1.53
1	B	162	SER	C-O	-6.91	1.16	1.24
1	B	255	GLY	C-O	-6.86	1.16	1.23
1	A	201	LEU	C-O	-6.85	1.15	1.24
1	B	200	ILE	C-O	-6.82	1.16	1.24
1	C	171	ILE	C-O	-6.79	1.16	1.24
1	B	220	ARG	C-O	-6.78	1.16	1.24
1	A	183	ASN	C-O	-6.76	1.16	1.24
1	B	263	THR	C-O	-6.75	1.18	1.24
1	A	295	LEU	C-O	-6.74	1.16	1.24
1	B	290	LEU	C-O	-6.73	1.16	1.24
1	D	156	ALA	C-O	-6.73	1.16	1.24
1	D	220	ARG	C-O	-6.72	1.16	1.24
1	C	259	LEU	C-O	-6.69	1.15	1.23
1	C	167	TYR	C-O	-6.68	1.15	1.24
1	C	199	TYR	C-O	-6.66	1.15	1.24
1	D	239	ALA	CA-CB	-6.62	1.44	1.53
1	B	325	LEU	C-O	-6.61	1.16	1.24
1	A	227	GLN	C-O	-6.59	1.15	1.23
1	A	321	ASN	CA-C	-6.57	1.44	1.52
1	D	288	ALA	CA-CB	-6.54	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	ASN	C-O	-6.52	1.16	1.23
1	D	293	ARG	C-O	-6.51	1.16	1.24
1	B	157	HIS	C-O	-6.48	1.16	1.24
1	B	332	HIS	C-O	-6.47	1.16	1.24
1	B	329	VAL	C-O	-6.44	1.16	1.24
1	C	178	ARG	C-O	-6.40	1.16	1.24
1	C	270	ALA	C-O	-6.40	1.16	1.24
1	A	329	VAL	C-O	-6.39	1.16	1.24
1	B	159	LEU	C-O	-6.39	1.16	1.24
1	B	338	ALA	CA-CB	-6.38	1.43	1.53
1	A	255	GLY	C-O	-6.38	1.16	1.24
1	B	146	ALA	CA-CB	-6.34	1.42	1.53
1	C	165	ILE	C-O	-6.33	1.17	1.24
1	C	128	SER	C-O	-6.32	1.16	1.24
1	D	269	PHE	C-O	-6.32	1.16	1.24
1	A	241	SER	C-O	-6.30	1.16	1.24
1	D	226	PRO	C-O	-6.29	1.16	1.23
1	C	162	SER	C-O	-6.28	1.16	1.24
1	C	298	ILE	C-O	-6.28	1.17	1.24
1	B	307	ASN	C-O	-6.28	1.16	1.23
1	C	268	LEU	C-O	-6.26	1.16	1.24
1	C	172	LEU	C-O	-6.25	1.16	1.24
1	A	230	THR	C-O	-6.25	1.16	1.23
1	D	178	ARG	C-O	-6.21	1.16	1.24
1	D	150	GLU	C-O	-6.18	1.16	1.23
1	C	151	LYS	C-O	-6.18	1.16	1.23
1	D	258	ILE	C-O	-6.16	1.17	1.24
1	A	161	TRP	C-O	-6.15	1.17	1.24
1	A	297	GLU	C-O	-6.15	1.17	1.24
1	B	165	ILE	C-O	-6.15	1.17	1.24
1	B	193	ALA	CA-CB	-6.13	1.43	1.53
1	D	310	ARG	C-O	-6.13	1.17	1.23
1	D	162	SER	C-O	-6.11	1.17	1.24
1	B	197	ARG	C-O	-6.10	1.16	1.23
1	B	262	ALA	C-O	-6.08	1.16	1.23
1	B	269	PHE	C-O	-6.07	1.17	1.24
1	D	304	GLU	C-O	-6.06	1.17	1.24
1	B	151	LYS	C-O	-6.05	1.16	1.24
1	D	329	VAL	C-O	-6.04	1.17	1.24
1	A	177	ALA	C-O	-6.00	1.17	1.24
1	C	337	GLU	C-O	-6.00	1.17	1.24
1	A	268	LEU	C-O	-5.99	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	180	ARG	C-O	-5.98	1.17	1.24
1	A	260	GLU	C-O	-5.98	1.16	1.23
1	B	179	ILE	C-O	-5.97	1.17	1.24
1	B	257	CYS	C-O	-5.95	1.16	1.23
1	A	165	ILE	C-O	-5.95	1.17	1.24
1	B	302	VAL	C-O	-5.95	1.17	1.24
1	A	256	ALA	CA-CB	-5.93	1.41	1.54
1	D	145	SER	C-O	-5.91	1.16	1.23
1	A	152	ASN	C-O	-5.90	1.18	1.23
1	D	179	ILE	C-O	-5.90	1.17	1.24
1	B	337	GLU	C-O	-5.90	1.17	1.24
1	C	242	ASN	C-O	-5.90	1.16	1.24
1	B	176	GLN	C-O	-5.89	1.17	1.24
1	B	270	ALA	C-O	-5.88	1.17	1.24
1	C	299	LEU	C-O	-5.88	1.16	1.24
1	D	257	CYS	C-O	-5.86	1.16	1.23
1	B	232	ARG	C-O	-5.84	1.16	1.23
1	A	246	GLU	C-O	-5.84	1.17	1.24
1	B	164	TYR	C-O	-5.84	1.17	1.24
1	B	312	ILE	C-O	-5.84	1.17	1.24
1	B	193	ALA	C-O	-5.83	1.17	1.24
1	B	140	ALA	C-O	-5.81	1.16	1.23
1	D	328	GLU	C-O	-5.80	1.17	1.24
1	D	166	GLY	C-O	-5.80	1.16	1.23
1	B	246	GLU	C-O	-5.79	1.17	1.23
1	D	155	VAL	C-O	-5.79	1.17	1.24
1	D	254	ALA	N-CA	5.79	1.53	1.46
1	A	148	CYS	C-O	-5.79	1.16	1.23
1	B	147	VAL	C-O	-5.78	1.17	1.24
1	A	193	ALA	CA-CB	-5.77	1.44	1.53
1	D	298	ILE	C-O	-5.77	1.17	1.24
1	C	173	PRO	C-O	-5.77	1.16	1.23
1	B	289	LYS	C-O	-5.76	1.17	1.24
1	A	147	VAL	C-O	-5.74	1.17	1.24
1	A	233	ALA	C-O	-5.74	1.17	1.23
1	D	247	LEU	C-O	-5.74	1.17	1.24
1	A	298	ILE	C-O	-5.74	1.17	1.24
1	C	161	TRP	C-O	-5.74	1.17	1.24
1	D	256	ALA	C-O	-5.72	1.17	1.23
1	B	334	ARG	C-O	-5.71	1.17	1.24
1	A	289	LYS	C-O	-5.71	1.17	1.24
1	C	149	GLU	C-O	-5.70	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	295	LEU	C-O	-5.69	1.17	1.24
1	B	154	ASN	C-O	-5.69	1.17	1.23
1	D	195	SER	C-O	-5.68	1.16	1.24
1	C	176	GLN	C-O	-5.68	1.17	1.24
1	A	175	LEU	C-O	-5.66	1.17	1.24
1	B	148	CYS	C-O	-5.66	1.17	1.23
1	B	267	THR	C-O	-5.65	1.17	1.24
1	A	226	PRO	C-O	-5.64	1.17	1.23
1	B	219	ILE	C-O	-5.64	1.17	1.24
1	B	150	GLU	C-O	-5.64	1.17	1.23
1	B	195	SER	C-O	-5.64	1.16	1.24
1	D	184	GLN	C-O	-5.63	1.17	1.24
1	C	308	HIS	C-O	-5.63	1.16	1.23
1	B	189	MET	C-O	-5.63	1.17	1.24
1	B	221	PHE	C-O	-5.63	1.17	1.23
1	C	328	GLU	C-O	-5.62	1.17	1.24
1	A	178	ARG	C-O	-5.62	1.17	1.24
1	D	146	ALA	C-O	-5.62	1.17	1.23
1	C	333	ILE	C-O	-5.61	1.17	1.24
1	D	285	LEU	C-O	-5.60	1.17	1.24
1	B	252	GLN	C-O	-5.59	1.17	1.24
1	B	315	GLN	C-O	-5.58	1.17	1.24
1	C	339	ALA	C-O	-5.57	1.17	1.24
1	C	311	LEU	C-O	-5.56	1.17	1.24
1	C	204	LEU	C-O	-5.56	1.16	1.24
1	B	188	ASN	C-O	-5.55	1.16	1.23
1	A	146	ALA	C-O	-5.54	1.16	1.23
1	D	326	SER	C-O	-5.54	1.17	1.24
1	D	294	THR	C-O	-5.52	1.17	1.24
1	D	336	GLU	C-O	-5.51	1.17	1.24
1	B	202	PHE	C-O	-5.50	1.17	1.24
1	B	167	TYR	CA-CB	5.50	1.62	1.53
1	D	318	GLU	C-O	-5.49	1.16	1.24
1	A	170	LEU	C-O	-5.49	1.17	1.24
1	B	242	ASN	C-O	-5.49	1.17	1.23
1	C	164	TYR	C-O	-5.49	1.17	1.24
1	C	131	ASN	C-O	-5.48	1.17	1.24
1	D	259	LEU	C-O	-5.48	1.17	1.23
1	D	146	ALA	CA-CB	-5.47	1.44	1.53
1	B	259	LEU	C-O	-5.47	1.17	1.23
1	B	282	GLU	C-O	-5.47	1.17	1.24
1	B	167	TYR	C-O	-5.46	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	288	ALA	C-O	-5.46	1.17	1.24
1	B	248	LEU	C-O	-5.45	1.16	1.23
1	D	271	MET	C-O	-5.45	1.17	1.24
1	B	295	LEU	C-O	-5.44	1.17	1.24
1	B	177	ALA	C-O	-5.44	1.17	1.24
1	A	145	SER	C-O	-5.42	1.16	1.24
1	A	328	GLU	C-O	-5.41	1.17	1.24
1	C	155	VAL	C-O	-5.41	1.18	1.24
1	D	196	ARG	C-O	-5.40	1.16	1.24
1	D	312	ILE	C-O	-5.39	1.18	1.24
1	B	243	SER	C-O	-5.39	1.17	1.23
1	B	238	ARG	C-O	-5.38	1.17	1.24
1	C	258	ILE	C-O	-5.38	1.18	1.24
1	D	203	PRO	C-O	-5.38	1.17	1.24
1	A	223	ASP	C-O	-5.38	1.17	1.23
1	C	209	PRO	C-O	-5.38	1.17	1.23
1	D	137	SER	N-CA	-5.38	1.40	1.46
1	A	330	LEU	C-O	-5.37	1.17	1.24
1	A	180	ARG	C-O	-5.37	1.17	1.24
1	D	208	VAL	C-O	-5.37	1.18	1.24
1	B	235	VAL	C-O	-5.36	1.16	1.24
1	C	310	ARG	C-O	-5.34	1.17	1.24
1	D	223	ASP	C-O	-5.34	1.18	1.23
1	A	221	PHE	C-O	-5.34	1.17	1.23
1	C	184	GLN	C-O	-5.34	1.17	1.24
1	B	256	ALA	C-O	-5.33	1.17	1.23
1	B	317	SER	C-O	-5.33	1.17	1.24
1	B	305	SER	C-O	-5.33	1.17	1.24
1	C	271	MET	C-O	-5.32	1.17	1.24
1	D	262	ALA	CA-CB	-5.32	1.46	1.53
1	D	222	ARG	C-O	-5.30	1.17	1.23
1	A	258	ILE	C-O	-5.30	1.18	1.24
1	A	257	CYS	C-O	-5.30	1.17	1.23
1	A	327	GLN	C-O	-5.29	1.18	1.24
1	C	168	LEU	C-O	-5.29	1.18	1.24
1	D	183	ASN	C-O	-5.29	1.18	1.24
1	B	327	GLN	C-O	-5.28	1.18	1.24
1	D	167	TYR	C-O	-5.28	1.17	1.24
1	B	310	ARG	C-O	-5.27	1.18	1.24
1	B	196	ARG	C-O	-5.27	1.15	1.23
1	C	314	TYR	C-O	-5.27	1.17	1.23
1	C	293	ARG	C-O	-5.26	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	197	ARG	C-O	-5.26	1.17	1.23
1	A	140	ALA	C-O	-5.25	1.17	1.23
1	D	215	ALA	C-O	-5.25	1.18	1.24
1	B	156	ALA	C-O	-5.24	1.17	1.24
1	C	202	PHE	C-O	-5.23	1.18	1.24
1	D	299	LEU	C-O	-5.23	1.17	1.24
1	A	331	ARG	C-O	-5.22	1.18	1.24
1	B	311	LEU	C-O	-5.22	1.17	1.24
1	A	160	ALA	C-O	-5.22	1.18	1.24
1	B	181	MET	C-O	-5.21	1.18	1.24
1	B	249	GLU	C-O	-5.21	1.18	1.24
1	C	211	ASP	C-O	-5.21	1.18	1.24
1	A	325	LEU	C-O	-5.21	1.18	1.24
1	A	254	ALA	CA-CB	-5.20	1.46	1.54
1	A	279	PHE	C-O	-5.19	1.17	1.24
1	D	300	ALA	C-O	-5.18	1.17	1.24
1	B	208	VAL	CA-CB	-5.15	1.49	1.54
1	D	199	TYR	C-O	-5.15	1.17	1.24
1	D	323	PHE	C-O	-5.15	1.17	1.23
1	A	309	CYS	C-O	-5.13	1.17	1.23
1	D	315	GLN	C-O	-5.13	1.18	1.24
1	B	236	LYS	C-O	-5.13	1.18	1.24
1	B	283	ASP	C-O	-5.13	1.18	1.24
1	D	159	LEU	C-O	-5.13	1.18	1.24
1	C	327	GLN	C-O	-5.12	1.18	1.24
1	A	308	HIS	C-O	-5.11	1.17	1.24
1	D	172	LEU	C-O	-5.11	1.17	1.24
1	D	221	PHE	C-O	-5.10	1.17	1.23
1	D	324	SER	C-O	-5.10	1.18	1.24
1	D	265	LEU	C-O	-5.08	1.18	1.24
1	A	283	ASP	C-O	-5.08	1.18	1.24
1	D	157	HIS	C-O	-5.08	1.18	1.24
1	A	313	VAL	C-O	-5.07	1.18	1.24
1	A	171	ILE	C-O	-5.07	1.18	1.24
1	B	285	LEU	C-O	-5.07	1.18	1.24
1	B	279	PHE	C-O	-5.07	1.17	1.23
1	A	195	SER	C-O	-5.06	1.17	1.24
1	D	171	ILE	C-O	-5.06	1.18	1.24
1	B	144	VAL	C-O	-5.06	1.17	1.24
1	B	241	SER	C-O	-5.05	1.18	1.24
1	D	174	GLY	C-O	-5.05	1.17	1.24
1	B	323	PHE	C-O	-5.05	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	LEU	C-O	-5.05	1.18	1.24
1	B	274	ASP	C-O	-5.05	1.17	1.23
1	C	300	ALA	CA-CB	-5.04	1.44	1.53
1	A	164	TYR	C-O	-5.02	1.18	1.24
1	C	262	ALA	CA-CB	-5.01	1.46	1.53
1	B	254	ALA	CA-CB	-5.01	1.47	1.54
1	A	274	ASP	C-O	-5.01	1.16	1.23
1	B	245	TYR	C-O	-5.01	1.17	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253	PRO	CA-N-CD	-16.53	88.85	112.00
1	C	128	SER	N-CA-C	10.34	122.13	111.07
1	B	319	GLU	N-CA-C	-10.03	91.81	108.76
1	D	253	PRO	N-CA-C	9.96	132.98	112.47
1	B	167	TYR	N-CA-C	9.28	130.56	110.80
1	A	274	ASP	N-CA-C	-9.07	91.38	108.17
1	C	171	ILE	N-CA-C	9.04	119.85	110.72
1	D	252	GLN	N-CA-C	-8.51	91.00	109.81
1	C	280	SER	N-CA-C	7.74	120.57	110.43
1	D	135	GLN	N-CA-C	7.53	120.59	110.35
1	D	254	ALA	N-CA-C	7.50	122.61	113.38
1	D	253	PRO	N-CA-CB	-7.01	95.89	103.25
1	D	170	LEU	N-CA-C	6.92	118.91	111.36
1	B	277	ALA	N-CA-CB	-6.84	103.05	114.27
1	B	274	ASP	N-CA-C	-6.80	100.16	110.70
1	D	239	ALA	N-CA-C	6.75	120.88	111.56
1	D	253	PRO	N-CD-CG	-6.62	93.27	103.20
1	A	320	GLY	N-CA-C	6.56	122.94	111.46
1	D	316	GLU	O-C-N	6.49	129.00	122.12
1	C	170	LEU	N-CA-C	6.45	118.39	111.36
1	D	316	GLU	N-CA-C	6.43	119.11	111.33
1	C	133	TYR	N-CA-C	6.10	118.01	111.36
1	B	320	GLY	N-CA-C	-5.92	96.12	113.30
1	C	276	LYS	N-CA-C	-5.88	104.78	111.07
1	D	254	ALA	CA-C-O	5.67	125.62	119.15
1	C	239	ALA	N-CA-C	5.61	118.05	110.88
1	C	128	SER	O-C-N	-5.50	116.41	122.07
1	C	128	SER	CA-C-N	5.40	131.42	121.70
1	C	128	SER	C-N-CA	5.40	131.42	121.70
1	A	321	ASN	CA-C-O	5.35	128.16	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	GLN	CB-CA-C	-5.08	101.42	109.80
1	A	152	ASN	CB-CA-C	-5.06	101.04	110.56
1	B	171	ILE	N-CA-C	5.06	119.53	112.50
1	B	257	CYS	N-CA-C	5.06	115.99	108.60
1	A	321	ASN	CA-CB-CG	-5.05	107.55	112.60
1	D	252	GLN	CA-C-N	-5.00	113.59	119.84
1	D	252	GLN	C-N-CA	-5.00	113.59	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	276	LYS	Peptide
1	C	128	SER	Peptide
1	D	250	ASN	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	1582	0	1547	25	1
1	B	1616	0	1576	38	0
1	C	1698	0	1643	26	1
1	D	1683	0	1631	32	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	139	0	0	4	0
3	B	152	0	0	4	0
3	C	147	0	0	3	0
3	D	162	0	0	6	0
All	All	7224	0	6397	115	1

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 9.

All (115) 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:B:274:ASP:CG	1:B:276:LYS:HD3	1.57	1.29
1:D:253:PRO:CD	1:D:253:PRO:N	1.89	1.28
1:B:274:ASP:OD1	1:B:276:LYS:HD3	1.41	1.16
1:B:153:PHE:HZ	1:B:278:GLY:HA3	1.21	1.03
1:B:274:ASP:OD1	1:B:276:LYS:CD	2.07	1.01
1:B:274:ASP:O	1:B:276:LYS:N	1.94	1.00
1:D:252:GLN:HB3	1:D:253:PRO:HD3	1.41	0.98
1:B:230:THR:HG22	1:B:232:ARG:H	1.29	0.97
1:D:252:GLN:HB3	1:D:253:PRO:CD	1.96	0.95
1:B:274:ASP:O	1:B:276:LYS:HD2	1.69	0.93
1:A:230:THR:HG22	1:A:232:ARG:H	1.35	0.91
1:D:230:THR:HG23	1:D:237:ASN:OD1	1.71	0.91
1:B:153:PHE:CZ	1:B:278:GLY:HA3	2.07	0.90
1:D:251:GLY:O	3:D:501:HOH:O	1.93	0.86
1:B:274:ASP:O	1:B:276:LYS:CD	2.25	0.83
1:C:327:GLN:HE21	1:D:321:ASN:HD21	1.29	0.80
1:C:281:ARG:HD3	1:C:284:ARG:NH2	1.97	0.79
1:A:275:GLY:HA2	3:A:501:HOH:O	1.82	0.79
1:B:215:ALA:HA	1:B:216:ASP:HB3	1.69	0.75
1:C:327:GLN:NE2	1:D:321:ASN:HD21	1.84	0.74
1:C:230:THR:HG23	1:C:237:ASN:OD1	1.88	0.74
1:B:214:VAL:O	1:B:215:ALA:HB3	1.90	0.72
1:A:320:GLY:C	1:A:321:ASN:OD1	2.34	0.70
1:B:274:ASP:CB	1:B:276:LYS:HD3	2.22	0.68
1:C:281:ARG:HD3	1:C:284:ARG:HH22	1.57	0.67
1:C:274:ASP:O	1:C:277:ALA:HB3	1.98	0.64
1:B:214:VAL:O	1:B:215:ALA:CB	2.46	0.63
1:B:214:VAL:HG12	1:B:215:ALA:N	2.12	0.62
1:A:152:ASN:OD1	1:A:152:ASN:C	2.41	0.62
1:B:222:ARG:NH2	1:B:246:GLU:OE1	2.34	0.61
1:B:215:ALA:HA	1:B:216:ASP:CB	2.28	0.60
1:D:252:GLN:C	1:D:253:PRO:CD	2.71	0.60
1:C:312:ILE:HG23	1:C:332:HIS:CE1	2.37	0.59
1:B:296:GLU:HG3	1:B:311:LEU:HD12	1.84	0.59
1:A:321:ASN:OD1	1:A:321:ASN:N	2.32	0.59
1:B:157:HIS:HB2	3:B:505:HOH:O	2.02	0.58
1:A:319:GLU:HA	1:A:319:GLU:OE1	2.04	0.58
1:B:274:ASP:O	1:B:275:GLY:C	2.45	0.58
1:B:228:GLN:HB2	1:B:230:THR:OG1	2.05	0.56
1:D:246:GLU:CD	1:D:253:PRO:HB3	2.31	0.56
1:B:214:VAL:HG12	1:B:215:ALA:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLY:HA2	3:C:582:HOH:O	2.06	0.56
1:A:335:GLN:C	3:A:509:HOH:O	2.49	0.56
1:D:252:GLN:NE2	1:D:252:GLN:HA	2.21	0.56
1:D:246:GLU:CD	1:D:253:PRO:CB	2.79	0.55
1:A:202:PHE:CE2	1:A:311:LEU:HD22	2.42	0.55
1:A:321:ASN:CG	1:A:322:SER:H	2.14	0.55
1:B:274:ASP:HB3	1:B:276:LYS:HG2	1.89	0.55
1:D:248:LEU:HD22	1:D:252:GLN:C	2.31	0.54
1:C:340:ALA:O	1:C:341:ALA:HB3	2.08	0.54
1:C:213:SER:HB3	1:C:220:ARG:HH12	1.74	0.52
1:A:156:ALA:HB3	1:A:290:LEU:HD23	1.91	0.52
1:B:217:PRO:HG2	1:C:253:PRO:O	2.11	0.51
1:D:263:THR:HB	1:D:264:PRO:HD3	1.91	0.51
1:B:222:ARG:NE	1:B:246:GLU:OE1	2.44	0.51
1:A:202:PHE:HE2	1:A:311:LEU:HD22	1.76	0.50
1:C:340:ALA:O	1:C:341:ALA:CB	2.59	0.50
1:C:263:THR:HB	1:C:264:PRO:HD3	1.93	0.49
1:D:276:LYS:O	1:D:278:GLY:N	2.46	0.49
1:A:210:ASP:HB3	3:A:606:HOH:O	2.13	0.49
1:B:273:GLN:O	1:B:275:GLY:N	2.46	0.47
1:D:181:MET:HE1	1:D:228:GLN:HG3	1.96	0.47
1:A:139:MET:HE1	1:C:263:THR:HA	1.94	0.47
1:A:205:ASP:HB2	3:A:585:HOH:O	2.14	0.47
1:B:202:PHE:CE1	1:B:292:CYS:HB2	2.49	0.47
1:D:246:GLU:CD	1:D:253:PRO:HB2	2.40	0.47
1:C:224:MET:HE3	1:C:241:SER:HB3	1.97	0.47
1:D:132:LEU:HD21	3:D:639:HOH:O	2.15	0.47
1:D:281:ARG:NE	1:D:284:ARG:HH22	2.13	0.47
1:B:196:ARG:HD3	3:B:556:HOH:O	2.14	0.47
1:D:133:TYR:CE1	1:D:271:MET:HE3	2.50	0.47
1:B:185:LEU:CD2	1:D:296:GLU:HB3	2.45	0.46
1:A:160:ALA:HA	1:A:291:PHE:HE1	1.80	0.46
1:A:273:GLN:O	1:A:275:GLY:N	2.48	0.46
1:B:274:ASP:OD1	1:B:276:LYS:HD2	2.09	0.46
1:D:196:ARG:HD3	3:D:590:HOH:O	2.15	0.46
1:C:273:GLN:HG3	3:C:637:HOH:O	2.15	0.46
1:D:210:ASP:HA	3:D:603:HOH:O	2.14	0.46
1:D:281:ARG:HD3	3:D:633:HOH:O	2.15	0.45
1:A:220:ARG:HG2	1:A:220:ARG:HH11	1.81	0.45
1:D:144:VAL:HG22	1:D:144:VAL:O	2.17	0.45
1:D:252:GLN:NE2	1:D:252:GLN:CA	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:PRO:HD2	1:A:265:LEU:CD1	2.48	0.44
1:C:132:LEU:HB2	3:C:562:HOH:O	2.17	0.44
1:D:253:PRO:O	1:D:253:PRO:HD2	2.17	0.44
1:D:276:LYS:C	1:D:278:GLY:N	2.69	0.44
1:A:274:ASP:O	1:A:277:ALA:HB3	2.18	0.43
1:B:153:PHE:CZ	1:B:278:GLY:CA	2.90	0.43
1:A:152:ASN:OD1	1:A:152:ASN:O	2.37	0.43
1:B:205:ASP:HB2	3:B:607:HOH:O	2.18	0.43
1:A:320:GLY:CA	1:A:321:ASN:OD1	2.67	0.43
1:D:281:ARG:NH2	3:D:513:HOH:O	2.51	0.42
1:A:318:GLU:O	1:A:319:GLU:C	2.62	0.42
1:B:218:ASN:ND2	3:B:506:HOH:O	2.43	0.42
1:B:247:LEU:HD13	1:B:330:LEU:HG	2.01	0.42
1:C:276:LYS:C	1:C:278:GLY:H	2.26	0.42
1:D:171:ILE:O	1:D:171:ILE:HD13	2.20	0.42
1:B:216:ASP:H	1:C:252:GLN:HE22	1.66	0.42
1:C:168:LEU:HA	1:C:171:ILE:HG22	2.01	0.42
1:B:274:ASP:O	1:B:276:LYS:CG	2.67	0.42
1:A:282:GLU:H	1:A:282:GLU:CD	2.28	0.41
1:B:220:ARG:HH11	1:B:220:ARG:HD3	1.73	0.41
1:C:147:VAL:O	1:C:148:CYS:HB3	2.20	0.41
1:C:179:ILE:HD13	1:C:196:ARG:HA	2.03	0.41
1:C:321:ASN:OD1	1:C:321:ASN:N	2.52	0.41
1:B:263:THR:N	1:B:264:PRO:CD	2.84	0.41
1:C:276:LYS:C	1:C:278:GLY:N	2.79	0.41
1:B:310:ARG:HE	1:B:336:GLU:CD	2.28	0.41
1:C:252:GLN:HA	1:C:253:PRO:HD3	1.95	0.41
1:D:263:THR:N	1:D:264:PRO:CD	2.83	0.41
1:C:128:SER:HB2	1:C:130:GLU:H	1.86	0.41
1:D:211:ASP:HB3	1:D:214:VAL:HG23	2.02	0.41
1:A:263:THR:N	1:A:264:PRO:CD	2.85	0.40
1:D:248:LEU:HD23	1:D:253:PRO:HA	2.03	0.40
1:A:216:ASP:OD1	1:A:217:PRO:HD2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:OE1	1:C:135:GLN:OE1[4_445]	1.22	0.98

5.3 Torsion angles

5.3.1 Protein backbone

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	198/225 (88%)	194 (98%)	3 (2%)	1 (0%)	24	12
1	B	203/225 (90%)	197 (97%)	3 (2%)	3 (2%)	8	1
1	C	214/225 (95%)	208 (97%)	6 (3%)	0	100	100
1	D	211/225 (94%)	205 (97%)	6 (3%)	0	100	100
All	All	826/900 (92%)	804 (97%)	18 (2%)	4 (0%)	24	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	ASN
1	B	275	GLY
1	B	216	ASP
1	B	215	ALA

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	170/189 (90%)	167 (98%)	3 (2%)	51	35
1	B	172/189 (91%)	169 (98%)	3 (2%)	53	37
1	C	180/189 (95%)	175 (97%)	5 (3%)	38	20
1	D	180/189 (95%)	172 (96%)	8 (4%)	25	8
All	All	702/756 (93%)	683 (97%)	19 (3%)	39	22

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	PHE
1	A	223	ASP
1	A	293	ARG
1	B	148	CYS
1	B	223	ASP
1	B	301	ASP
1	C	128	SER
1	C	224	MET
1	C	252	GLN
1	C	290	LEU
1	C	321	ASN
1	D	127	SER
1	D	171	ILE
1	D	220	ARG
1	D	225	LEU
1	D	252	GLN
1	D	253	PRO
1	D	276	LYS
1	D	290	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	273	GLN
1	A	327	GLN
1	B	227	GLN
1	B	327	GLN
1	C	252	GLN
1	C	273	GLN
1	C	327	GLN
1	C	332	HIS
1	D	135	GLN
1	D	252	GLN
1	D	287	GLN

5.3.3 RNA ⓘ

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](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	401	-	4,4,4	0.28	0	6,6,6	0.44	0
2	SO4	C	403	-	4,4,4	0.29	0	6,6,6	0.13	0
2	SO4	B	401	-	4,4,4	0.25	0	6,6,6	0.29	0
2	SO4	A	402	-	4,4,4	0.24	0	6,6,6	0.25	0
2	SO4	D	401	-	4,4,4	0.25	0	6,6,6	0.17	0
2	SO4	C	402	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	D	402	-	4,4,4	0.33	0	6,6,6	0.46	0
2	SO4	D	403	-	4,4,4	0.22	0	6,6,6	0.16	0
2	SO4	C	401	-	4,4,4	0.09	0	6,6,6	0.40	0

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, 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	200/225 (88%)	0.23	9 (4%) 38 40	12, 22, 56, 88	0
1	B	205/225 (91%)	0.18	13 (6%) 26 27	10, 20, 51, 84	0
1	C	216/225 (96%)	0.46	25 (11%) 9 9	12, 24, 59, 91	0
1	D	213/225 (94%)	0.33	19 (8%) 15 16	11, 21, 50, 88	0
All	All	834/900 (92%)	0.30	66 (7%) 18 19	10, 22, 55, 91	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	252	GLN	5.9
1	D	275	GLY	5.2
1	B	277	ALA	5.1
1	D	251	GLY	5.0
1	D	277	ALA	4.8
1	D	253	PRO	4.6
1	D	278	GLY	4.6
1	C	132	LEU	4.6
1	B	215	ALA	4.5
1	C	275	GLY	4.3
1	B	320	GLY	4.3
1	B	275	GLY	4.1
1	C	341	ALA	4.1
1	C	136	GLY	3.9
1	A	322	SER	3.8
1	D	132	LEU	3.8
1	D	135	GLN	3.8
1	B	276	LYS	3.7
1	B	341	ALA	3.7
1	C	278	GLY	3.6
1	C	279	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	277	ALA	3.4
1	C	126	HIS	3.3
1	D	321	ASN	3.2
1	B	321	ASN	3.1
1	D	276	LYS	3.0
1	D	134	PHE	3.0
1	B	274	ASP	3.0
1	C	135	GLN	3.0
1	A	320	GLY	3.0
1	A	275	GLY	2.9
1	A	276	LYS	2.9
1	C	128	SER	2.9
1	C	134	PHE	2.9
1	A	319	GLU	2.9
1	C	321	ASN	2.9
1	C	276	LYS	2.9
1	D	279	PHE	2.8
1	D	133	TYR	2.7
1	B	319	GLU	2.7
1	A	136	GLY	2.7
1	C	274	ASP	2.6
1	C	320	GLY	2.6
1	A	215	ALA	2.6
1	D	136	GLY	2.6
1	D	224	MET	2.5
1	D	339	ALA	2.5
1	B	278	GLY	2.5
1	C	191	SER	2.5
1	A	321	ASN	2.4
1	B	153	PHE	2.4
1	C	230	THR	2.4
1	D	230	THR	2.3
1	B	137	SER	2.2
1	C	234	GLY	2.2
1	C	217	PRO	2.2
1	B	210	ASP	2.1
1	C	127	SER	2.1
1	D	254	ALA	2.1
1	D	320	GLY	2.1
1	C	190	LEU	2.1
1	C	273	GLN	2.1
1	A	274	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	249	GLU	2.0
1	C	282	GLU	2.0
1	C	133	TYR	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	SO4	D	401	5/5	0.88	0.11	53,53,57,58	0
2	SO4	D	403	5/5	0.91	0.11	37,46,50,54	0
2	SO4	C	403	5/5	0.92	0.13	34,38,45,48	0
2	SO4	B	401	5/5	0.95	0.07	36,43,51,51	0
2	SO4	D	402	5/5	0.97	0.10	23,24,26,26	0
2	SO4	A	402	5/5	0.98	0.06	21,22,27,29	0
2	SO4	A	401	5/5	0.98	0.05	13,16,19,23	0
2	SO4	C	401	5/5	0.98	0.05	16,17,22,29	0
2	SO4	C	402	5/5	0.98	0.06	24,26,30,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.