



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:55 AM UTC

PDB ID : 5O3Z / pdb_00005o3z
Title : Crystal structure of Sorbitol-6-Phosphate 2-dehydrogenase SrlD from *Erwinia amylovora*
Authors : Salomone-Stagni, M.; Bartho, J.D.; Bellini, D.; Walsh, M.A.; Benini, S.
Deposited on : 2017-05-25
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:

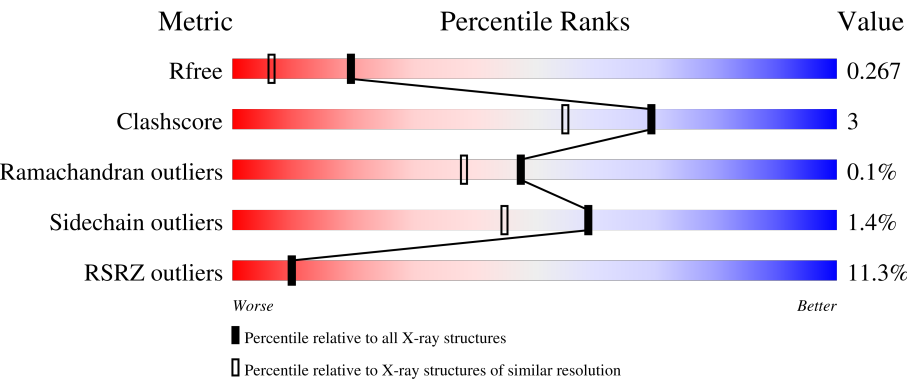
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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	263	16% 88%10%.
1	B	263	27% 87%9%..
1	C	263	3% 90%6%..
1	D	263	5% 88%9%.
1	E	263	2% 90%6%..

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Mol	Chain	Length	Quality of chain
1	F	263	6% 90% 8%
1	G	263	9% 89% 9%
1	H	263	4% 89% 9%
1	I	263	5% 80% 17%
1	J	263	10% 85% 11%
1	K	263	28% 84% 13%
1	L	263	17% 83% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24163 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 Sorbitol-6-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1948	1236	329	375	8			
1	B	257	Total	C	N	O	S	0	0	0
			1939	1231	328	372	8			
1	C	258	Total	C	N	O	S	0	0	0
			1948	1236	329	375	8			
1	D	258	Total	C	N	O	S	0	0	0
			1948	1236	329	375	8			
1	E	258	Total	C	N	O	S	0	0	0
			1948	1236	329	375	8			
1	F	259	Total	C	N	O	S	0	1	0
			1964	1246	333	376	9			
1	G	258	Total	C	N	O	S	0	0	0
			1948	1236	329	375	8			
1	H	258	Total	C	N	O	S	0	0	0
			1948	1236	329	375	8			
1	I	258	Total	C	N	O	S	0	0	0
			1948	1236	329	375	8			
1	J	259	Total	C	N	O	S	0	0	0
			1956	1241	330	376	9			
1	K	258	Total	C	N	O	S	0	0	0
			1948	1236	329	375	8			
1	L	256	Total	C	N	O	S	0	0	0
			1930	1226	326	370	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP D4I194
A	-2	ALA	-	expression tag	UNP D4I194
A	-1	MET	-	expression tag	UNP D4I194
A	0	ALA	-	expression tag	UNP D4I194
B	-3	GLY	-	expression tag	UNP D4I194

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	expression tag	UNP D4I194
B	-1	MET	-	expression tag	UNP D4I194
B	0	ALA	-	expression tag	UNP D4I194
C	-3	GLY	-	expression tag	UNP D4I194
C	-2	ALA	-	expression tag	UNP D4I194
C	-1	MET	-	expression tag	UNP D4I194
C	0	ALA	-	expression tag	UNP D4I194
D	-3	GLY	-	expression tag	UNP D4I194
D	-2	ALA	-	expression tag	UNP D4I194
D	-1	MET	-	expression tag	UNP D4I194
D	0	ALA	-	expression tag	UNP D4I194
E	-3	GLY	-	expression tag	UNP D4I194
E	-2	ALA	-	expression tag	UNP D4I194
E	-1	MET	-	expression tag	UNP D4I194
E	0	ALA	-	expression tag	UNP D4I194
F	-3	GLY	-	expression tag	UNP D4I194
F	-2	ALA	-	expression tag	UNP D4I194
F	-1	MET	-	expression tag	UNP D4I194
F	0	ALA	-	expression tag	UNP D4I194
G	-3	GLY	-	expression tag	UNP D4I194
G	-2	ALA	-	expression tag	UNP D4I194
G	-1	MET	-	expression tag	UNP D4I194
G	0	ALA	-	expression tag	UNP D4I194
H	-3	GLY	-	expression tag	UNP D4I194
H	-2	ALA	-	expression tag	UNP D4I194
H	-1	MET	-	expression tag	UNP D4I194
H	0	ALA	-	expression tag	UNP D4I194
I	-3	GLY	-	expression tag	UNP D4I194
I	-2	ALA	-	expression tag	UNP D4I194
I	-1	MET	-	expression tag	UNP D4I194
I	0	ALA	-	expression tag	UNP D4I194
J	-3	GLY	-	expression tag	UNP D4I194
J	-2	ALA	-	expression tag	UNP D4I194
J	-1	MET	-	expression tag	UNP D4I194
J	0	ALA	-	expression tag	UNP D4I194
K	-3	GLY	-	expression tag	UNP D4I194
K	-2	ALA	-	expression tag	UNP D4I194
K	-1	MET	-	expression tag	UNP D4I194
K	0	ALA	-	expression tag	UNP D4I194
L	-3	GLY	-	expression tag	UNP D4I194
L	-2	ALA	-	expression tag	UNP D4I194
L	-1	MET	-	expression tag	UNP D4I194

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Chain	Residue	Modelled	Actual	Comment	Reference
L	0	ALA	-	expression tag	UNP D4I194

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0
2	K	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	32	Total O 32 32	0	0
3	B	45	Total O 45 45	0	0
3	C	77	Total O 77 77	0	0
3	D	100	Total O 100 100	0	0
3	E	79	Total O 79 79	0	0

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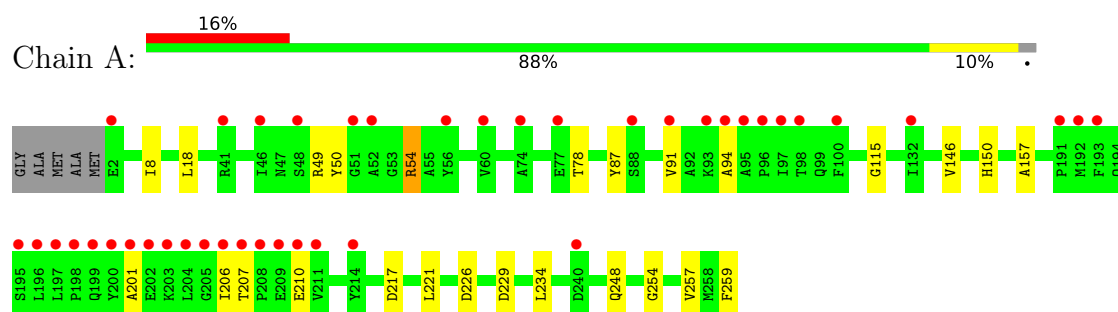
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	102	Total 102	O 102	0	0
3	G	81	Total 81	O 81	0	0
3	H	86	Total 86	O 86	0	0
3	I	68	Total 68	O 68	0	0
3	J	66	Total 66	O 66	0	0
3	K	15	Total 15	O 15	0	0
3	L	27	Total 27	O 27	0	0

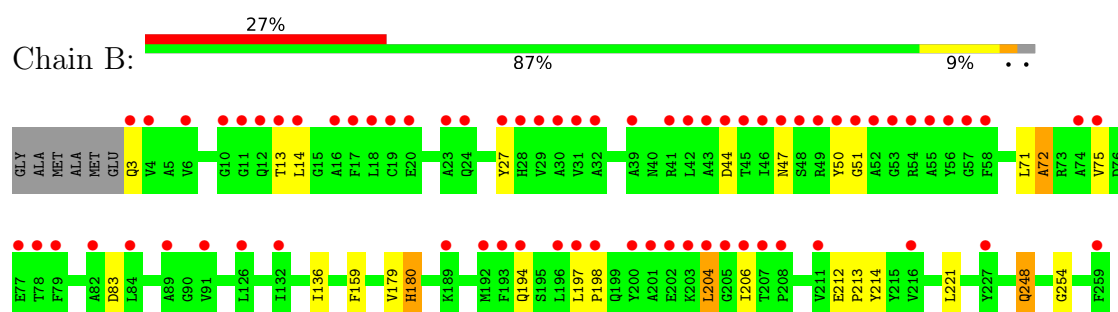
3 Residue-property plots [i](#)

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.

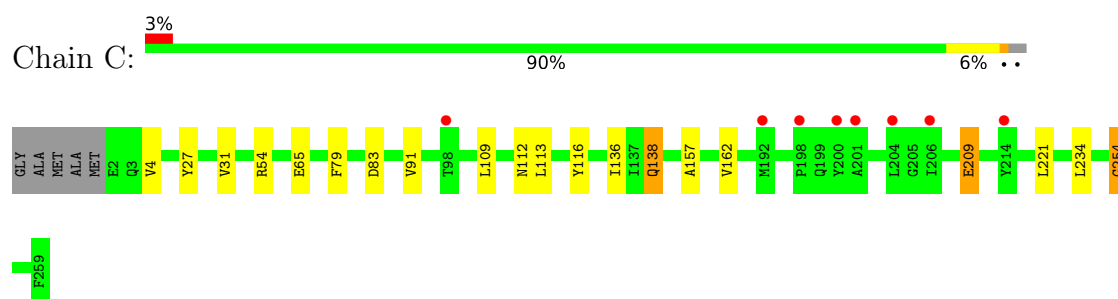
- Molecule 1: Sorbitol-6-phosphate dehydrogenase



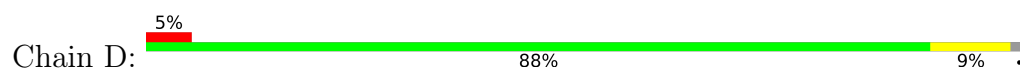
- Molecule 1: Sorbitol-6-phosphate dehydrogenase

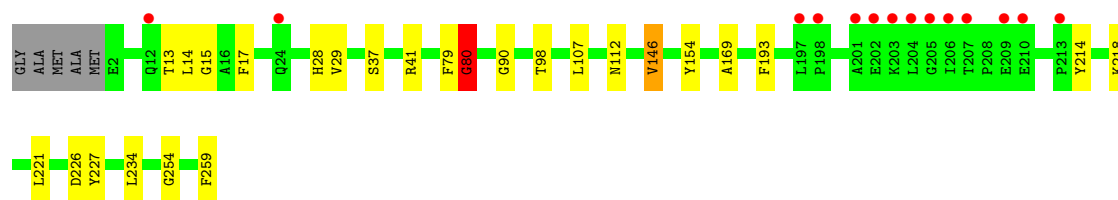


- Molecule 1: Sorbitol-6-phosphate dehydrogenase

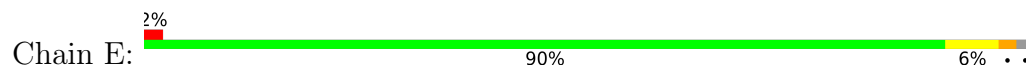


- Molecule 1: Sorbitol-6-phosphate dehydrogenase

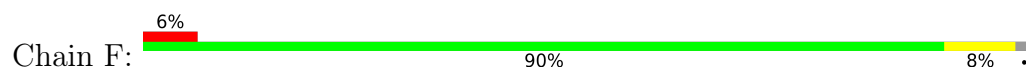




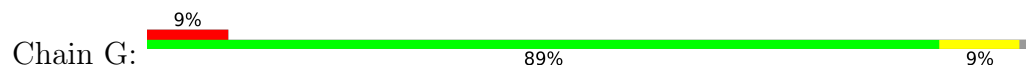
- Molecule 1: Sorbitol-6-phosphate dehydrogenase



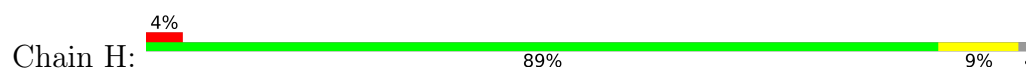
- Molecule 1: Sorbitol-6-phosphate dehydrogenase



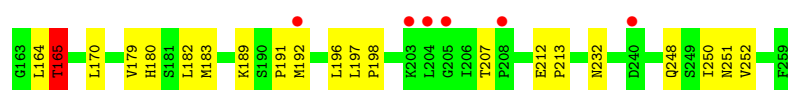
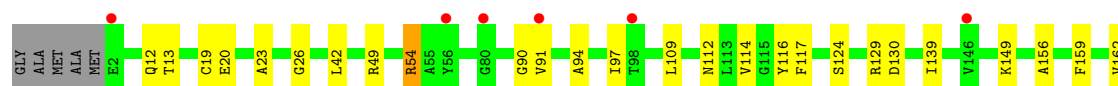
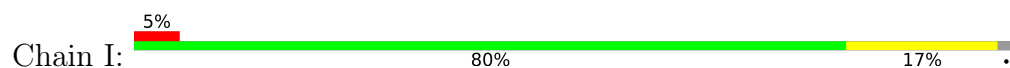
- Molecule 1: Sorbitol-6-phosphate dehydrogenase



- Molecule 1: Sorbitol-6-phosphate dehydrogenase

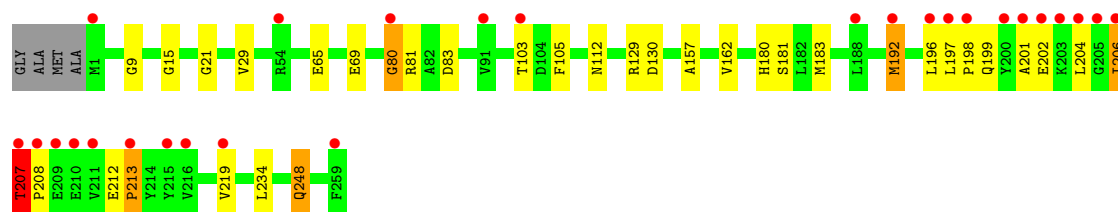


- Molecule 1: Sorbitol-6-phosphate dehydrogenase



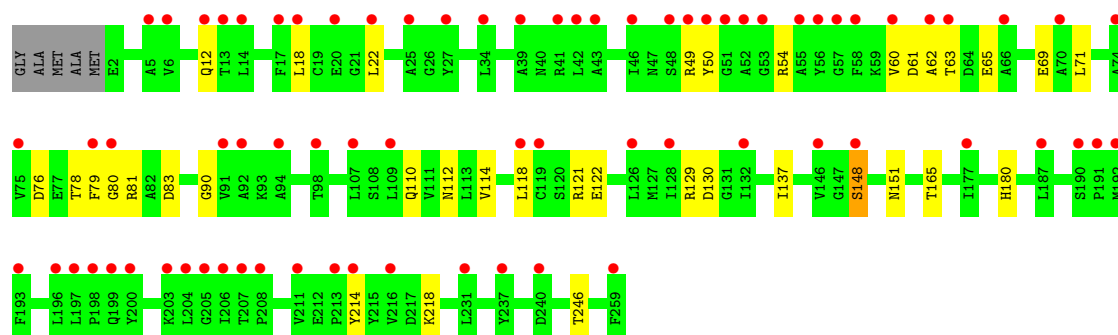
- Molecule 1: Sorbitol-6-phosphate dehydrogenase

Chain J:  10% 85% 11% ..



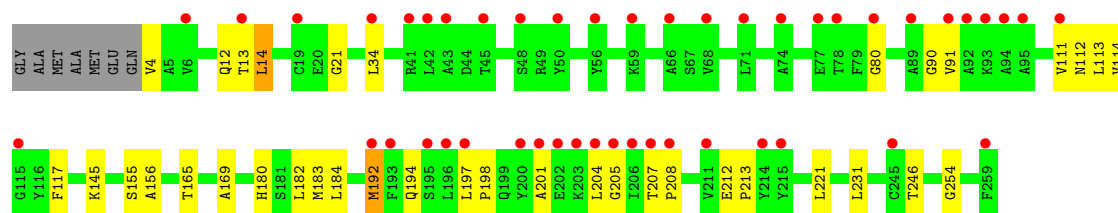
- Molecule 1: Sorbitol-6-phosphate dehydrogenase

Chain K:  28% 84% 13% .



- Molecule 1: Sorbitol-6-phosphate dehydrogenase

Chain L:  17% 83% 14% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.71Å 138.06Å 199.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.51 – 1.84 113.51 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.0 (113.51-1.84) 98.0 (113.51-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.209 , 0.255 0.221 , 0.267	Depositor DCC
R_{free} test set	14179 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24163	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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:
CL

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	1.24	4/1980 (0.2%)	1.12	2/2676 (0.1%)
1	B	1.29	3/1971 (0.2%)	1.16	2/2664 (0.1%)
1	C	1.37	6/1980 (0.3%)	1.18	1/2676 (0.0%)
1	D	1.34	7/1980 (0.4%)	1.23	5/2676 (0.2%)
1	E	1.33	5/1980 (0.3%)	1.21	4/2676 (0.1%)
1	F	1.35	2/1999 (0.1%)	1.20	4/2700 (0.1%)
1	G	1.39	3/1980 (0.2%)	1.25	5/2676 (0.2%)
1	H	1.39	6/1980 (0.3%)	1.21	2/2676 (0.1%)
1	I	1.48	17/1980 (0.9%)	1.22	2/2676 (0.1%)
1	J	1.40	10/1988 (0.5%)	1.23	5/2686 (0.2%)
1	K	1.26	2/1980 (0.1%)	1.13	4/2676 (0.1%)
1	L	1.24	3/1962 (0.2%)	1.16	6/2652 (0.2%)
All	All	1.34	68/23760 (0.3%)	1.19	42/32110 (0.1%)

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	D	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	5

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	159	PHE	N-CA	6.89	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	15	GLY	C-O	-6.85	1.15	1.23
1	C	162	VAL	C-O	-6.84	1.16	1.24
1	I	162	VAL	N-CA	6.75	1.54	1.46
1	I	250	ILE	C-O	6.61	1.31	1.24
1	I	109	LEU	CA-C	-6.60	1.43	1.52
1	K	137	ILE	C-O	6.41	1.30	1.24
1	G	140	ASN	C-O	-6.37	1.17	1.24
1	I	182	LEU	CA-C	-6.36	1.45	1.52
1	I	156	ALA	CA-C	-6.18	1.44	1.52
1	D	226	ASP	C-O	6.16	1.31	1.23
1	J	9	GLY	C-O	-6.16	1.16	1.24
1	C	83	ASP	N-CA	6.14	1.54	1.46
1	D	29	VAL	CA-CB	-6.06	1.46	1.54
1	E	88	SER	N-CA	-5.99	1.39	1.46
1	J	181	SER	N-CA	5.98	1.53	1.46
1	L	182	LEU	C-O	-5.96	1.16	1.24
1	A	229	ASP	C-O	-5.96	1.17	1.24
1	H	23	ALA	C-O	-5.92	1.17	1.24
1	B	83	ASP	N-CA	5.91	1.53	1.46
1	I	117	PHE	C-O	5.89	1.30	1.24
1	I	165	THR	C-N	-5.88	1.25	1.33
1	K	122	GLU	N-CA	5.85	1.53	1.46
1	J	29	VAL	C-O	-5.85	1.18	1.24
1	E	171	ASP	N-CA	5.79	1.53	1.46
1	C	31	VAL	N-CA	-5.77	1.39	1.46
1	D	169	ALA	N-CA	5.75	1.53	1.46
1	L	169	ALA	N-CA	-5.66	1.39	1.46
1	J	219	VAL	N-CA	5.66	1.51	1.46
1	E	166	GLN	CA-C	5.65	1.60	1.52
1	A	257	VAL	C-O	-5.62	1.18	1.24
1	J	21	GLY	CA-C	-5.58	1.45	1.52
1	L	156	ALA	C-O	5.54	1.30	1.24
1	I	252	VAL	C-O	5.52	1.30	1.24
1	I	164	LEU	N-CA	-5.48	1.39	1.46
1	F	75	VAL	N-CA	5.47	1.53	1.46
1	I	116	TYR	N-CA	5.47	1.52	1.46
1	D	154	TYR	C-O	-5.45	1.17	1.24
1	D	107	LEU	C-O	-5.45	1.17	1.24
1	B	159	PHE	N-CA	5.39	1.52	1.46
1	I	170	LEU	C-O	5.39	1.30	1.24
1	H	187	LEU	C-O	-5.35	1.18	1.23
1	I	26	GLY	C-O	-5.35	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	113	LEU	CA-C	-5.33	1.48	1.52
1	J	219	VAL	CA-C	5.33	1.57	1.53
1	I	232	ASN	N-CA	5.33	1.52	1.46
1	H	31	VAL	N-CA	-5.31	1.40	1.46
1	C	254	GLY	N-CA	-5.29	1.38	1.45
1	H	133	LYS	CA-C	-5.20	1.47	1.53
1	A	157	ALA	C-O	-5.17	1.17	1.24
1	H	190	SER	CA-C	5.15	1.59	1.53
1	F	183	MET	C-O	5.14	1.30	1.23
1	G	252	VAL	N-CA	5.14	1.52	1.46
1	I	124	SER	CA-C	5.13	1.59	1.52
1	B	180	HIS	CA-C	-5.13	1.46	1.52
1	I	114	VAL	CA-CB	5.13	1.60	1.54
1	D	193	PHE	C-O	-5.12	1.18	1.24
1	E	182	LEU	C-O	5.11	1.30	1.24
1	C	136	ILE	CA-C	-5.10	1.46	1.52
1	J	162	VAL	N-CA	5.09	1.52	1.46
1	G	165	THR	N-CA	-5.08	1.40	1.46
1	H	20	GLU	N-CA	5.08	1.52	1.46
1	J	206	ILE	CA-CB	5.07	1.59	1.55
1	C	138	GLN	C-O	5.06	1.30	1.23
1	I	139	ILE	CA-C	-5.05	1.47	1.52
1	D	15	GLY	N-CA	-5.03	1.39	1.45
1	A	8	ILE	C-O	5.03	1.30	1.24
1	J	183	MET	C-O	5.02	1.30	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	212	GLU	CA-C-N	-7.60	111.89	119.56
1	E	212	GLU	C-N-CA	-7.60	111.89	119.56
1	D	79	PHE	O-C-N	-7.33	113.65	123.10
1	F	157	ALA	N-CA-C	6.77	118.66	111.28
1	E	65	GLU	N-CA-C	6.74	118.28	111.07
1	D	80	GLY	N-CA-C	6.61	121.74	114.40
1	H	29	VAL	N-CA-C	6.44	117.12	108.11
1	L	14	LEU	N-CA-C	6.35	117.87	111.07
1	G	78	THR	N-CA-C	6.13	117.76	111.14
1	L	111	VAL	CB-CA-C	-6.12	104.16	111.81
1	A	78	THR	N-CA-C	6.06	117.68	111.14
1	G	106	ASP	N-CA-C	6.04	117.53	111.07
1	J	80	GLY	N-CA-C	6.02	121.70	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	34	LEU	N-CA-C	-5.95	104.80	111.28
1	I	94	ALA	N-CA-C	5.92	119.90	109.96
1	E	146	VAL	CB-CA-C	-5.87	101.76	110.33
1	G	118	LEU	N-CA-C	5.71	117.18	111.07
1	J	208	PRO	N-CA-C	5.69	121.03	113.40
1	H	54	ARG	NE-CZ-NH2	-5.64	114.13	119.20
1	B	72	ALA	N-CA-C	5.59	117.38	111.28
1	F	2	GLU	N-CA-CB	-5.54	108.56	114.10
1	D	79	PHE	CA-C-N	-5.51	109.55	121.17
1	D	79	PHE	C-N-CA	-5.51	109.55	121.17
1	D	146	VAL	CB-CA-C	-5.45	102.38	110.33
1	A	248	GLN	N-CA-C	5.34	118.81	110.32
1	K	118	LEU	N-CA-C	5.31	116.75	111.07
1	L	184	LEU	N-CA-C	5.30	118.58	110.20
1	I	54	ARG	CG-CD-NE	-5.27	100.41	112.00
1	F	111	VAL	CB-CA-C	-5.25	105.16	112.04
1	B	248	GLN	N-CA-C	5.22	118.25	110.52
1	K	78	THR	N-CA-C	5.17	116.61	110.97
1	G	78	THR	CB-CA-C	-5.12	102.82	110.90
1	J	207	THR	N-CA-C	5.10	117.55	110.20
1	J	105	PHE	N-CA-C	-5.08	105.20	111.40
1	G	204	LEU	N-CA-C	-5.08	100.97	109.24
1	K	62	ALA	CA-C-N	5.06	128.77	120.63
1	K	62	ALA	C-N-CA	5.06	128.77	120.63
1	C	65	GLU	N-CA-C	5.05	117.18	111.11
1	F	113	LEU	N-CA-C	5.05	118.89	112.12
1	L	155	SER	CA-C-N	-5.01	113.57	120.28
1	L	155	SER	C-N-CA	-5.01	113.57	120.28
1	J	248	GLN	N-CA-C	5.00	117.93	110.52

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	80	GLY	Peptide
1	I	12	GLN	Peptide
1	J	80	GLY	Peptide
1	K	80	GLY	Peptide
1	L	80	GLY	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	1948	0	1943	16	0
1	B	1939	0	1937	21	0
1	C	1948	0	1943	7	0
1	D	1948	0	1943	13	0
1	E	1948	0	1943	8	0
1	F	1964	0	1968	10	0
1	G	1948	0	1943	11	0
1	H	1948	0	1943	10	0
1	I	1948	0	1943	14	0
1	J	1956	0	1955	21	0
1	K	1948	0	1943	17	0
1	L	1930	0	1929	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	32	0	0	1	0
3	B	45	0	0	10	0
3	C	77	0	0	0	0
3	D	100	0	0	3	0
3	E	79	0	0	0	0
3	F	102	0	0	1	0
3	G	81	0	0	0	0
3	H	86	0	0	2	1
3	I	68	0	0	0	0
3	J	66	0	0	2	1
3	K	15	0	0	0	0
3	L	27	0	0	1	0
All	All	24163	0	23333	163	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 3.

All (163) 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:72:ALA:C	3:B:401:HOH:O	2.02	1.02
1:D:80:GLY:HA3	3:D:484:HOH:O	1.65	0.96
1:J:201:ALA:HA	1:J:206:ILE:CG2	1.96	0.95
1:B:27:TYR:HA	3:B:402:HOH:O	1.68	0.92
1:J:201:ALA:HA	1:J:206:ILE:HG23	1.55	0.88
1:F:226:ASP:OD2	3:F:401:HOH:O	1.92	0.85
1:K:18:LEU:O	1:K:22:LEU:HD13	1.81	0.81
1:B:71:LEU:O	3:B:401:HOH:O	2.01	0.79
1:G:209:GLU:O	1:G:209:GLU:OE2	2.03	0.77
1:L:201:ALA:O	1:L:204:LEU:O	2.02	0.76
1:B:3:GLN:O	3:B:402:HOH:O	2.02	0.76
1:B:72:ALA:O	3:B:401:HOH:O	1.99	0.75
1:I:192:MET:HE3	1:I:196:LEU:HD11	1.67	0.74
1:L:13:THR:HG23	1:L:14:LEU:H	1.55	0.72
1:L:4:VAL:N	3:L:401:HOH:O	2.22	0.72
1:A:146:VAL:CG1	1:A:259:PHE:HZ	2.04	0.71
1:J:129:ARG:HD3	1:J:130:ASP:OD1	1.91	0.70
1:G:201:ALA:O	1:G:204:LEU:O	2.12	0.68
1:G:204:LEU:HD22	1:G:206:ILE:HG23	1.77	0.66
1:F:234:LEU:C	1:F:234:LEU:HD23	2.21	0.65
1:J:81:ARG:HD3	1:J:83:ASP:OD1	1.98	0.64
1:J:201:ALA:O	1:J:204:LEU:O	2.16	0.64
1:J:192:MET:HE1	1:J:196:LEU:HD11	1.80	0.63
1:A:207:THR:CG2	1:A:210:GLU:HG3	2.30	0.62
1:B:204:LEU:HD11	1:B:214:TYR:CE1	2.36	0.61
1:I:23:ALA:O	1:I:54:ARG:NH2	2.33	0.61
1:F:61:ASP:OD1	1:F:63:THR:HG22	2.01	0.61
1:J:206:ILE:HG13	1:J:207:THR:O	2.01	0.60
1:F:91:VAL:HG21	1:F:192:MET:HE2	1.84	0.59
1:G:37:SER:O	1:G:41:ARG:HG3	2.03	0.58
1:B:47:ASN:O	1:B:51:GLY:O	2.21	0.57
1:B:204:LEU:HD11	1:B:214:TYR:CZ	2.41	0.56
1:L:90:GLY:HA3	1:L:112:ASN:OD1	2.06	0.56
1:A:221:LEU:HD12	1:A:254:GLY:HA2	1.87	0.56
1:H:73:ARG:O	1:H:77:GLU:HG2	2.05	0.56
1:I:20:GLU:OE1	1:I:49:ARG:NH1	2.39	0.55
1:I:212:GLU:HB2	1:I:213:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:VAL:N	3:B:401:HOH:O	2.34	0.55
1:B:72:ALA:CA	3:B:401:HOH:O	2.51	0.54
1:J:201:ALA:HA	1:J:206:ILE:HG22	1.87	0.54
1:G:192:MET:SD	1:G:196:LEU:HD23	2.47	0.54
1:G:209:GLU:O	1:G:209:GLU:CD	2.50	0.54
1:B:50:TYR:O	3:B:403:HOH:O	2.19	0.53
1:D:28:HIS:NE2	3:D:401:HOH:O	2.34	0.53
1:H:191:PRO:HD2	1:H:192:MET:HE3	1.90	0.53
1:I:13:THR:HG21	1:I:191:PRO:HG2	1.91	0.52
1:J:103:THR:HG23	3:J:453:HOH:O	2.10	0.52
1:D:90:GLY:HA3	1:D:112:ASN:OD1	2.10	0.52
1:I:90:GLY:HA3	1:I:112:ASN:OD1	2.10	0.52
1:C:221:LEU:HD12	1:C:254:GLY:HA2	1.93	0.51
1:E:51:GLY:O	1:E:54:ARG:HG2	2.11	0.51
1:L:212:GLU:HB2	1:L:213:PRO:HD3	1.91	0.51
1:J:129:ARG:CD	1:J:130:ASP:OD1	2.58	0.51
1:D:37:SER:OG	1:D:41:ARG:NH2	2.44	0.50
1:H:201:ALA:HB1	1:H:206:ILE:O	2.12	0.50
1:L:180:HIS:CE1	1:L:246:THR:HA	2.47	0.50
1:L:13:THR:HG23	1:L:14:LEU:N	2.25	0.50
1:A:207:THR:HG22	1:A:210:GLU:HG3	1.93	0.50
1:K:65:GLU:O	1:K:69:GLU:HG3	2.12	0.49
1:H:206:ILE:HB	1:H:210:GLU:CG	2.42	0.49
1:E:180:HIS:HD2	1:E:248:GLN:HB2	1.77	0.49
1:I:19:CYS:HB2	1:I:42:LEU:HD21	1.95	0.49
1:J:206:ILE:HD12	1:J:207:THR:H	1.76	0.49
1:A:50:TYR:HB3	1:A:54:ARG:CD	2.43	0.49
1:L:91:VAL:HG23	1:L:192:MET:HE2	1.95	0.49
1:D:13:THR:HG21	3:D:482:HOH:O	2.12	0.49
1:H:180:HIS:HD2	1:H:248:GLN:HB2	1.78	0.49
1:L:12:GLN:HG3	1:L:13:THR:HG22	1.95	0.49
1:J:201:ALA:CA	1:J:206:ILE:HG23	2.35	0.49
1:K:148:SER:HB2	1:K:151:ASN:HB2	1.95	0.49
1:G:90:GLY:HA3	1:G:112:ASN:OD1	2.13	0.48
1:K:129:ARG:NH1	1:K:130:ASP:OD1	2.46	0.48
1:F:180:HIS:CE1	1:F:246:THR:HA	2.49	0.48
1:G:234:LEU:C	1:G:234:LEU:HD23	2.39	0.47
1:I:180:HIS:HD2	1:I:248:GLN:HB2	1.80	0.47
1:J:199:GLN:HG2	1:J:199:GLN:O	2.14	0.47
1:C:209:GLU:H	1:C:209:GLU:CD	2.22	0.47
1:G:146:VAL:HG22	1:G:259:PHE:HZ	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:N	1:B:198:PRO:CD	2.78	0.47
1:A:207:THR:HG23	1:A:210:GLU:HG3	1.97	0.47
1:K:60:VAL:CB	1:K:71:LEU:HD22	2.44	0.47
1:B:44:ASP:HA	1:B:47:ASN:HB2	1.95	0.47
1:B:221:LEU:HD12	1:B:254:GLY:HA2	1.95	0.47
1:K:49:ARG:HG2	1:K:50:TYR:CE1	2.49	0.47
1:L:204:LEU:HD23	1:L:205:GLY:N	2.30	0.47
1:D:13:THR:CG2	1:D:227:TYR:OH	2.64	0.46
1:F:90:GLY:HA3	1:F:112:ASN:OD1	2.15	0.46
1:F:201:ALA:HB1	1:F:206:ILE:O	2.14	0.46
1:J:180:HIS:HE1	3:J:424:HOH:O	1.98	0.46
1:K:18:LEU:O	1:K:22:LEU:CD1	2.60	0.46
1:A:206:ILE:HG12	1:A:210:GLU:OE1	2.15	0.46
1:K:60:VAL:HB	1:K:71:LEU:HD22	1.96	0.46
1:C:27:TYR:O	1:C:54:ARG:NH2	2.48	0.46
1:F:146:VAL:HG22	1:F:259:PHE:HZ	1.81	0.46
1:E:146:VAL:HG22	1:E:259:PHE:HZ	1.80	0.46
1:J:212:GLU:HB2	1:J:213:PRO:CD	2.45	0.46
1:E:116:TYR:CD2	1:E:164:LEU:HD23	2.51	0.46
1:A:146:VAL:CG1	1:A:259:PHE:CZ	2.93	0.46
1:K:61:ASP:OD1	1:K:63:THR:HB	2.15	0.46
1:L:197:LEU:HB2	1:L:198:PRO:HD3	1.98	0.46
1:C:112:ASN:HB2	1:C:157:ALA:HB1	1.98	0.45
1:H:90:GLY:HA3	1:H:112:ASN:OD1	2.16	0.45
1:H:180:HIS:HE1	3:H:433:HOH:O	1.99	0.45
1:I:129:ARG:NH1	1:I:130:ASP:OD1	2.48	0.45
1:I:189:LYS:NZ	1:I:212:GLU:OE1	2.49	0.45
1:B:212:GLU:HB2	1:B:213:PRO:HD3	1.98	0.45
1:K:81:ARG:NH2	1:K:83:ASP:OD2	2.50	0.45
1:J:112:ASN:HB2	1:J:157:ALA:HB1	1.99	0.44
1:H:3:GLN:NE2	3:H:402:HOH:O	2.50	0.44
1:D:13:THR:HG22	1:D:14:LEU:N	2.32	0.44
1:E:113:LEU:HA	1:E:113:LEU:HD23	1.81	0.44
1:E:45:THR:HG22	1:E:49:ARG:HD3	1.99	0.44
1:G:148:SER:HB3	1:G:151:ASN:HB2	2.00	0.44
1:C:4:VAL:HG21	1:C:79:PHE:HB3	2.00	0.43
1:D:214:TYR:CE2	1:D:218:LYS:HE3	2.54	0.43
1:D:13:THR:HG23	1:D:227:TYR:OH	2.18	0.43
1:D:221:LEU:HD12	1:D:254:GLY:HA2	2.00	0.43
1:C:116:TYR:CZ	1:C:138:GLN:HB2	2.54	0.43
1:A:94:ALA:HA	1:A:150:HIS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:197:LEU:HB2	1:J:198:PRO:HD3	2.01	0.42
1:A:50:TYR:HB3	1:A:54:ARG:HD3	2.01	0.42
1:F:146:VAL:CG2	1:F:259:PHE:HZ	2.32	0.42
1:K:214:TYR:CZ	1:K:218:LYS:NZ	2.88	0.42
1:B:136:ILE:O	1:B:179:VAL:HA	2.19	0.42
1:D:234:LEU:C	1:D:234:LEU:HD23	2.44	0.42
1:L:221:LEU:HD12	1:L:254:GLY:HA2	2.01	0.42
1:A:50:TYR:HB3	1:A:54:ARG:HD2	2.01	0.42
1:B:180:HIS:HD2	1:B:248:GLN:HB2	1.84	0.42
1:I:183:MET:HB2	1:I:251:ASN:HD22	1.85	0.42
1:K:90:GLY:HA3	1:K:112:ASN:OD1	2.19	0.42
1:L:114:VAL:O	1:L:117:PHE:HB3	2.19	0.42
1:B:13:THR:O	1:B:14:LEU:C	2.62	0.42
1:J:201:ALA:HB1	1:J:206:ILE:O	2.20	0.42
1:D:146:VAL:HG22	1:D:259:PHE:HZ	1.85	0.42
1:K:76:ASP:O	1:K:79:PHE:O	2.37	0.42
1:A:18:LEU:HD22	1:A:234:LEU:HD13	2.01	0.42
1:L:207:THR:HB	1:L:208:PRO:CD	2.50	0.42
1:J:65:GLU:O	1:J:69:GLU:HG3	2.20	0.41
1:L:145:LYS:HD3	1:L:183:MET:HG3	2.02	0.41
1:A:226:ASP:CG	3:A:425:HOH:O	2.62	0.41
1:H:112:ASN:HB2	1:H:157:ALA:HB1	2.01	0.41
1:C:234:LEU:C	1:C:234:LEU:HD23	2.46	0.41
1:E:65:GLU:O	1:E:69:GLU:HG3	2.20	0.41
1:H:13:THR:HG21	1:H:192:MET:HE1	2.02	0.41
1:A:87:TYR:OH	1:A:115:GLY:HA3	2.21	0.41
1:B:214:TYR:CD1	1:B:214:TYR:C	2.97	0.41
1:B:3:GLN:N	3:B:405:HOH:O	2.53	0.41
1:A:201:ALA:HB1	1:A:206:ILE:O	2.20	0.41
1:E:2:GLU:N	1:E:2:GLU:OE1	2.54	0.41
1:F:197:LEU:HB2	1:F:198:PRO:HD3	2.02	0.41
1:G:180:HIS:CE1	1:G:246:THR:HA	2.56	0.41
1:B:75:VAL:HB	3:B:401:HOH:O	2.20	0.41
1:D:17:PHE:CD1	1:D:227:TYR:HB3	2.55	0.41
1:A:49:ARG:HG2	1:A:50:TYR:CD2	2.56	0.41
1:K:54:ARG:HD3	1:K:54:ARG:HA	1.87	0.41
1:K:180:HIS:CE1	1:K:246:THR:HA	2.56	0.41
1:I:97:ILE:O	1:K:121:ARG:HG3	2.21	0.40
1:K:110:GLN:HA	1:K:114:VAL:HB	2.04	0.40
1:I:165:THR:HG23	1:I:179:VAL:HG12	2.03	0.40
1:I:197:LEU:HB2	1:I:198:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:180:HIS:HD2	1:J:248:GLN:HB2	1.87	0.40
1:J:234:LEU:C	1:J:234:LEU:HD23	2.46	0.40
1:L:21:GLY:HA3	1:L:231:LEU:HD21	2.04	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)
3:H:485:HOH:O	3:J:425:HOH:O[3_454]	2.13	0.07

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	256/263 (97%)	247 (96%)	9 (4%)	0	100	100
1	B	255/263 (97%)	247 (97%)	8 (3%)	0	100	100
1	C	256/263 (97%)	250 (98%)	6 (2%)	0	100	100
1	D	256/263 (97%)	250 (98%)	6 (2%)	0	100	100
1	E	256/263 (97%)	251 (98%)	5 (2%)	0	100	100
1	F	258/263 (98%)	251 (97%)	7 (3%)	0	100	100
1	G	256/263 (97%)	250 (98%)	6 (2%)	0	100	100
1	H	256/263 (97%)	252 (98%)	4 (2%)	0	100	100
1	I	256/263 (97%)	252 (98%)	4 (2%)	0	100	100
1	J	257/263 (98%)	245 (95%)	10 (4%)	2 (1%)	16	5
1	K	256/263 (97%)	246 (96%)	10 (4%)	0	100	100
1	L	254/263 (97%)	246 (97%)	8 (3%)	0	100	100
All	All	3072/3156 (97%)	2987 (97%)	83 (3%)	2 (0%)	48	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	202	GLU
1	J	213	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	203/205 (99%)	200 (98%)	3 (2%)	57	42
1	B	202/205 (98%)	199 (98%)	3 (2%)	57	42
1	C	203/205 (99%)	199 (98%)	4 (2%)	48	32
1	D	203/205 (99%)	202 (100%)	1 (0%)	81	75
1	E	203/205 (99%)	201 (99%)	2 (1%)	68	58
1	F	205/205 (100%)	203 (99%)	2 (1%)	68	58
1	G	203/205 (99%)	199 (98%)	4 (2%)	48	32
1	H	203/205 (99%)	200 (98%)	3 (2%)	57	42
1	I	203/205 (99%)	199 (98%)	4 (2%)	48	32
1	J	204/205 (100%)	202 (99%)	2 (1%)	68	58
1	K	203/205 (99%)	200 (98%)	3 (2%)	57	42
1	L	201/205 (98%)	197 (98%)	4 (2%)	48	32
All	All	2436/2460 (99%)	2401 (99%)	35 (1%)	59	45

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	91	VAL
1	A	217	ASP
1	B	194	GLN
1	B	204	LEU
1	B	206	ILE
1	C	91	VAL

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Mol	Chain	Res	Type
1	C	109	LEU
1	C	113	LEU
1	C	209	GLU
1	D	98	THR
1	E	49	ARG
1	E	165	THR
1	F	91	VAL
1	F	165	THR
1	G	137	ILE
1	G	165	THR
1	G	197	LEU
1	G	204	LEU
1	H	24	GLN
1	H	192	MET
1	H	203	LYS
1	I	91	VAL
1	I	149	LYS
1	I	165	THR
1	I	207	THR
1	J	192	MET
1	J	207	THR
1	K	12	GLN
1	K	148	SER
1	K	165	THR
1	L	113	LEU
1	L	165	THR
1	L	192	MET
1	L	194	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	28	HIS
1	A	40	ASN
1	A	110	GLN
1	A	186	ASN
1	A	251	ASN
1	B	150	HIS
1	B	151	ASN
1	B	180	HIS
1	B	248	GLN

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Mol	Chain	Res	Type
1	B	251	ASN
1	C	194	GLN
1	C	228	GLN
1	D	40	ASN
1	D	110	GLN
1	D	251	ASN
1	E	3	GLN
1	E	180	HIS
1	E	251	ASN
1	F	12	GLN
1	F	38	ASN
1	G	99	GLN
1	G	228	GLN
1	G	251	ASN
1	H	3	GLN
1	H	24	GLN
1	H	150	HIS
1	H	180	HIS
1	H	194	GLN
1	I	24	GLN
1	I	99	GLN
1	I	110	GLN
1	I	180	HIS
1	I	251	ASN
1	I	256	GLN
1	J	110	GLN
1	J	180	HIS
1	K	24	GLN
1	K	150	HIS
1	K	151	ASN
1	K	186	ASN
1	K	228	GLN
1	K	251	ASN
1	L	24	GLN
1	L	99	GLN
1	L	110	GLN
1	L	151	ASN
1	L	166	GLN
1	L	186	ASN

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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	258/263 (98%)	1.06	42 (16%) 4 4	18, 31, 60, 80	0
1	B	257/263 (97%)	1.40	71 (27%) 1 1	17, 31, 59, 71	0
1	C	258/263 (98%)	0.27	8 (3%) 51 56	15, 23, 42, 58	0
1	D	258/263 (98%)	0.36	14 (5%) 31 34	15, 23, 48, 77	0
1	E	258/263 (98%)	0.20	6 (2%) 61 67	15, 23, 40, 60	0
1	F	259/263 (98%)	0.23	16 (6%) 26 28	11, 22, 49, 73	1 (0%)
1	G	258/263 (98%)	0.47	24 (9%) 14 15	14, 23, 60, 93	0
1	H	258/263 (98%)	0.23	11 (4%) 40 42	15, 22, 44, 70	0
1	I	258/263 (98%)	0.72	12 (4%) 36 38	17, 27, 44, 64	0
1	J	259/263 (98%)	0.70	27 (10%) 11 12	16, 24, 62, 91	0
1	K	258/263 (98%)	1.65	74 (28%) 1 1	22, 35, 66, 91	0
1	L	256/263 (97%)	1.30	46 (17%) 3 3	21, 33, 64, 87	0
All	All	3095/3156 (98%)	0.72	351 (11%) 10 10	11, 27, 54, 93	1 (0%)

All (351) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	56	TYR	7.3
1	J	204	LEU	7.2
1	K	204	LEU	6.8
1	B	53	GLY	6.5
1	B	204	LEU	6.5
1	B	57	GLY	6.4
1	B	50	TYR	6.3
1	J	206	ILE	6.1
1	B	54	ARG	6.0
1	B	52	ALA	5.9
1	J	208	PRO	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	42	LEU	5.8
1	A	206	ILE	5.8
1	G	204	LEU	5.8
1	B	46	ILE	5.7
1	L	204	LEU	5.4
1	J	203	LYS	5.3
1	J	1	MET	5.3
1	K	91	VAL	5.2
1	L	206	ILE	5.0
1	F	205	GLY	4.9
1	J	198	PRO	4.9
1	G	203	LYS	4.8
1	K	42	LEU	4.8
1	K	206	ILE	4.7
1	L	91	VAL	4.7
1	K	53	GLY	4.6
1	D	202	GLU	4.5
1	B	206	ILE	4.5
1	G	208	PRO	4.5
1	B	55	ALA	4.5
1	G	201	ALA	4.4
1	G	196	LEU	4.4
1	D	204	LEU	4.3
1	K	34	LEU	4.3
1	L	192	MET	4.2
1	L	92	ALA	4.2
1	J	197	LEU	4.2
1	G	200	TYR	4.1
1	G	206	ILE	4.1
1	B	47	ASN	4.1
1	J	207	THR	4.1
1	H	205	GLY	4.1
1	B	48	SER	4.0
1	F	1	MET	4.0
1	J	200	TYR	4.0
1	G	205	GLY	4.0
1	H	203	LYS	4.0
1	B	31	VAL	4.0
1	D	206	ILE	3.9
1	K	211	VAL	3.9
1	I	80	GLY	3.9
1	B	43	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	206	ILE	3.9
1	A	204	LEU	3.8
1	A	91	VAL	3.8
1	B	19	CYS	3.8
1	A	208	PRO	3.8
1	K	199	GLN	3.7
1	K	51	GLY	3.7
1	K	203	LYS	3.7
1	A	211	VAL	3.7
1	K	80	GLY	3.7
1	K	198	PRO	3.7
1	J	211	VAL	3.6
1	B	203	LYS	3.6
1	B	49	ARG	3.6
1	K	207	THR	3.6
1	D	205	GLY	3.6
1	K	197	LEU	3.6
1	D	207	THR	3.5
1	A	197	LEU	3.5
1	B	196	LEU	3.5
1	B	197	LEU	3.5
1	K	193	PHE	3.5
1	D	201	ALA	3.5
1	B	28	HIS	3.5
1	K	56	TYR	3.5
1	K	205	GLY	3.4
1	G	197	LEU	3.4
1	B	10	GLY	3.4
1	L	197	LEU	3.4
1	A	93	LYS	3.3
1	H	206	ILE	3.3
1	K	192	MET	3.3
1	D	203	LYS	3.3
1	G	191	PRO	3.3
1	A	192	MET	3.3
1	K	50	TYR	3.3
1	B	78	THR	3.3
1	K	126	LEU	3.3
1	L	13	THR	3.3
1	L	196	LEU	3.3
1	F	209	GLU	3.2
1	B	45	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	204	LEU	3.2
1	G	207	THR	3.2
1	K	22	LEU	3.2
1	L	205	GLY	3.2
1	B	41	ARG	3.2
1	G	214	TYR	3.2
1	H	201	ALA	3.2
1	B	77	GLU	3.2
1	L	93	LYS	3.2
1	A	98	THR	3.2
1	D	209	GLU	3.2
1	K	74	ALA	3.2
1	L	208	PRO	3.2
1	F	204	LEU	3.2
1	B	39	ALA	3.1
1	J	201	ALA	3.1
1	L	95	ALA	3.1
1	K	146	VAL	3.1
1	B	30	ALA	3.1
1	L	195	SER	3.1
1	B	189	LYS	3.1
1	B	23	ALA	3.1
1	A	46	ILE	3.1
1	B	79	PHE	3.1
1	A	207	THR	3.1
1	L	207	THR	3.1
1	F	208	PRO	3.1
1	K	208	PRO	3.1
1	B	211	VAL	3.0
1	J	216	VAL	3.0
1	K	60	VAL	3.0
1	G	192	MET	3.0
1	G	202	GLU	3.0
1	K	190	SER	3.0
1	J	205	GLY	3.0
1	I	203	LYS	3.0
1	G	37	SER	3.0
1	A	198	PRO	3.0
1	B	44	ASP	3.0
1	J	192	MET	3.0
1	B	259	PHE	3.0
1	B	198	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	41	ARG	3.0
1	C	192	MET	3.0
1	D	197	LEU	2.9
1	I	204	LEU	2.9
1	L	259	PHE	2.9
1	B	82	ALA	2.9
1	K	66	ALA	2.9
1	L	89	ALA	2.9
1	L	94	ALA	2.9
1	F	206	ILE	2.9
1	B	18	LEU	2.9
1	E	204	LEU	2.9
1	J	209	GLU	2.9
1	B	29	VAL	2.9
1	K	200	TYR	2.9
1	K	18	LEU	2.9
1	L	80	GLY	2.9
1	J	91	VAL	2.8
1	A	201	ALA	2.8
1	L	66	ALA	2.8
1	J	202	GLU	2.8
1	H	204	LEU	2.8
1	K	187	LEU	2.8
1	H	200	TYR	2.8
1	E	2	GLU	2.8
1	A	48	SER	2.8
1	K	43	ALA	2.8
1	K	92	ALA	2.8
1	B	11	GLY	2.8
1	A	132	ILE	2.8
1	B	13	THR	2.8
1	H	207	THR	2.8
1	B	192	MET	2.8
1	F	192	MET	2.8
1	K	52	ALA	2.8
1	K	58	PHE	2.8
1	A	56	TYR	2.7
1	A	200	TYR	2.7
1	K	237	TYR	2.7
1	B	24	GLN	2.7
1	K	13	THR	2.7
1	A	196	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	240	ASP	2.7
1	G	211	VAL	2.7
1	A	95	ALA	2.7
1	A	203	LYS	2.7
1	K	231	LEU	2.7
1	E	208	PRO	2.7
1	J	213	PRO	2.7
1	K	46	ILE	2.7
1	G	93	LYS	2.7
1	L	111	VAL	2.7
1	A	52	ALA	2.7
1	A	94	ALA	2.7
1	J	215	TYR	2.7
1	K	79	PHE	2.7
1	A	51	GLY	2.6
1	B	51	GLY	2.6
1	F	89	ALA	2.6
1	J	259	PHE	2.6
1	L	193	PHE	2.6
1	A	96	PRO	2.6
1	B	208	PRO	2.6
1	K	196	LEU	2.6
1	A	205	GLY	2.6
1	L	74	ALA	2.6
1	K	119	CYS	2.6
1	K	177	ILE	2.6
1	B	194	GLN	2.6
1	E	209	GLU	2.6
1	G	195	SER	2.6
1	G	198	PRO	2.6
1	A	97	ILE	2.6
1	B	20	GLU	2.6
1	B	205	GLY	2.6
1	K	27	TYR	2.5
1	K	214	TYR	2.5
1	A	77	GLU	2.5
1	E	203	LYS	2.5
1	E	206	ILE	2.5
1	H	192	MET	2.5
1	A	2	GLU	2.5
1	G	209	GLU	2.5
1	B	4	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	58	PHE	2.5
1	B	132	ILE	2.5
1	B	3	GLN	2.5
1	A	74	ALA	2.5
1	K	70	ALA	2.5
1	I	91	VAL	2.5
1	A	191	PRO	2.5
1	K	191	PRO	2.5
1	L	56	TYR	2.4
1	L	48	SER	2.4
1	C	98	THR	2.4
1	K	98	THR	2.4
1	D	198	PRO	2.4
1	K	6	VAL	2.4
1	I	192	MET	2.4
1	I	240	ASP	2.4
1	B	91	VAL	2.4
1	K	107	LEU	2.4
1	K	109	LEU	2.4
1	L	215	TYR	2.4
1	L	43	ALA	2.4
1	F	202	GLU	2.4
1	K	49	ARG	2.3
1	A	193	PHE	2.3
1	B	32	ALA	2.3
1	B	89	ALA	2.3
1	K	55	ALA	2.3
1	K	213	PRO	2.3
1	B	75	VAL	2.3
1	L	211	VAL	2.3
1	A	240	ASP	2.3
1	K	41	ARG	2.3
1	J	210	GLU	2.3
1	D	24	GLN	2.3
1	F	196	LEU	2.3
1	J	188	LEU	2.3
1	K	14	LEU	2.3
1	C	214	TYR	2.3
1	I	98	THR	2.3
1	L	50	TYR	2.3
1	L	200	TYR	2.3
1	L	214	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	41	ARG	2.3
1	L	202	GLU	2.3
1	B	126	LEU	2.3
1	K	63	THR	2.3
1	B	227	TYR	2.3
1	K	128	ILE	2.3
1	K	132	ILE	2.3
1	A	195	SER	2.3
1	K	48	SER	2.3
1	A	209	GLU	2.3
1	B	216	VAL	2.3
1	J	54	ARG	2.2
1	A	100	PHE	2.2
1	B	16	ALA	2.2
1	H	202	GLU	2.2
1	I	205	GLY	2.2
1	K	259	PHE	2.2
1	L	201	ALA	2.2
1	G	199	GLN	2.2
1	K	216	VAL	2.2
1	L	6	VAL	2.2
1	F	63	THR	2.2
1	F	98	THR	2.2
1	L	45	THR	2.2
1	K	5	ALA	2.2
1	K	62	ALA	2.2
1	K	17	PHE	2.2
1	B	207	THR	2.2
1	J	103	THR	2.2
1	A	199	GLN	2.2
1	B	74	ALA	2.2
1	B	201	ALA	2.2
1	K	39	ALA	2.2
1	L	203	LYS	2.2
1	A	88	SER	2.2
1	L	245	CYS	2.2
1	B	14	LEU	2.2
1	J	196	LEU	2.2
1	K	25	ALA	2.2
1	B	27	TYR	2.1
1	B	200	TYR	2.1
1	D	210	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	56	TYR	2.1
1	I	2	GLU	2.1
1	J	219	VAL	2.1
1	J	80	GLY	2.1
1	L	34	LEU	2.1
1	L	42	LEU	2.1
1	A	202	GLU	2.1
1	L	77	GLU	2.1
1	K	148	SER	2.1
1	A	41	ARG	2.1
1	K	75	VAL	2.1
1	B	202	GLU	2.1
1	F	198	PRO	2.1
1	L	19	CYS	2.1
1	B	17	PHE	2.1
1	B	193	PHE	2.1
1	A	214	TYR	2.1
1	C	200	TYR	2.1
1	F	77	GLU	2.1
1	L	59	LYS	2.1
1	K	57	GLY	2.1
1	B	12	GLN	2.1
1	D	12	GLN	2.1
1	D	213	PRO	2.1
1	G	213	PRO	2.1
1	K	118	LEU	2.1
1	C	201	ALA	2.1
1	K	94	ALA	2.1
1	A	210	GLU	2.0
1	K	20	GLU	2.0
1	I	56	TYR	2.0
1	L	115	GLY	2.0
1	K	12	GLN	2.0
1	B	84	LEU	2.0
1	L	71	LEU	2.0
1	F	93	LYS	2.0
1	F	207	THR	2.0
1	L	78	THR	2.0
1	G	215	TYR	2.0
1	H	50	TYR	2.0
1	C	198	PRO	2.0
1	I	208	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	60	VAL	2.0
1	B	6	VAL	2.0
1	I	146	VAL	2.0
1	L	68	VAL	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($\text{\AA}^2$)	Q<0.9
2	CL	L	301	1/1	0.93	0.13	33,33,33,33	0
2	CL	J	301	1/1	0.96	0.08	31,31,31,31	0
2	CL	K	301	1/1	0.97	0.06	31,31,31,31	0
2	CL	A	301	1/1	0.98	0.06	32,32,32,32	0
2	CL	B	301	1/1	0.98	0.05	34,34,34,34	0
2	CL	H	301	1/1	0.98	0.04	23,23,23,23	0
2	CL	I	301	1/1	0.99	0.04	26,26,26,26	0
2	CL	E	301	1/1	0.99	0.05	21,21,21,21	0
2	CL	G	301	1/1	0.99	0.04	26,26,26,26	0
2	CL	C	301	1/1	0.99	0.03	22,22,22,22	0
2	CL	D	301	1/1	1.00	0.04	25,25,25,25	0
2	CL	F	301	1/1	1.00	0.03	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.