



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 09:45 AM EDT

PDB ID : 5O3Z
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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

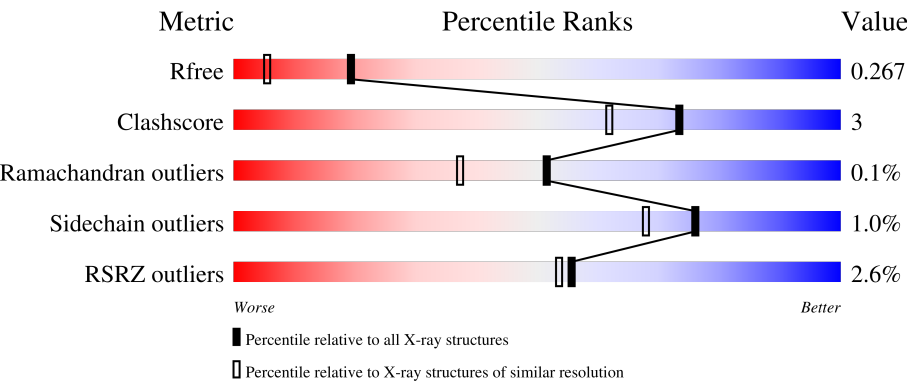
1 Overall quality at a glance i

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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	<div><div>2%</div><div><div></div><div>91%</div><div>7%</div><div></div></div><div></div></div>
1	B	263	<div><div>7%</div><div><div></div><div>90%</div><div>8%</div><div></div></div><div></div></div>
1	C	263	<div><div></div><div><div></div><div>93%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	D	263	<div><div>2%</div><div><div></div><div>91%</div><div>6%</div><div></div></div><div></div></div>
1	E	263	<div><div></div><div><div></div><div>92%</div><div>6%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	263	<div><div><div>%</div><div><div></div><div>91%</div><div>7%</div><div></div></div><div></div></div></div>
1	G	263	<div><div><div>5%</div><div><div></div><div>88%</div><div>10%</div><div></div></div><div></div></div></div>
1	H	263	<div><div><div>%</div><div><div></div><div>92%</div><div>6%</div><div></div></div><div></div></div></div>
1	I	263	<div><div><div>%</div><div><div></div><div>87%</div><div>11%</div><div></div></div><div></div></div></div>
1	J	263	<div><div><div>4%</div><div><div></div><div>89%</div><div>8%</div><div></div></div><div></div></div></div>
1	K	263	<div><div><div>5%</div><div><div></div><div>87%</div><div>11%</div><div></div></div><div></div></div></div>
1	L	263	<div><div><div>5%</div><div><div></div><div>86%</div><div>11%</div><div></div></div><div></div></div></div>

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 (three-letter code: 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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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

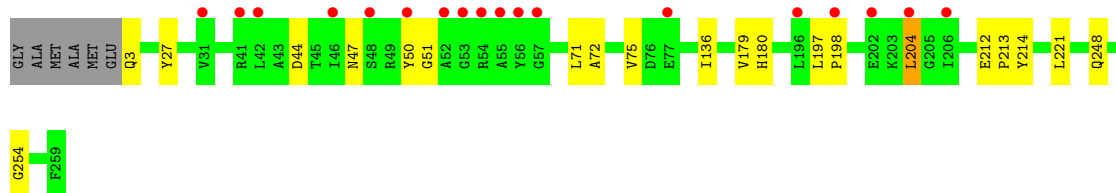
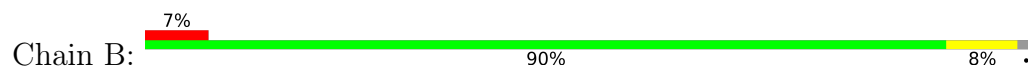
3 Residue-property plots [i](#)

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.

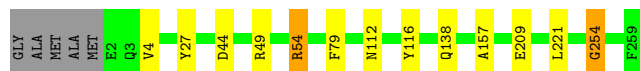
- Molecule 1: Sorbitol-6-phosphate dehydrogenase



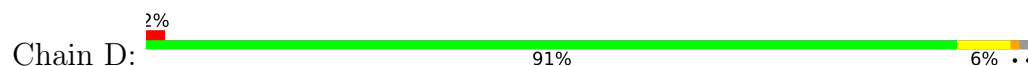
- Molecule 1: Sorbitol-6-phosphate dehydrogenase



- Molecule 1: Sorbitol-6-phosphate dehydrogenase



- Molecule 1: Sorbitol-6-phosphate dehydrogenase

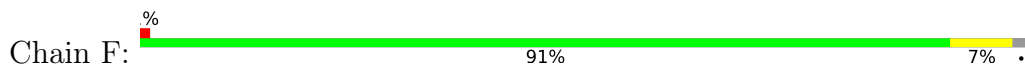


- Molecule 1: Sorbitol-6-phosphate dehydrogenase

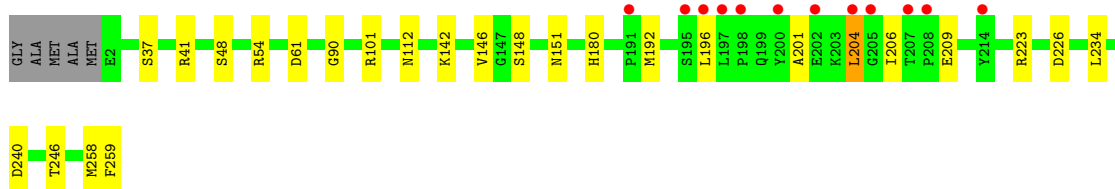
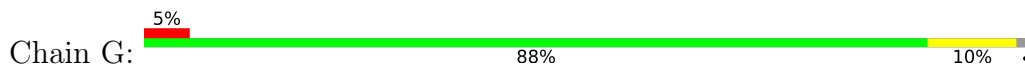




- Molecule 1: Sorbitol-6-phosphate dehydrogenase



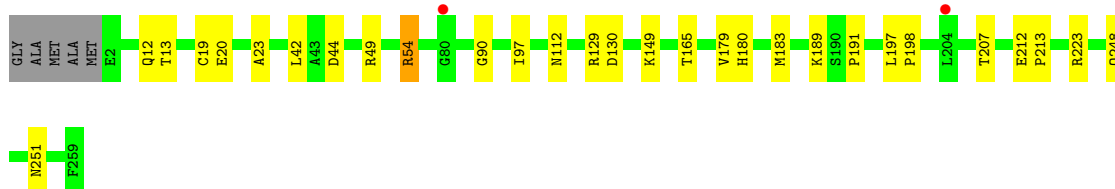
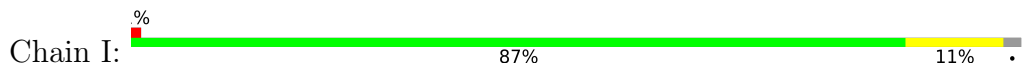
- Molecule 1: Sorbitol-6-phosphate dehydrogenase



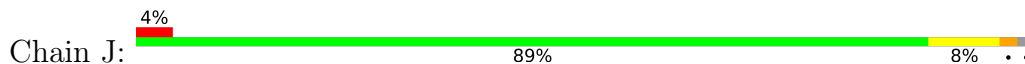
- Molecule 1: Sorbitol-6-phosphate dehydrogenase



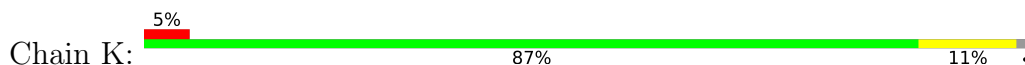
- Molecule 1: Sorbitol-6-phosphate dehydrogenase

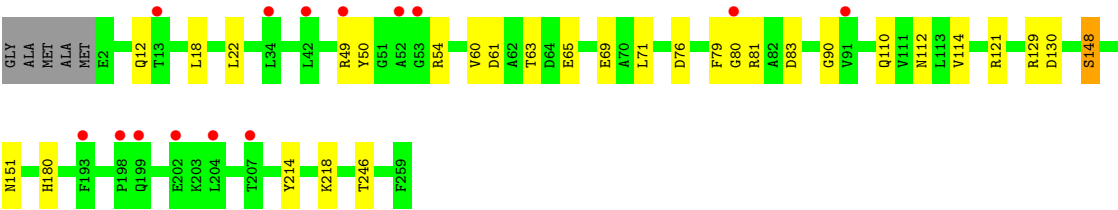


- Molecule 1: Sorbitol-6-phosphate dehydrogenase

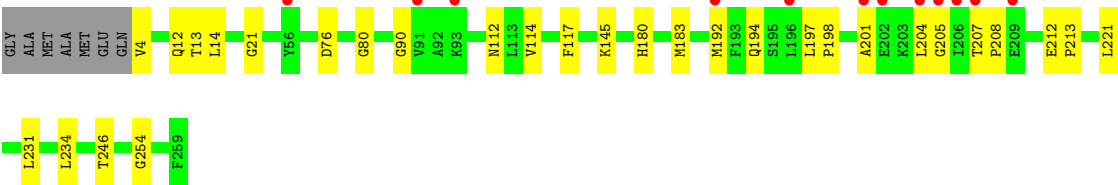
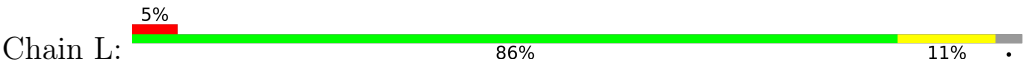


- Molecule 1: Sorbitol-6-phosphate dehydrogenase





● Molecule 1: Sorbitol-6-phosphate dehydrogenase



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 (5.04%)	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)	0.34 , 36.4	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 [i](#)

5.1 Standard geometry [i](#)

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	0.89	0/1980	0.89	0/2676
1	B	0.95	0/1971	0.90	0/2664
1	C	0.99	1/1980 (0.1%)	0.99	3/2676 (0.1%)
1	D	0.99	0/1980	1.00	4/2676 (0.1%)
1	E	1.00	0/1980	1.01	6/2676 (0.2%)
1	F	1.03	0/1999	1.01	4/2700 (0.1%)
1	G	1.04	0/1980	1.04	8/2676 (0.3%)
1	H	1.00	0/1980	0.99	2/2676 (0.1%)
1	I	1.05	0/1980	1.00	5/2676 (0.2%)
1	J	1.05	1/1988 (0.1%)	1.02	4/2686 (0.1%)
1	K	0.94	0/1980	0.87	0/2676
1	L	0.92	0/1962	0.90	1/2652 (0.0%)
All	All	0.99	2/23760 (0.0%)	0.97	37/32110 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	254	GLY	N-CA	-5.27	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	15	GLY	C-O	-5.06	1.15	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	54	ARG	NE-CZ-NH2	-12.35	114.13	120.30
1	J	129	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	J	81	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	J	81	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	C	54	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	J	129	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	C	49	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	I	54	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	G	101	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	G	54	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	E	49	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	F	121	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	I	54	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	E	73	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	D	101	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	I	223	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	C	44	ASP	CB-CG-OD1	6.28	123.95	118.30
1	D	79	PHE	C-N-CA	-6.07	109.55	122.30
1	G	226	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	F	135	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	G	61	ASP	CB-CG-OD1	5.74	123.47	118.30
1	D	223	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	G	240	ASP	CB-CG-OD1	5.63	123.37	118.30
1	G	54	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	79	PHE	O-C-N	-5.62	113.65	123.20
1	F	135	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	H	54	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	I	54	ARG	CG-CD-NE	-5.42	100.41	111.80
1	G	258	MET	CG-SD-CE	5.42	108.87	100.20
1	I	44	ASP	CB-CG-OD1	5.38	123.14	118.30
1	F	54	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	L	76	ASP	CB-CG-OD1	5.33	123.10	118.30
1	E	44	ASP	CB-CG-OD1	5.26	123.03	118.30
1	G	223	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	E	184	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	E	49	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	E	146	VAL	CB-CA-C	-5.07	101.76	111.40

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	15	0
1	B	1939	0	1937	19	0
1	C	1948	0	1943	6	0
1	D	1948	0	1943	12	0
1	E	1948	0	1943	8	0
1	F	1964	0	1968	9	0
1	G	1948	0	1943	11	0
1	H	1948	0	1943	9	0
1	I	1948	0	1943	13	0
1	J	1956	0	1955	20	0
1	K	1948	0	1943	17	0
1	L	1930	0	1929	15	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	153	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 (153) 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	0.96
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:72:ALA:O	3:B:401:HOH:O	1.99	0.80
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:234:LEU:C	1:F:234:LEU:HD23	2.21	0.60
1:J:206:ILE:HG13	1:J:207:THR:O	2.01	0.60
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
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: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: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:D:13:THR:HG21	3:D:482:HOH:O	2.12	0.49
1:G:209:GLU:O	1:G:209:GLU:CD	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:146:VAL:HG22	1:G:259:PHE:HZ	1.80	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:192:MET:HE3	1:H:192:MET:H	1.82	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:G:234:LEU:C	1:G:234:LEU:HD23	2.39	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
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: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:J:192:MET:CE	1:J:196:LEU:HD11	2.50	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:C:209:GLU:CD	1:C:209:GLU:H	2.22	0.41
1:L:145:LYS:HD3	1:L:183:MET:HG3	2.02	0.41
1:H:112:ASN:HB2	1:H:157:ALA:HB1	2.01	0.41
1:E:65:GLU:O	1:E:69:GLU:HG3	2.20	0.41
1:A:87:TYR:OH	1:A:115:GLY:HA3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:180:HIS:HD2	1:J:248:GLN:HB2	1.87	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%)	19	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	51	37

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%)	65	52
1	B	202/205 (98%)	201 (100%)	1 (0%)	88	85
1	C	203/205 (99%)	203 (100%)	0	100	100
1	D	203/205 (99%)	202 (100%)	1 (0%)	88	85
1	E	203/205 (99%)	203 (100%)	0	100	100
1	F	205/205 (100%)	202 (98%)	3 (2%)	65	52
1	G	203/205 (99%)	200 (98%)	3 (2%)	65	52
1	H	203/205 (99%)	199 (98%)	4 (2%)	55	40
1	I	203/205 (99%)	201 (99%)	2 (1%)	76	68
1	J	204/205 (100%)	201 (98%)	3 (2%)	65	52
1	K	203/205 (99%)	201 (99%)	2 (1%)	76	68
1	L	201/205 (98%)	198 (98%)	3 (2%)	65	52
All	All	2436/2460 (99%)	2411 (99%)	25 (1%)	76	68

All (25) 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	204	LEU
1	D	37	SER
1	F	91	VAL
1	F	209	GLU
1	F	226	ASP
1	G	48	SER
1	G	142	LYS
1	G	204	LEU
1	H	24	GLN
1	H	192	MET
1	H	202	GLU
1	H	203	LYS
1	I	149	LYS
1	I	207	THR
1	J	129	ARG
1	J	192	MET
1	J	207	THR
1	K	12	GLN
1	K	148	SER
1	L	192	MET
1	L	194	GLN
1	L	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	28	HIS
1	A	40	ASN
1	A	251	ASN
1	B	150	HIS
1	B	180	HIS
1	B	248	GLN
1	B	251	ASN
1	C	186	ASN
1	C	194	GLN
1	D	40	ASN
1	D	186	ASN
1	D	194	GLN
1	E	3	GLN

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Mol	Chain	Res	Type
1	E	12	GLN
1	E	24	GLN
1	E	180	HIS
1	E	251	ASN
1	F	3	GLN
1	F	38	ASN
1	G	3	GLN
1	G	251	ASN
1	H	3	GLN
1	H	24	GLN
1	H	110	GLN
1	H	180	HIS
1	H	194	GLN
1	H	251	ASN
1	I	24	GLN
1	I	99	GLN
1	I	180	HIS
1	I	251	ASN
1	J	180	HIS
1	J	251	ASN
1	K	24	GLN
1	K	150	HIS
1	K	251	ASN
1	L	24	GLN
1	L	166	GLN
1	L	251	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.18	4 (1%) 72 71	18, 31, 60, 80	0
1	B	257/263 (97%)	0.42	18 (7%) 16 14	17, 31, 59, 71	0
1	C	258/263 (98%)	-0.14	0 100 100	15, 23, 42, 58	0
1	D	258/263 (98%)	-0.08	4 (1%) 72 71	15, 23, 48, 77	0
1	E	258/263 (98%)	-0.23	1 (0%) 92 92	15, 23, 40, 60	0
1	F	259/263 (98%)	-0.13	2 (0%) 86 86	14, 22, 49, 73	0
1	G	258/263 (98%)	-0.02	12 (4%) 31 28	14, 23, 60, 93	0
1	H	258/263 (98%)	-0.17	2 (0%) 86 86	15, 22, 44, 70	0
1	I	258/263 (98%)	-0.01	2 (0%) 86 86	17, 27, 44, 64	0
1	J	259/263 (98%)	0.06	11 (4%) 36 33	16, 24, 62, 91	0
1	K	258/263 (98%)	0.56	14 (5%) 25 23	22, 35, 66, 91	0
1	L	256/263 (97%)	0.36	12 (4%) 31 28	21, 33, 64, 87	0
All	All	3095/3156 (98%)	0.07	82 (2%) 56 53	14, 27, 54, 93	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	56	TYR	6.3
1	K	204	LEU	6.2
1	G	202	GLU	6.2
1	J	208	PRO	5.6
1	K	53	GLY	5.2
1	L	192	MET	5.0
1	G	204	LEU	4.9
1	K	34	LEU	4.8
1	G	205	GLY	4.7
1	B	53	GLY	4.7
1	J	206	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	42	LEU	4.3
1	F	205	GLY	4.2
1	L	204	LEU	4.2
1	D	204	LEU	4.1
1	L	206	ILE	3.8
1	K	42	LEU	3.8
1	B	57	GLY	3.7
1	B	204	LEU	3.6
1	J	202	GLU	3.6
1	L	207	THR	3.2
1	B	52	ALA	3.2
1	L	202	GLU	3.2
1	G	196	LEU	3.2
1	K	199	GLN	3.1
1	B	50	TYR	3.1
1	B	48	SER	3.0
1	L	91	VAL	3.0
1	B	77	GLU	2.9
1	B	46	ILE	2.9
1	K	91	VAL	2.9
1	J	197	LEU	2.9
1	J	204	LEU	2.9
1	A	204	LEU	2.8
1	D	202	GLU	2.8
1	L	56	TYR	2.8
1	K	207	THR	2.8
1	J	203	LYS	2.7
1	B	198	PRO	2.7
1	G	197	LEU	2.7
1	L	93	LYS	2.7
1	L	201	ALA	2.6
1	B	196	LEU	2.6
1	G	195	SER	2.6
1	I	80	GLY	2.6
1	B	41	ARG	2.6
1	B	54	ARG	2.5
1	J	200	TYR	2.5
1	K	80	GLY	2.5
1	B	55	ALA	2.5
1	K	198	PRO	2.5
1	K	49	ARG	2.5
1	B	202	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	207	THR	2.5
1	B	206	ILE	2.4
1	D	209	GLU	2.4
1	G	191	PRO	2.4
1	K	202	GLU	2.4
1	L	196	LEU	2.4
1	H	207	THR	2.4
1	L	209	GLU	2.3
1	G	208	PRO	2.3
1	B	31	VAL	2.3
1	J	209	GLU	2.3
1	A	91	VAL	2.3
1	I	204	LEU	2.3
1	G	200	TYR	2.2
1	J	201	ALA	2.2
1	J	207	THR	2.2
1	K	13	THR	2.2
1	F	202	GLU	2.2
1	K	52	ALA	2.1
1	A	205	GLY	2.1
1	E	198	PRO	2.1
1	G	214	TYR	2.1
1	H	205	GLY	2.1
1	A	202	GLU	2.1
1	L	205	GLY	2.1
1	G	207	THR	2.1
1	J	210	GLU	2.1
1	G	198	PRO	2.0
1	K	193	PHE	2.0

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 monosaccharides 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	CL	J	301	1/1	0.96	0.14	31,31,31,31	0
2	CL	L	301	1/1	0.96	0.09	33,33,33,33	0
2	CL	K	301	1/1	0.97	0.08	31,31,31,31	0
2	CL	A	301	1/1	0.97	0.10	32,32,32,32	0
2	CL	H	301	1/1	0.98	0.13	23,23,23,23	0
2	CL	B	301	1/1	0.98	0.10	34,34,34,34	0
2	CL	E	301	1/1	0.99	0.14	21,21,21,21	0
2	CL	G	301	1/1	0.99	0.11	26,26,26,26	0
2	CL	C	301	1/1	0.99	0.10	22,22,22,22	0
2	CL	D	301	1/1	1.00	0.13	25,25,25,25	0
2	CL	F	301	1/1	1.00	0.11	24,24,24,24	0
2	CL	I	301	1/1	1.00	0.12	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.