



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 02:34 AM EDT

PDB ID : 3C5Y
Title : Crystal structure of a putative ribose 5-phosphate isomerase (saro_3514) from novosphingobium aromaticivorans dsm at 1.81 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : unknown
Resolution : 1.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

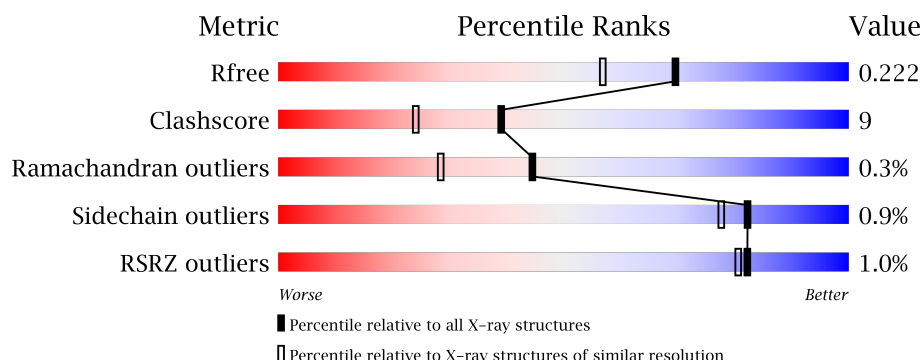
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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}	100719	5868 (1.84-1.80)
Clashscore	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)
RSRZ outliers	101464	5947 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	<div> <div>82%</div> <div>10%</div> <div>9%</div> </div>
1	B	231	<div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	C	231	<div> <div>78%</div> <div>13%</div> <div>8%</div> </div>
1	D	231	<div> <div>77%</div> <div>14%</div> <div>9%</div> </div>
1	E	231	<div> <div>83%</div> <div>10%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	231	
1	G	231	
1	H	231	
1	I	231	
1	J	231	
1	K	231	
1	L	231	
1	M	231	
1	N	231	
1	O	231	
1	P	231	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	213	-	-	-	X
2	EDO	A	215	-	-	-	X
2	EDO	A	217	-	-	-	X
2	EDO	A	219	-	-	-	X
2	EDO	A	220	-	-	-	X
2	EDO	B	216	-	-	-	X
2	EDO	B	217	-	-	-	X
2	EDO	B	218	-	-	-	X
2	EDO	D	214	-	-	-	X
2	EDO	E	215	-	-	X	X
2	EDO	E	216	-	-	-	X
2	EDO	F	217	-	-	-	X
2	EDO	F	219	-	-	-	X
2	EDO	F	220	-	-	-	X
2	EDO	G	216	-	-	-	X
2	EDO	G	218	-	-	-	X
2	EDO	G	221	-	-	-	X
2	EDO	H	216	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	H	217	-	-	-	X
2	EDO	H	218	-	-	-	X
2	EDO	I	217	-	-	-	X
2	EDO	M	216	-	-	-	X
2	EDO	N	215	-	-	-	X
3	NO3	F	213	-	-	-	X
3	NO3	F	215	-	-	-	X
3	NO3	G	213	-	-	-	X
3	NO3	G	214	-	-	-	X
3	NO3	P	213	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28863 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 Ribose/galactose isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	Se	0	6	0
			1630	1037	274	303	4	12			
1	B	212	Total	C	N	O	S	Se	0	3	0
			1612	1024	271	301	4	12			
1	C	212	Total	C	N	O	S	Se	0	6	0
			1625	1034	269	303	4	15			
1	D	211	Total	C	N	O	S	Se	0	4	0
			1605	1020	269	300	4	12			
1	E	215	Total	C	N	O	S	Se	0	3	0
			1652	1046	280	312	4	10			
1	F	213	Total	C	N	O	S	Se	0	4	0
			1634	1035	278	306	4	11			
1	G	211	Total	C	N	O	S	Se	0	4	0
			1622	1029	275	302	4	12			
1	H	214	Total	C	N	O	S	Se	0	6	0
			1663	1059	280	309	4	11			
1	I	212	Total	C	N	O	S	Se	0	5	0
			1633	1036	276	305	4	12			
1	J	212	Total	C	N	O	S	Se	0	3	0
			1618	1025	275	303	4	11			
1	K	212	Total	C	N	O	S	Se	0	3	0
			1615	1024	276	301	4	10			
1	L	213	Total	C	N	O	S	Se	0	3	0
			1616	1026	271	303	4	12			
1	M	212	Total	C	N	O	S	Se	0	4	0
			1616	1025	269	306	4	12			
1	N	212	Total	C	N	O	S	Se	0	5	0
			1616	1029	267	304	4	12			
1	O	211	Total	C	N	O	S	Se	0	3	0
			1568	1001	259	293	4	11			
1	P	211	Total	C	N	O	S	Se	0	2	0
			1597	1012	268	303	4	10			

There are 304 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
A	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
A	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
A	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
A	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
A	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
A	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
A	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
A	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
A	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
A	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
A	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
A	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
A	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
A	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
A	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
A	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
A	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
A	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
B	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
B	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
B	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
B	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
B	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
B	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
B	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
B	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
B	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
B	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
B	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
B	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
B	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
B	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
B	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
B	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
B	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
B	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
B	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
C	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
C	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
C	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
C	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
C	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
C	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
C	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
C	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
C	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
C	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
C	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
C	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
C	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
C	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
C	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
C	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
C	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
C	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
D	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
D	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
D	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
D	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
D	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
D	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
D	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
D	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
D	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
D	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
D	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
D	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
D	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
D	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
D	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
D	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
D	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
D	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
D	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
E	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
E	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
E	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
E	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
E	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
E	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
E	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
E	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
E	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
E	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
E	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
E	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
E	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
E	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
E	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
E	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
E	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
E	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
F	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
F	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
F	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
F	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
F	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
F	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
F	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
F	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
F	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
F	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
F	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
F	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
F	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
F	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
F	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
F	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
F	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
F	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
F	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
G	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
G	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
G	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
G	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
G	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
G	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
G	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
G	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
G	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
G	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
G	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
G	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
G	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
G	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
G	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
G	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
G	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
G	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
H	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
H	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
H	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
H	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
H	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
H	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
H	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
H	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
H	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
H	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
H	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
H	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
H	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
H	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
H	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
H	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
H	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
H	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
H	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
I	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
I	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
I	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
I	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
I	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
I	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
I	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
I	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
I	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
I	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
I	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
I	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
I	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
I	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
I	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
I	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
I	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
I	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
J	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
J	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
J	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
J	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
J	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
J	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
J	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
J	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
J	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
J	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
J	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
J	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
J	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
J	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
J	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
J	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
J	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
J	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
J	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
K	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
K	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
K	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
K	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
K	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
K	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
K	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
K	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
K	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
K	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
K	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
K	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
K	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
K	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
K	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
K	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
K	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
K	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
K	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
L	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
L	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
L	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
L	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
L	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
L	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
L	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
L	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
L	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
L	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
L	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
L	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
L	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
L	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
L	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
L	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
L	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
L	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
M	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
M	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
M	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
M	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
M	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
M	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
M	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
M	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
M	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
M	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
M	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
M	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
M	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
M	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
M	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
M	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
M	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
M	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
M	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
N	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
N	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
N	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
N	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
N	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3

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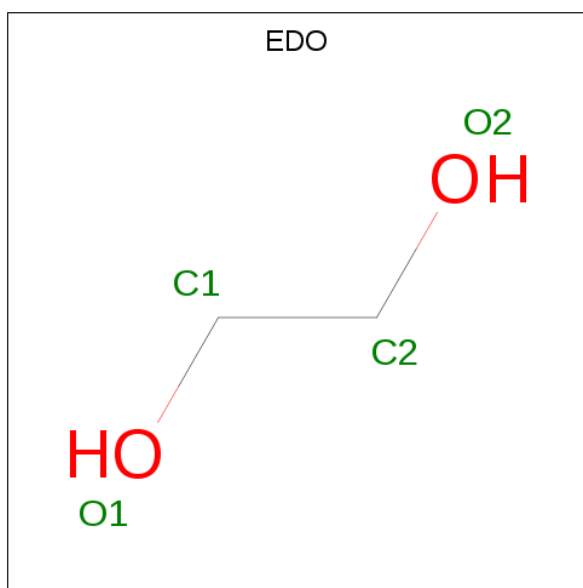
Chain	Residue	Modelled	Actual	Comment	Reference
N	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
N	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
N	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
N	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
N	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
N	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
N	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
N	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
O	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
O	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
O	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
O	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
O	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
O	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
O	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
O	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
O	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
O	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
O	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
O	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
O	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
O	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
O	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
O	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
O	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
O	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
O	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3
P	-18	MSE	-	LEADER SEQUENCE	UNP A4XEL3
P	-17	GLY	-	LEADER SEQUENCE	UNP A4XEL3
P	-16	SER	-	LEADER SEQUENCE	UNP A4XEL3
P	-15	ASP	-	LEADER SEQUENCE	UNP A4XEL3
P	-14	LYS	-	LEADER SEQUENCE	UNP A4XEL3
P	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
P	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
P	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
P	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
P	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
P	-7	HIS	-	LEADER SEQUENCE	UNP A4XEL3
P	-6	GLU	-	LEADER SEQUENCE	UNP A4XEL3
P	-5	ASN	-	LEADER SEQUENCE	UNP A4XEL3
P	-4	LEU	-	LEADER SEQUENCE	UNP A4XEL3
P	-3	TYR	-	LEADER SEQUENCE	UNP A4XEL3
P	-2	PHE	-	LEADER SEQUENCE	UNP A4XEL3
P	-1	GLN	-	LEADER SEQUENCE	UNP A4XEL3
P	0	GLY	-	LEADER SEQUENCE	UNP A4XEL3

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

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

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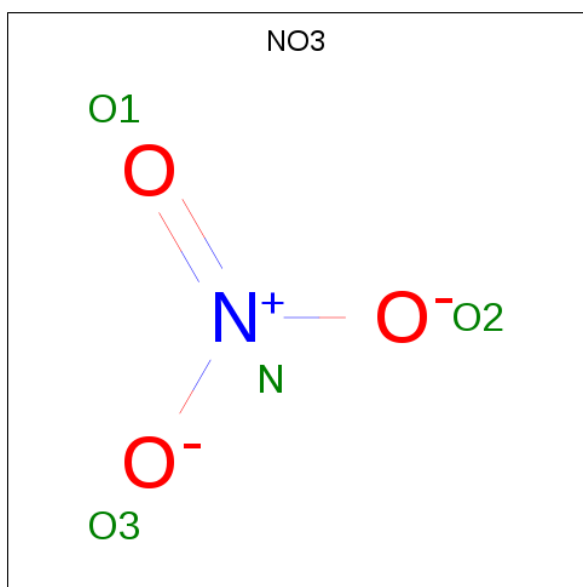
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	I	1	Total 4	C 2	O 2	0	0
2	I	1	Total 4	C 2	O 2	0	0
2	I	1	Total 4	C 2	O 2	0	0
2	I	1	Total 4	C 2	O 2	0	0
2	J	1	Total 4	C 2	O 2	0	0
2	J	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total 4	C 2	O 2	0	0
2	K	1	Total 4	C 2	O 2	0	0
2	K	1	Total 4	C 2	O 2	0	0
2	K	1	Total 4	C 2	O 2	0	0
2	L	1	Total 4	C 2	O 2	0	0
2	M	1	Total 4	C 2	O 2	0	0
2	M	1	Total 4	C 2	O 2	0	0
2	M	1	Total 4	C 2	O 2	0	0
2	M	1	Total 4	C 2	O 2	0	0
2	N	1	Total 4	C 2	O 2	0	0
2	N	1	Total 4	C 2	O 2	0	0
2	N	1	Total 4	C 2	O 2	0	0
2	P	1	Total 4	C 2	O 2	0	0

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	N	O	0	0
			4	1	3		
3	F	1	Total	N	O	0	0
			4	1	3		
3	F	1	Total	N	O	0	0
			4	1	3		
3	F	1	Total	N	O	0	0
			4	1	3		
3	G	1	Total	N	O	0	0
			4	1	3		
3	G	1	Total	N	O	0	0
			4	1	3		
3	I	1	Total	N	O	0	0
			4	1	3		
3	P	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	192	Total	O	0	0
			192	192		
4	B	210	Total	O	0	1
			211	211		
4	C	120	Total	O	0	0
			120	120		
4	D	74	Total	O	0	0
			74	74		

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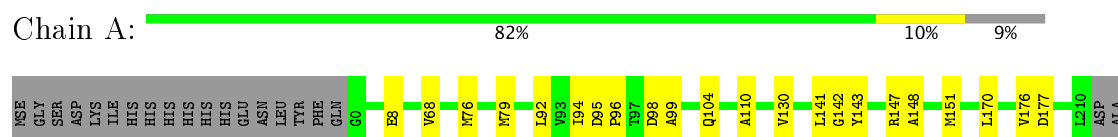
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	233	Total 235	O 235	0	2
4	F	210	Total 212	O 212	0	2
4	G	223	Total 223	O 223	0	0
4	H	203	Total 204	O 204	0	1
4	I	186	Total 187	O 187	0	1
4	J	167	Total 168	O 168	0	1
4	K	153	Total 153	O 153	0	0
4	L	145	Total 146	O 146	0	1
4	M	210	Total 210	O 210	0	0
4	N	141	Total 142	O 142	0	1
4	O	91	Total 91	O 91	0	0
4	P	97	Total 97	O 97	0	0

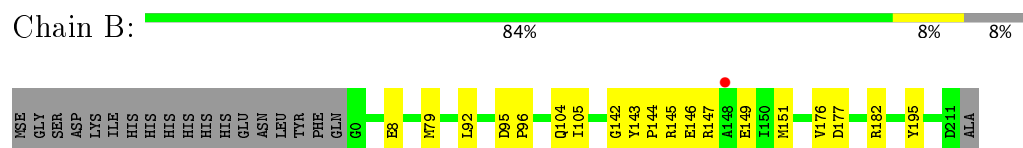
3 Residue-property plots [i](#)

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

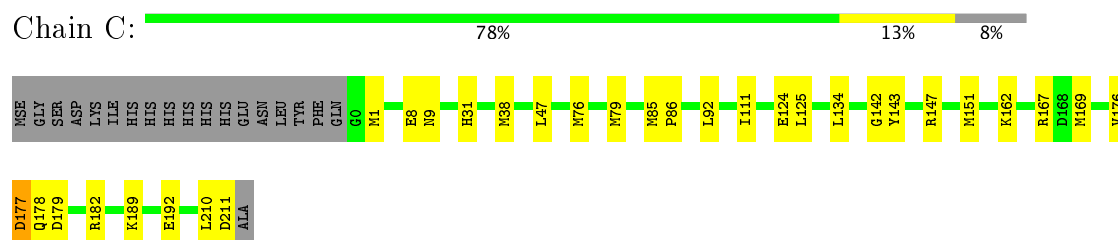
- Molecule 1: Ribose/galactose isomerase



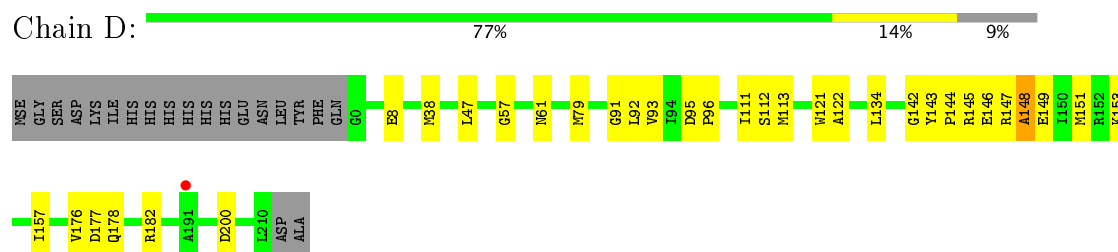
- Molecule 1: Ribose/galactose isomerase



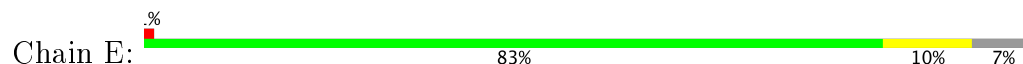
- Molecule 1: Ribose/galactose isomerase

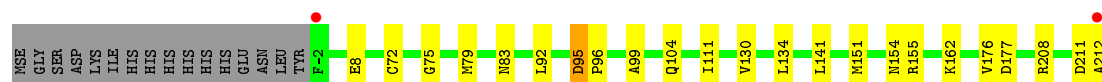


- Molecule 1: Ribose/galactose isomerase

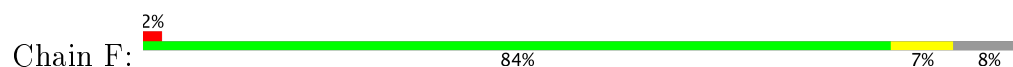


- Molecule 1: Ribose/galactose isomerase

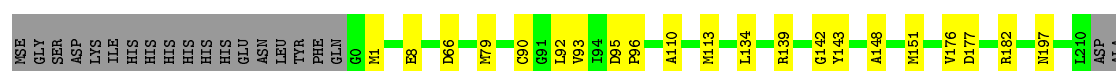




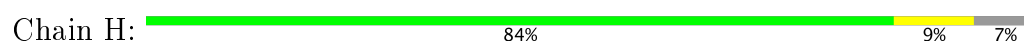
- Molecule 1: Ribose/galactose isomerase



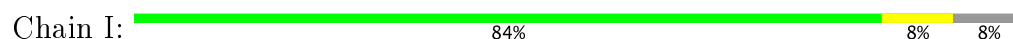
- Molecule 1: Ribose/galactose isomerase



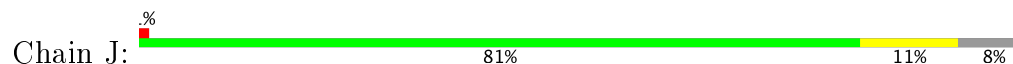
- Molecule 1: Ribose/galactose isomerase



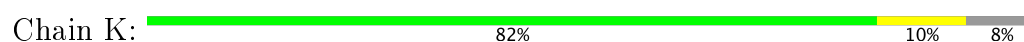
- Molecule 1: Ribose/galactose isomerase



- Molecule 1: Ribose/galactose isomerase

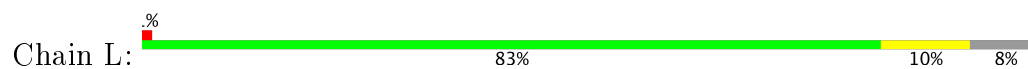


- Molecule 1: Ribose/galactose isomerase

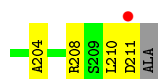
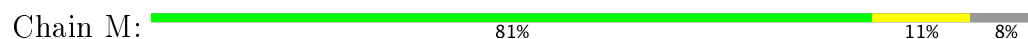




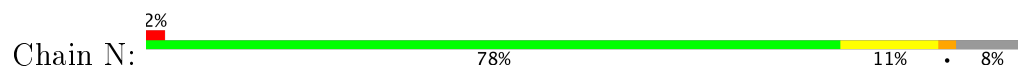
- Molecule 1: Ribose/galactose isomerase



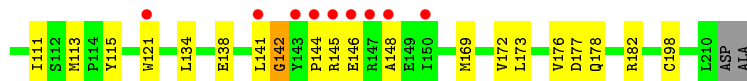
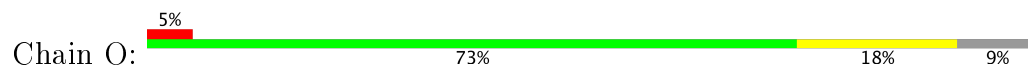
- Molecule 1: Ribose/galactose isomerase



- Molecule 1: Ribose/galactose isomerase



- Molecule 1: Ribose/galactose isomerase



- Molecule 1: Ribose/galactose isomerase



G108	R109	A110	I111	S112	Q128	R132	Y143	E149	I150	M151	R152	I157	K162	S165	L170	K174	I175	V176	D177	Q178	D179	R182	I185	E188	K189	F190	L193	N197	I210	ASP	ALA
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.75Å 109.46Å 167.57Å 90.00° 102.92° 90.00°	Depositor
Resolution (Å)	49.15 – 1.81 49.14 – 1.81	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.15-1.81) 96.9 (49.14-1.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.81Å)	Xtriage
Refinement program	PHENIX, REFMAC 5.4.0067	Depositor
R, R_{free}	0.170 , 0.220 0.176 , 0.222	Depositor DCC
R_{free} test set	16702 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28863	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: CSD, EDO, NO3

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	0.86	0/1657	0.87	0/2217
1	B	0.88	1/1630 (0.1%)	0.88	1/2184 (0.0%)
1	C	0.75	0/1652	0.83	0/2214
1	D	0.71	0/1626	0.86	0/2180
1	E	0.96	0/1671	0.96	3/2238 (0.1%)
1	F	0.91	1/1655 (0.1%)	0.98	3/2217 (0.1%)
1	G	0.91	0/1643	0.90	1/2200 (0.0%)
1	H	0.83	0/1692	0.87	1/2266 (0.0%)
1	I	0.85	0/1657	0.87	0/2219
1	J	0.85	0/1636	0.86	0/2193
1	K	0.73	0/1633	0.82	0/2189
1	L	0.76	0/1634	0.85	0/2189
1	M	0.80	0/1637	0.83	0/2195
1	N	0.70	0/1640	0.91	3/2199 (0.1%)
1	O	0.66	0/1586	0.82	0/2131
1	P	0.66	0/1612	0.84	2/2163 (0.1%)
All	All	0.81	2/26261 (0.0%)	0.87	14/35194 (0.0%)

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	N	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	195	TYR	CD2-CE2	-5.44	1.31	1.39
1	F	195	TYR	CE1-CZ	-5.18	1.31	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	146	GLU	N-CA-C	-13.88	73.52	111.00
1	N	145	ARG	N-CA-C	-8.66	87.60	111.00
1	F	167	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	F	182	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	E	155	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	F	167	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	E	155	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	E	95	ASP	CB-CG-OD1	5.27	123.05	118.30
1	N	145	ARG	O-C-N	-5.27	114.26	122.70
1	P	132	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	P	132	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	182	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	H	117	LYS	CD-CE-NZ	5.06	123.33	111.70
1	G	182	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	145	ARG	Mainchain,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	1630	0	1655	25	0
1	B	1612	0	1618	19	0
1	C	1625	0	1631	54	0
1	D	1605	0	1604	35	0
1	E	1652	0	1649	19	0
1	F	1634	0	1641	15	0
1	G	1622	0	1635	25	0
1	H	1663	0	1673	20	0
1	I	1633	0	1643	20	0
1	J	1618	0	1617	25	0
1	K	1615	0	1617	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1616	0	1616	28	0
1	M	1616	0	1611	26	0
1	N	1616	0	1620	34	0
1	O	1568	0	1551	52	0
1	P	1597	0	1587	37	0
2	A	32	0	48	7	0
2	B	24	0	36	2	0
2	C	8	0	12	3	0
2	D	8	0	12	0	0
2	E	20	0	30	4	0
2	F	24	0	36	5	0
2	G	28	0	42	4	0
2	H	24	0	36	0	0
2	I	16	0	24	0	0
2	J	12	0	18	1	0
2	K	12	0	18	0	0
2	L	4	0	6	0	0
2	M	16	0	24	0	0
2	N	12	0	18	1	0
2	P	4	0	6	0	0
3	F	16	0	0	0	0
3	G	8	0	0	0	0
3	I	4	0	0	0	0
3	P	4	0	0	0	0
4	A	192	0	0	3	0
4	B	211	0	0	3	0
4	C	120	0	0	3	0
4	D	74	0	0	0	0
4	E	235	0	0	0	0
4	F	212	0	0	2	0
4	G	223	0	0	2	0
4	H	204	0	0	1	0
4	I	187	0	0	0	0
4	J	168	0	0	1	0
4	K	153	0	0	0	0
4	L	146	0	0	0	0
4	M	210	0	0	0	0
4	N	142	0	0	1	0
4	O	91	0	0	0	0
4	P	97	0	0	0	0
All	All	28863	0	26334	448	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 9.

All (448) 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:O:54:LEU:HA	1:O:85:MSE:CE	1.35	1.54
1:L:142:GLY:HA2	1:L:151[B]:MSE:CE	1.49	1.43
1:I:142:GLY:CA	1:I:151[B]:MSE:HE1	1.56	1.35
1:O:54:LEU:CD1	1:O:85:MSE:HE1	1.59	1.31
1:O:61:ASN:ND2	1:O:169[B]:MSE:HE3	1.44	1.30
1:C:85[B]:MSE:HE1	1:C:169:MSE:CE	1.61	1.30
1:C:85[B]:MSE:CE	1:C:169:MSE:HE1	1.64	1.26
1:L:142:GLY:CA	1:L:151[B]:MSE:HE1	1.66	1.24
1:C:38[B]:MSE:HE2	1:C:47:LEU:N	1.53	1.22
1:H:142:GLY:CA	1:H:151[A]:MSE:HE1	1.70	1.18
1:N:145:ARG:O	1:N:148:ALA:HB2	1.44	1.16
1:I:142:GLY:HA3	1:I:151[B]:MSE:HE1	1.18	1.14
1:O:54:LEU:HD12	1:O:85:MSE:HE1	1.22	1.12
1:H:142:GLY:HA3	1:H:151[A]:MSE:HE1	1.26	1.12
1:O:86:PRO:HG2	1:O:169[B]:MSE:HE2	1.18	1.12
1:O:86:PRO:HG2	1:O:169[B]:MSE:CE	1.80	1.11
1:N:149:GLU:OE2	1:N:149:GLU:HA	1.45	1.11
1:O:54:LEU:CA	1:O:85:MSE:CE	2.27	1.11
1:L:142:GLY:CA	1:L:151[B]:MSE:CE	2.25	1.11
1:I:148:ALA:HA	1:I:151[B]:MSE:HE2	1.31	1.10
1:O:54:LEU:HA	1:O:85:MSE:HE3	1.27	1.10
1:O:54:LEU:HD12	1:O:85:MSE:CE	1.81	1.10
1:L:105:ILE:HA	1:L:151[B]:MSE:HE3	1.34	1.08
1:C:9:ASN:HB3	1:C:38[B]:MSE:HE1	1.29	1.06
1:C:85[B]:MSE:CE	1:C:169:MSE:SE	2.53	1.06
1:O:54:LEU:CA	1:O:85:MSE:HE2	1.84	1.06
1:C:38[B]:MSE:CE	1:C:47:LEU:H	1.69	1.06
1:N:143:TYR:HA	1:N:144:PRO:O	1.56	1.03
1:E:211:ASP:HB3	1:E:212:ALA:HB2	1.38	1.03
1:N:148:ALA:HA	1:N:151[B]:MSE:HE2	1.36	1.03
1:G:142:GLY:CA	1:G:151[B]:MSE:HE1	1.89	1.02
1:N:1[A]:MSE:SE	1:N:139:ARG:NH2	2.43	1.02
1:C:85[B]:MSE:HE3	1:C:169:MSE:SE	2.10	1.01
1:I:142:GLY:HA3	1:I:151[B]:MSE:CE	1.90	1.01
1:C:85[B]:MSE:CE	1:C:169:MSE:CE	2.30	1.01
1:O:54:LEU:HD13	1:O:85:MSE:HE1	1.42	1.01
1:O:54:LEU:HA	1:O:85:MSE:HE2	1.01	1.00
1:G:142:GLY:HA2	1:G:151[B]:MSE:HE1	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1[A]:MSE:SE	1:N:139:ARG:HH21	1.96	0.98
1:I:142:GLY:CA	1:I:151[B]:MSE:CE	2.42	0.97
1:I:142:GLY:HA2	1:I:151[B]:MSE:HE1	1.47	0.96
1:L:142:GLY:HA2	1:L:151[B]:MSE:HE1	0.97	0.95
1:C:85[B]:MSE:HE1	1:C:169:MSE:HE1	0.97	0.95
1:C:142:GLY:CA	1:C:151[B]:MSE:HE1	1.96	0.95
1:O:86:PRO:CG	1:O:169[B]:MSE:HE2	1.96	0.95
1:C:142:GLY:HA2	1:C:151[B]:MSE:HE1	1.47	0.92
1:N:143:TYR:H	1:N:151[B]:MSE:HE1	1.34	0.92
1:I:79[A]:MSE:SE	1:J:79[A]:MSE:SE	2.90	0.90
1:M:79[A]:MSE:SE	1:N:79[A]:MSE:SE	2.90	0.90
1:H:142:GLY:HA3	1:H:151[A]:MSE:CE	2.02	0.90
1:L:142:GLY:HA2	1:L:151[B]:MSE:HE2	1.54	0.89
1:G:79[A]:MSE:SE	1:H:79[A]:MSE:SE	2.91	0.88
1:C:142:GLY:HA2	1:C:151[B]:MSE:CE	2.03	0.87
1:A:142:GLY:CA	1:A:151[B]:MSE:HE1	2.04	0.87
1:C:142:GLY:CA	1:C:151[B]:MSE:CE	2.52	0.87
1:O:54:LEU:CD1	1:O:85:MSE:CE	2.44	0.87
1:A:79[A]:MSE:SE	1:B:79[A]:MSE:SE	2.91	0.87
1:E:79[A]:MSE:SE	1:F:79[A]:MSE:SE	2.93	0.87
1:A:143:TYR:H	1:A:151[B]:MSE:HE1	1.38	0.86
1:N:145:ARG:O	1:N:148:ALA:CB	2.22	0.85
2:A:215:EDO:H12	4:A:356:HOH:O	1.76	0.85
1:O:61:ASN:HD21	1:O:169[B]:MSE:HE3	1.39	0.84
1:C:85[B]:MSE:HE1	1:C:169:MSE:SE	2.24	0.84
1:P:48:THR:HG23	1:P:51:MSE:HE3	1.60	0.84
1:G:1[B]:MSE:HG2	1:G:66:ASP:HB2	1.59	0.83
1:M:143:TYR:H	1:M:151[B]:MSE:HE1	1.43	0.83
1:C:79[A]:MSE:SE	1:D:79[A]:MSE:SE	2.96	0.83
1:A:143:TYR:N	1:A:151[B]:MSE:HE1	1.93	0.82
1:C:9:ASN:CB	1:C:38[B]:MSE:HE1	2.09	0.82
1:H:142:GLY:HA2	1:H:151[A]:MSE:HE1	1.60	0.82
1:F:13:ALA:HB3	2:F:220:EDO:H21	1.60	0.81
1:A:142:GLY:HA2	1:A:151[B]:MSE:CE	2.10	0.81
1:K:124:GLU:HG2	1:K:125:LEU:HD12	1.62	0.81
1:A:142:GLY:HA2	1:A:151[B]:MSE:HE1	1.60	0.81
1:B:143:TYR:H	1:B:151[B]:MSE:HE1	1.45	0.81
1:C:143:TYR:H	1:C:151[B]:MSE:HE1	1.45	0.81
1:K:79[A]:MSE:SE	1:L:79[A]:MSE:SE	2.99	0.81
1:O:144:PRO:C	1:O:146:GLU:H	1.80	0.80
1:O:79[A]:MSE:SE	1:P:79[A]:MSE:SE	3.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLY:HA2	1:D:151[B]:MSE:HE1	1.63	0.80
1:A:142:GLY:CA	1:A:151[B]:MSE:CE	2.59	0.80
2:A:216:EDO:H11	4:A:400:HOH:O	1.80	0.80
1:M:143:TYR:N	1:M:151[B]:MSE:HE1	1.97	0.80
1:G:148:ALA:HA	1:G:151[B]:MSE:HE2	1.63	0.80
1:L:143:TYR:N	1:L:151[B]:MSE:HE1	1.96	0.80
1:L:142:GLY:CA	1:L:151[B]:MSE:HE2	2.09	0.79
1:F:79[A]:MSE:SE	1:F:92:LEU:HB2	2.32	0.79
1:D:142:GLY:CA	1:D:151[B]:MSE:HE1	2.13	0.79
1:M:210:LEU:O	1:M:211:ASP:HB2	1.82	0.78
1:M:142:GLY:CA	1:M:151[B]:MSE:HE1	2.14	0.78
1:N:143:TYR:CA	1:N:144:PRO:O	2.31	0.78
1:M:143:TYR:O	1:M:151[A]:MSE:HE1	1.84	0.78
1:F:149:GLU:HA	1:F:149:GLU:OE1	1.82	0.77
1:C:143:TYR:N	1:C:151[B]:MSE:HE1	1.99	0.76
1:N:149:GLU:OE2	1:N:149:GLU:CA	2.31	0.76
2:B:217:EDO:H22	4:B:421:HOH:O	1.85	0.76
1:N:171:THR:O	1:N:175:THR:HG23	1.85	0.76
1:J:210:LEU:O	1:J:211:ASP:HB2	1.85	0.76
1:O:54:LEU:CA	1:O:85:MSE:HE3	2.06	0.76
1:L:143:TYR:H	1:L:151[B]:MSE:HE1	1.49	0.76
1:C:178:GLN:O	1:C:182:ARG:HG3	1.87	0.75
1:H:142:GLY:CA	1:H:151[A]:MSE:CE	2.59	0.74
1:H:103:GLY:HA3	1:H:139[A]:ARG:HH21	1.53	0.74
1:N:143:TYR:CD1	1:N:143:TYR:C	2.61	0.73
1:O:86:PRO:CG	1:O:169[B]:MSE:CE	2.60	0.73
1:O:61:ASN:ND2	1:O:169[B]:MSE:CE	2.40	0.73
2:C:214:EDO:C2	4:C:253:HOH:O	2.37	0.72
1:N:143:TYR:N	1:N:151[B]:MSE:HE1	2.05	0.72
1:B:147:ARG:HD3	1:B:151[A]:MSE:HE3	1.72	0.72
1:G:142:GLY:HA2	1:G:151[B]:MSE:CE	2.19	0.71
1:L:147:ARG:HH11	1:L:151[A]:MSE:HE3	1.56	0.71
1:P:176:VAL:HG22	1:P:177:ASP:N	2.06	0.71
1:E:154:ASN:HD22	2:E:215:EDO:H12	1.56	0.70
1:M:176:VAL:HG22	1:M:177:ASP:N	2.06	0.70
2:E:215:EDO:H21	2:F:219:EDO:H12	1.73	0.70
1:O:86:PRO:HD2	1:O:169[B]:MSE:HE1	1.72	0.69
1:O:61:ASN:HD22	1:O:169[B]:MSE:HE3	1.53	0.69
1:G:142:GLY:HA3	1:G:151[B]:MSE:HE1	1.73	0.69
1:C:210:LEU:O	1:C:211:ASP:C	2.31	0.68
1:I:142:GLY:HA2	1:I:151[B]:MSE:CE	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1[B]:MSE:SE	1:J:139:ARG:HH22	2.27	0.68
1:C:9:ASN:N	1:C:38[B]:MSE:HE3	2.08	0.68
1:C:142:GLY:HA3	1:C:151[B]:MSE:CE	2.23	0.68
1:C:85[A]:MSE:HE2	1:C:85[A]:MSE:HA	1.75	0.68
1:L:142:GLY:C	1:L:151[B]:MSE:HE1	2.14	0.68
1:G:176:VAL:HG22	1:G:177:ASP:N	2.09	0.68
1:M:142:GLY:HA2	1:M:151[B]:MSE:HE1	1.77	0.67
1:C:1[A]:MSE:HG3	1:C:31:HIS:CE1	2.30	0.66
1:O:54:LEU:HD12	1:O:85:MSE:HE3	1.75	0.66
1:K:1:MSE:HG3	1:K:31:HIS:CE1	2.31	0.65
1:A:76:MSE:SE	1:A:79[A]:MSE:HE1	2.47	0.64
1:I:1[A]:MSE:HG3	1:I:31:HIS:CE1	2.33	0.64
1:O:79[A]:MSE:SE	1:O:92:LEU:HB2	2.47	0.64
1:P:1:MSE:HG3	1:P:31:HIS:CE1	2.33	0.64
1:P:188:GLU:HG3	1:P:189:LYS:HG2	1.80	0.64
1:P:79[A]:MSE:SE	1:P:92:LEU:HB2	2.48	0.64
2:C:214:EDO:H22	4:C:253:HOH:O	1.97	0.63
1:H:148:ALA:HA	1:H:151[A]:MSE:HE2	1.81	0.63
1:B:105:ILE:HG12	1:B:151[B]:MSE:HE1	1.81	0.63
1:C:147:ARG:O	1:C:151[B]:MSE:HG3	1.99	0.63
1:A:170:LEU:HD23	2:A:216:EDO:H22	1.81	0.62
1:P:170:LEU:HG	1:P:174:LYS:HE3	1.81	0.62
1:M:142:GLY:CA	1:M:151[B]:MSE:CE	2.78	0.61
1:O:86:PRO:CD	1:O:169[B]:MSE:HE1	2.29	0.61
1:C:76[B]:MSE:HE1	1:C:79[B]:MSE:HE1	1.82	0.61
1:D:143:TYR:O	1:D:151[A]:MSE:HE1	2.00	0.61
1:G:142:GLY:CA	1:G:151[B]:MSE:CE	2.73	0.61
1:K:1:MSE:HG3	1:K:31:HIS:ND1	2.16	0.60
1:B:143:TYR:H	1:B:151[B]:MSE:CE	2.15	0.60
1:J:79[A]:MSE:SE	1:J:92:LEU:HB2	2.52	0.60
1:E:154:ASN:HD22	2:E:215:EDO:C1	2.13	0.60
1:M:142:GLY:HA2	1:M:151[B]:MSE:CE	2.32	0.60
1:A:147:ARG:O	1:A:151[B]:MSE:HG3	2.01	0.60
1:J:1[A]:MSE:CE	1:J:139:ARG:HH12	2.15	0.60
1:J:143:TYR:HA	1:J:144:PRO:C	2.21	0.59
1:A:142:GLY:HA3	1:A:151[B]:MSE:CE	2.32	0.59
1:J:1[A]:MSE:HE1	1:J:139:ARG:HH12	1.67	0.59
1:O:144:PRO:C	1:O:146:GLU:N	2.51	0.59
1:C:85[B]:MSE:HE2	1:C:169:MSE:HE1	1.72	0.59
2:G:220:EDO:H21	4:G:383:HOH:O	2.01	0.59
1:C:38[B]:MSE:HE2	1:C:47:LEU:H	0.72	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLU:HG2	1:C:125:LEU:HD12	1.83	0.59
1:P:176:VAL:HG22	1:P:177:ASP:H	1.68	0.59
1:F:143:TYR:CD1	1:F:143:TYR:C	2.76	0.59
1:F:13:ALA:HB3	2:F:220:EDO:C2	2.33	0.58
1:D:143:TYR:H	1:D:151[B]:MSE:HE1	1.68	0.58
1:B:79[A]:MSE:SE	1:B:92:LEU:HB2	2.53	0.58
1:M:103:GLY:HA3	1:M:139:ARG:HH11	1.68	0.58
1:L:172:VAL:O	1:L:176:VAL:HG13	2.04	0.58
1:A:76:MSE:SE	1:A:79[A]:MSE:CE	3.02	0.57
1:D:143:TYR:CD1	1:D:143:TYR:C	2.77	0.57
1:K:124:GLU:HG2	1:K:125:LEU:CD1	2.33	0.57
1:L:142:GLY:HA3	1:L:151[B]:MSE:CE	2.29	0.57
1:P:178:GLN:O	1:P:182:ARG:HG3	2.03	0.57
1:E:151:MSE:HG2	2:E:215:EDO:O1	2.04	0.57
1:F:76:MSE:SE	1:F:92:LEU:HD22	2.55	0.57
1:C:9:ASN:N	1:C:38[B]:MSE:CE	2.68	0.56
1:E:111:ILE:HD13	1:E:134:LEU:HD11	1.86	0.56
1:F:149:GLU:CA	1:F:149:GLU:OE1	2.51	0.56
1:D:143:TYR:H	1:D:151[A]:MSE:SE	2.39	0.56
1:G:134:LEU:O	1:G:139:ARG:NH1	2.39	0.56
1:M:176:VAL:CG2	1:M:177:ASP:N	2.68	0.56
1:D:149:GLU:HA	1:D:149:GLU:OE1	2.06	0.56
1:D:142:GLY:HA2	1:D:151[B]:MSE:CE	2.35	0.55
1:B:105:ILE:HG12	1:B:151[B]:MSE:CE	2.36	0.55
1:O:102:PHE:CZ	1:O:108:GLY:HA3	2.42	0.55
1:I:147:ARG:O	1:I:151[B]:MSE:HG3	2.07	0.55
1:C:86:PRO:HG3	1:C:167:ARG:O	2.07	0.55
1:N:1[B]:MSE:SE	1:N:139:ARG:NH2	2.89	0.54
1:C:38[B]:MSE:CE	1:C:47:LEU:O	2.55	0.54
1:G:93:VAL:O	1:G:113:MSE:HG2	2.08	0.54
1:I:148:ALA:HA	1:I:151[B]:MSE:CE	2.23	0.54
1:A:176:VAL:HG22	1:A:177:ASP:N	2.23	0.54
2:N:215:EDO:H11	4:N:297:HOH:O	2.06	0.54
1:G:1[B]:MSE:CG	1:G:66:ASP:HB2	2.34	0.54
1:H:143:TYR:C	1:H:143:TYR:CD1	2.81	0.54
1:D:79[A]:MSE:SE	1:D:92:LEU:HB2	2.58	0.54
1:C:76[B]:MSE:HE1	1:D:91:GLY:HA2	1.90	0.54
1:P:76:MSE:SE	1:P:79[A]:MSE:CE	3.06	0.53
1:L:143:TYR:CD1	1:L:143:TYR:C	2.82	0.53
1:I:149:GLU:OE1	1:I:149:GLU:HA	2.06	0.53
1:N:105:ILE:HG23	1:N:151[A]:MSE:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:GLY:HA3	1:L:151[B]:MSE:HE2	1.88	0.53
1:O:176:VAL:HG22	1:O:177:ASP:N	2.24	0.53
1:O:54:LEU:CB	1:O:85:MSE:CE	2.86	0.53
1:P:128:GLN:OE1	1:P:132:ARG:NH2	2.41	0.53
1:C:38[A]:MSE:SE	1:C:47:LEU:H	2.40	0.53
1:D:121:TRP:O	1:D:122:ALA:HB3	2.09	0.53
1:J:144:PRO:HG2	1:J:147:ARG:HG3	1.90	0.53
1:N:95:ASP:O	1:N:98:ASP:HB2	2.09	0.53
1:J:149:GLU:HA	1:J:149:GLU:OE1	2.09	0.52
1:P:76:MSE:SE	1:P:79[A]:MSE:HE1	2.59	0.52
1:B:147:ARG:HG2	1:B:147:ARG:O	2.08	0.52
1:K:31:HIS:C	1:K:32:LYS:HD2	2.30	0.52
1:N:147:ARG:O	1:N:151[A]:MSE:CG	2.57	0.52
1:O:50:VAL:HG11	1:P:157:ILE:HG22	1.91	0.52
1:C:76[B]:MSE:SE	1:C:92:LEU:HD22	2.59	0.52
1:G:197:ASN:HD21	2:G:219:EDO:C2	2.23	0.52
1:J:138:GLU:OE1	1:J:141:LEU:HD11	2.09	0.52
2:C:214:EDO:H11	4:C:259:HOH:O	2.10	0.52
1:L:99:ALA:HB2	1:L:130:VAL:HG13	1.92	0.51
1:N:38:MSE:CE	1:N:43:ASP:HB2	2.40	0.51
1:F:134:LEU:O	1:F:139:ARG:NH1	2.43	0.51
1:H:79[A]:MSE:SE	1:H:92:LEU:HB2	2.60	0.51
1:I:142:GLY:C	1:I:151[B]:MSE:HE1	2.26	0.51
1:A:143:TYR:O	1:A:151[A]:MSE:HE1	2.11	0.51
1:D:93:VAL:O	1:D:113:MSE:HG2	2.11	0.51
1:F:176:VAL:HG23	4:F:242:HOH:O	2.11	0.51
1:H:142:GLY:HA2	1:H:151[A]:MSE:CE	2.33	0.51
1:B:105:ILE:HA	1:B:151[B]:MSE:HE3	1.93	0.51
1:B:149:GLU:HA	1:B:149:GLU:OE1	2.09	0.51
2:B:217:EDO:H12	4:H:369:HOH:O	2.10	0.51
1:J:111:ILE:HD13	1:J:134:LEU:HD11	1.93	0.51
1:F:153:LYS:HE2	1:F:157:ILE:HD11	1.93	0.51
1:K:104:GLN:OE1	1:K:141:LEU:HB2	2.11	0.51
1:A:142:GLY:C	1:A:151[B]:MSE:HE1	2.32	0.50
1:C:76[B]:MSE:HE1	1:C:79[B]:MSE:CE	2.41	0.50
1:E:211:ASP:HB3	1:E:212:ALA:CB	2.26	0.50
1:F:17:VAL:HG23	4:F:282:HOH:O	2.09	0.50
1:G:176:VAL:CG2	1:G:177:ASP:N	2.73	0.50
1:G:79[A]:MSE:SE	1:G:92:LEU:HB2	2.60	0.50
1:A:148:ALA:HA	1:A:151[B]:MSE:HE2	1.94	0.50
2:A:217:EDO:H12	4:B:250:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79[A]:MSE:SE	1:C:92:LEU:HB2	2.62	0.50
1:J:1[A]:MSE:HE1	1:J:139:ARG:NH1	2.26	0.50
1:K:143:TYR:CD1	1:K:143:TYR:C	2.84	0.49
1:N:79[A]:MSE:SE	1:N:92:LEU:HB2	2.62	0.49
1:P:176:VAL:CG2	1:P:177:ASP:N	2.72	0.49
1:M:204:ALA:O	1:M:208:ARG:HG3	2.11	0.49
1:O:86:PRO:HD2	1:O:169[B]:MSE:CE	2.43	0.49
1:J:143:TYR:CD1	1:J:143:TYR:C	2.85	0.49
1:K:79[A]:MSE:SE	1:K:92:LEU:HB2	2.62	0.49
1:B:95:ASP:HB2	1:B:96:PRO:CD	2.43	0.49
1:D:147:ARG:O	1:D:151[A]:MSE:HG3	2.13	0.49
1:P:176:VAL:CG2	1:P:177:ASP:H	2.26	0.49
1:N:121:TRP:O	1:N:122:ALA:HB3	2.13	0.49
2:A:215:EDO:C1	4:A:356:HOH:O	2.49	0.49
1:O:86:PRO:CD	1:O:169[B]:MSE:CE	2.89	0.49
1:P:1:MSE:HG3	1:P:31:HIS:ND1	2.28	0.49
1:B:143:TYR:O	1:B:151[A]:MSE:HE1	2.13	0.48
1:E:208:ARG:O	1:E:211:ASP:HB2	2.13	0.48
1:H:149:GLU:OE2	1:H:152:ARG:NH1	2.45	0.48
1:N:143:TYR:HA	1:N:144:PRO:C	2.21	0.48
1:C:142:GLY:C	1:C:151[B]:MSE:HE1	2.33	0.48
1:D:142:GLY:CA	1:D:151[B]:MSE:CE	2.90	0.48
1:L:79[A]:MSE:SE	1:L:92:LEU:HB2	2.64	0.48
1:G:197:ASN:HD21	2:G:219:EDO:H12	1.78	0.48
1:H:122:ALA:HB1	1:H:125:LEU:HD22	1.96	0.48
1:P:102:PHE:CZ	1:P:108:GLY:HA3	2.49	0.48
1:D:144:PRO:C	1:D:146:GLU:H	2.17	0.48
1:I:79[A]:MSE:SE	1:I:92:LEU:HB2	2.64	0.48
1:P:193:LEU:O	1:P:197:ASN:ND2	2.29	0.48
1:P:57:GLY:O	1:P:61:ASN:HB2	2.13	0.48
1:P:149:GLU:OE2	1:P:152:ARG:NH1	2.46	0.48
1:O:178:GLN:O	1:O:182:ARG:HG3	2.14	0.48
1:M:79[A]:MSE:SE	1:M:92:LEU:HB2	2.64	0.47
1:H:143:TYR:HA	1:H:144:PRO:C	2.35	0.47
1:J:210:LEU:O	1:J:211:ASP:CB	2.53	0.47
1:N:143:TYR:C	1:N:143:TYR:HD1	2.17	0.47
1:O:104:GLN:O	1:O:142:GLY:HA2	2.14	0.47
1:C:142:GLY:HA3	1:C:151[B]:MSE:HE2	1.96	0.47
1:A:143:TYR:C	1:A:143:TYR:CD1	2.88	0.47
1:E:72:CSD:OD1	1:E:75:GLY:N	2.41	0.47
1:C:124:GLU:HG2	1:C:125:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:TYR:HA	1:D:144:PRO:C	2.34	0.47
1:N:38:MSE:HE3	1:N:43:ASP:HB2	1.96	0.47
1:C:189:LYS:HD2	1:C:192:GLU:OE1	2.14	0.47
1:D:178:GLN:O	1:D:182:ARG:HG3	2.15	0.47
1:K:176:VAL:HG22	1:K:177:ASP:N	2.29	0.47
1:O:93:VAL:O	1:O:113:MSE:HG2	2.14	0.47
1:D:143:TYR:N	1:D:151[B]:MSE:HE1	2.29	0.47
1:O:57:GLY:O	1:O:61:ASN:HB2	2.14	0.47
1:D:148:ALA:HA	1:D:151[B]:MSE:HE2	1.97	0.47
1:G:142:GLY:HA3	1:G:151[B]:MSE:CE	2.41	0.46
1:C:38[B]:MSE:HE2	1:C:47:LEU:CA	2.37	0.46
1:K:125:LEU:N	1:K:125:LEU:CD1	2.79	0.46
1:C:176:VAL:HG22	1:C:177:ASP:N	2.31	0.46
1:E:176:VAL:HG22	1:E:177:ASP:N	2.31	0.46
1:A:68:VAL:O	1:A:110:ALA:HA	2.15	0.46
1:G:176:VAL:HG23	4:G:259:HOH:O	2.15	0.46
1:C:111:ILE:HD13	1:C:134:LEU:CD1	2.46	0.46
1:D:92:LEU:HD12	1:D:112:SER:O	2.15	0.46
1:N:102:PHE:CZ	1:N:108:GLY:HA3	2.50	0.46
1:C:9:ASN:CA	1:C:38[B]:MSE:HE1	2.45	0.46
1:J:188:GLU:HG3	1:J:189:LYS:HG2	1.98	0.46
1:K:134:LEU:O	1:K:139[A]:ARG:NH1	2.49	0.46
1:N:150:ILE:HG22	1:N:154:ASN:ND2	2.30	0.46
1:G:143:TYR:CD1	1:G:143:TYR:C	2.88	0.46
1:N:176:VAL:HG22	1:N:177:ASP:N	2.30	0.46
2:A:217:EDO:H11	4:B:278:HOH:O	2.16	0.46
1:A:147:ARG:HE	2:A:217:EDO:H21	1.80	0.46
1:K:27:GLU:HB2	1:K:28:PRO:HD3	1.98	0.45
1:M:116[A]:SER:HB3	1:O:121:TRP:HB2	1.98	0.45
1:P:12:ALA:CB	1:P:38:MSE:HE2	2.46	0.45
1:E:95:ASP:HB2	1:E:96:PRO:CD	2.46	0.45
1:K:86:PRO:HG3	1:K:167:ARG:O	2.16	0.45
1:P:38:MSE:SE	1:P:47:LEU:H	2.49	0.45
1:E:83:ASN:O	1:E:162:LYS:NZ	2.36	0.45
1:G:95:ASP:HB2	1:G:96:PRO:CD	2.46	0.45
1:H:122:ALA:O	1:H:125:LEU:HB2	2.16	0.45
1:H:111:ILE:HD13	1:H:134:LEU:HD11	1.99	0.45
1:M:85:MSE:HE2	1:M:85:MSE:HA	1.99	0.45
1:O:11:GLN:NE2	1:O:73:GLY:HA2	2.32	0.45
1:B:95:ASP:HB2	1:B:96:PRO:HD2	1.98	0.45
1:E:104:GLN:OE1	1:E:141:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:MSE:HE2	2:F:219:EDO:H22	1.98	0.45
1:P:189:LYS:O	1:P:193:LEU:HG	2.17	0.45
1:P:177:ASP:C	1:P:177:ASP:OD1	2.55	0.45
1:A:142:GLY:HA2	1:A:151[B]:MSE:HE3	1.97	0.45
1:I:95:ASP:HB2	1:I:96:PRO:CD	2.47	0.45
1:L:1[A]:MSE:SE	1:L:31:HIS:CE1	3.19	0.45
1:L:85:MSE:HE2	1:L:85:MSE:HA	1.99	0.45
1:N:147:ARG:O	1:N:151[A]:MSE:HG3	2.17	0.45
1:O:121:TRP:HA	1:O:121:TRP:CE3	2.51	0.45
1:A:79[A]:MSE:SE	1:A:92:LEU:HB2	2.67	0.45
1:J:149:GLU:CA	1:J:149:GLU:OE1	2.65	0.45
1:K:38:MSE:HE3	1:K:43:ASP:HB2	1.99	0.45
1:A:104:GLN:OE1	1:A:141:LEU:HB2	2.17	0.44
1:F:143:TYR:HD1	1:F:143:TYR:C	2.20	0.44
1:L:147:ARG:NH1	1:L:151[A]:MSE:HE3	2.27	0.44
1:O:85:MSE:SE	1:O:169[A]:MSE:HE1	2.68	0.44
1:C:189:LYS:HD3	1:C:189:LYS:HA	1.62	0.44
1:D:176:VAL:HG22	1:D:177:ASP:N	2.32	0.44
1:D:57:GLY:O	1:D:61:ASN:HB2	2.17	0.44
1:M:142:GLY:C	1:M:151[B]:MSE:HE1	2.37	0.44
1:E:151:MSE:HE2	2:F:219:EDO:C2	2.46	0.44
1:J:148:ALA:HB3	4:J:285:HOH:O	2.18	0.44
1:M:95:ASP:HB2	1:M:96:PRO:CD	2.47	0.44
1:O:62:SER:HB2	1:O:198:CYS:SG	2.58	0.44
1:A:94:ILE:HB	1:A:98:ASP:OD2	2.17	0.44
1:N:111:ILE:HD13	1:N:134:LEU:HD11	1.99	0.44
1:N:143:TYR:CD1	1:N:144:PRO:N	2.85	0.44
1:P:70:THR:HG23	1:P:71:GLY:N	2.32	0.44
1:C:85[B]:MSE:HE2	1:C:169:MSE:CE	2.37	0.44
1:D:95:ASP:HB2	1:D:96:PRO:CD	2.47	0.44
1:J:143:TYR:HA	1:J:145:ARG:N	2.32	0.44
1:P:143:TYR:O	1:P:151:MSE:HE1	2.18	0.44
1:P:170:LEU:O	1:P:174:LYS:HG3	2.18	0.44
1:P:185:ILE:HG22	1:P:190:PHE:CE1	2.53	0.44
1:M:142:GLY:HA3	1:M:151[B]:MSE:CE	2.48	0.44
1:C:76[B]:MSE:CE	1:C:79[B]:MSE:CE	2.96	0.44
1:E:79[A]:MSE:HE1	1:F:91:GLY:HA2	2.00	0.44
1:P:27:GLU:HB2	1:P:28:PRO:HD3	1.99	0.44
1:J:170:LEU:HD23	2:J:214:EDO:H22	1.99	0.44
1:L:95:ASP:HB2	1:L:96:PRO:CD	2.48	0.44
1:H:128:GLN:O	1:H:132[A]:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ILE:HD13	1:D:134:LEU:CD1	2.47	0.43
1:K:79[B]:MSE:SE	1:L:79[B]:MSE:SE	3.36	0.43
1:N:148:ALA:HA	1:N:151[A]:MSE:SE	2.68	0.43
1:O:111:ILE:HD13	1:O:134:LEU:CD1	2.49	0.43
1:P:85:MSE:O	1:P:162:LYS:HE2	2.18	0.43
1:B:144:PRO:HD2	1:B:147:ARG:HB3	1.99	0.43
1:M:38:MSE:HE3	1:M:43:ASP:HB2	1.99	0.43
1:O:14:LYS:HE2	1:O:115:TYR:O	2.18	0.43
1:B:144:PRO:O	1:B:146:GLU:N	2.51	0.43
1:M:111:ILE:HD13	1:M:134:LEU:HD11	2.01	0.43
1:M:148:ALA:HA	1:M:151[B]:MSE:HE2	2.01	0.43
1:O:95:ASP:HB2	1:O:96:PRO:CD	2.48	0.43
1:J:1[A]:MSE:CE	1:J:139:ARG:NH1	2.81	0.43
1:B:147:ARG:HD3	1:B:151[A]:MSE:CE	2.44	0.43
1:O:27:GLU:HB2	1:O:28:PRO:HD3	2.01	0.43
1:D:111:ILE:HD13	1:D:134:LEU:HD11	2.00	0.43
1:E:99:ALA:HB2	1:E:130:VAL:HG13	2.00	0.43
1:E:79[A]:MSE:SE	1:E:92:LEU:HB2	2.68	0.43
1:O:138:GLU:CB	1:O:141:LEU:HD11	2.49	0.43
1:D:153:LYS:O	1:D:157:ILE:HG12	2.19	0.43
1:I:143:TYR:N	1:I:151[B]:MSE:HE1	2.34	0.43
1:J:102:PHE:CZ	1:J:108:GLY:HA3	2.54	0.43
1:J:83:ASN:O	1:J:162:LYS:NZ	2.48	0.43
1:M:99:ALA:HB2	1:M:130:VAL:HG13	2.01	0.42
1:O:146:GLU:C	1:O:148:ALA:H	2.23	0.42
1:J:1[B]:MSE:SE	1:J:139:ARG:HH12	2.52	0.42
1:L:94:ILE:HB	1:L:98:ASP:OD2	2.18	0.42
1:G:197:ASN:HD21	2:G:219:EDO:C1	2.32	0.42
1:H:-2:PHE:HB2	1:H:30:GLY:O	2.19	0.42
1:A:99:ALA:HB2	1:A:130:VAL:HG13	2.01	0.42
1:D:38:MSE:SE	1:D:47:LEU:H	2.53	0.42
1:D:95:ASP:HB2	1:D:96:PRO:HD2	2.00	0.42
1:E:177:ASP:OD1	1:E:177:ASP:C	2.57	0.42
1:N:148:ALA:HA	1:N:151[A]:MSE:HG3	2.01	0.42
1:P:68:VAL:O	1:P:110:ALA:HA	2.19	0.42
1:B:176:VAL:HG22	1:B:177:ASP:N	2.34	0.42
1:G:176:VAL:HG22	1:G:177:ASP:H	1.82	0.42
1:L:79[B]:MSE:HE3	1:L:79[B]:MSE:HB3	1.85	0.42
1:D:147:ARG:O	1:D:151[B]:MSE:HG3	2.19	0.42
1:C:79[B]:MSE:SE	1:D:79[B]:MSE:SE	3.38	0.42
1:G:79[B]:MSE:SE	1:H:79[B]:MSE:SE	3.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:68:VAL:O	1:J:110:ALA:HA	2.19	0.42
1:N:145:ARG:O	1:N:148:ALA:N	2.53	0.42
1:O:144:PRO:O	1:O:146:GLU:N	2.52	0.42
1:L:105:ILE:CA	1:L:151[B]:MSE:HE3	2.25	0.42
1:I:134:LEU:O	1:I:139[A]:ARG:CZ	2.68	0.42
1:K:125:LEU:N	1:K:125:LEU:HD12	2.35	0.42
1:I:143:TYR:C	1:I:143:TYR:CD1	2.93	0.41
1:P:12:ALA:HB2	1:P:38:MSE:HE2	2.02	0.41
1:O:76:MSE:SE	1:O:92:LEU:HD22	2.70	0.41
1:M:111:ILE:HD13	1:M:134:LEU:CD1	2.49	0.41
1:B:144:PRO:O	1:B:147:ARG:N	2.50	0.41
1:C:9:ASN:CA	1:C:38[B]:MSE:CE	2.98	0.41
1:G:90:CYS:HA	1:G:110:ALA:O	2.21	0.41
1:P:177:ASP:OD1	1:P:179:ASP:N	2.46	0.41
1:I:86:PRO:HG3	1:I:167:ARG:O	2.20	0.41
1:A:95:ASP:HB2	1:A:96:PRO:CD	2.51	0.41
1:O:172:VAL:HG22	1:P:165:SER:HA	2.02	0.41
1:P:76:MSE:SE	1:P:79[A]:MSE:HE2	2.71	0.41
1:C:142:GLY:HA2	1:C:151[B]:MSE:HE3	1.96	0.41
1:G:95:ASP:HB2	1:G:96:PRO:HD2	2.02	0.41
1:L:93:VAL:O	1:L:113:MSE:HG2	2.21	0.41
1:O:176:VAL:CG2	1:O:177:ASP:N	2.82	0.41
1:F:176:VAL:HG22	1:F:177:ASP:N	2.35	0.41
1:P:92:LEU:HD12	1:P:112:SER:O	2.20	0.41
1:C:79[A]:MSE:HE1	1:D:91:GLY:HA2	2.02	0.41
1:M:210:LEU:O	1:M:211:ASP:CB	2.60	0.41
1:N:138:GLU:HB2	1:N:141:LEU:HD11	2.02	0.41
1:K:79[A]:MSE:HE1	1:L:91:GLY:HA2	2.02	0.40
1:M:79[B]:MSE:SE	1:M:83:ASN:HD22	2.54	0.40
1:C:177:ASP:OD1	1:C:179:ASP:N	2.52	0.40
1:D:149:GLU:CA	1:D:149:GLU:OE1	2.68	0.40
1:P:8:GLU:OE2	1:P:10:SER:OG	2.37	0.40
1:D:200:ASP:OD1	1:D:200:ASP:C	2.60	0.40
1:I:143:TYR:HA	1:I:144:PRO:C	2.42	0.40
1:K:188:GLU:HG3	1:K:189:LYS:HG2	2.03	0.40
1:B:104:GLN:O	1:B:142:GLY:HA2	2.21	0.40
1:D:144:PRO:C	1:D:146:GLU:N	2.75	0.40
1:J:138:GLU:CB	1:J:141:LEU:HD11	2.52	0.40

There are no symmetry-related clashes.

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	214/231 (93%)	211 (99%)	3 (1%)	0	100	100
1	B	212/231 (92%)	209 (99%)	2 (1%)	1 (0%)	32	17
1	C	215/231 (93%)	211 (98%)	4 (2%)	0	100	100
1	D	212/231 (92%)	206 (97%)	4 (2%)	2 (1%)	20	6
1	E	215/231 (93%)	212 (99%)	3 (1%)	0	100	100
1	F	214/231 (93%)	210 (98%)	4 (2%)	0	100	100
1	G	212/231 (92%)	209 (99%)	3 (1%)	0	100	100
1	H	217/231 (94%)	212 (98%)	5 (2%)	0	100	100
1	I	214/231 (93%)	212 (99%)	2 (1%)	0	100	100
1	J	212/231 (92%)	207 (98%)	4 (2%)	1 (0%)	32	17
1	K	212/231 (92%)	209 (99%)	3 (1%)	0	100	100
1	L	213/231 (92%)	209 (98%)	4 (2%)	0	100	100
1	M	213/231 (92%)	209 (98%)	4 (2%)	0	100	100
1	N	214/231 (93%)	206 (96%)	5 (2%)	3 (1%)	13	3
1	O	211/231 (91%)	206 (98%)	3 (1%)	2 (1%)	20	6
1	P	210/231 (91%)	204 (97%)	6 (3%)	0	100	100
All	All	3410/3696 (92%)	3342 (98%)	59 (2%)	9 (0%)	44	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	147	ARG
1	B	145	ARG
1	J	148	ALA
1	D	145	ARG
1	D	148	ALA
1	N	145	ARG

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Mol	Chain	Res	Type
1	O	145	ARG
1	O	142	GLY
1	N	144	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	168/171 (98%)	167 (99%)	1 (1%)	89	86
1	B	164/171 (96%)	163 (99%)	1 (1%)	89	86
1	C	166/171 (97%)	164 (99%)	2 (1%)	75	69
1	D	162/171 (95%)	161 (99%)	1 (1%)	89	86
1	E	168/171 (98%)	167 (99%)	1 (1%)	89	86
1	F	167/171 (98%)	165 (99%)	2 (1%)	75	69
1	G	166/171 (97%)	165 (99%)	1 (1%)	89	86
1	H	170/171 (99%)	169 (99%)	1 (1%)	89	86
1	I	167/171 (98%)	165 (99%)	2 (1%)	75	69
1	J	164/171 (96%)	163 (99%)	1 (1%)	89	86
1	K	163/171 (95%)	162 (99%)	1 (1%)	89	86
1	L	163/171 (95%)	162 (99%)	1 (1%)	89	86
1	M	165/171 (96%)	164 (99%)	1 (1%)	89	86
1	N	165/171 (96%)	160 (97%)	5 (3%)	46	29
1	O	155/171 (91%)	154 (99%)	1 (1%)	89	86
1	P	162/171 (95%)	161 (99%)	1 (1%)	89	86
All	All	2635/2736 (96%)	2612 (99%)	23 (1%)	82	77

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU

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Mol	Chain	Res	Type
1	B	8	GLU
1	C	8	GLU
1	C	177	ASP
1	D	8	GLU
1	E	8	GLU
1	F	8	GLU
1	F	149	GLU
1	G	8	GLU
1	H	8	GLU
1	I	8	GLU
1	I	146	GLU
1	J	8	GLU
1	K	8	GLU
1	L	8	GLU
1	M	8	GLU
1	N	8	GLU
1	N	143	TYR
1	N	149	GLU
1	N	151[A]	MSE
1	N	151[B]	MSE
1	O	8	GLU
1	P	8	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	154	ASN
1	G	197	ASN
1	K	11	GLN
1	L	11	GLN
1	O	11	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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$
1	CSD	A	72	1	4,7,8	1.04	0	2,8,10	1.59	1 (50%)
1	CSD	B	72	1	4,7,8	1.03	0	2,8,10	1.12	0
1	CSD	C	72	1	4,7,8	1.12	0	2,8,10	3.71	1 (50%)
1	CSD	D	72	1	4,7,8	1.18	0	2,8,10	2.41	1 (50%)
1	CSD	E	72	1	4,7,8	0.90	0	2,8,10	2.08	1 (50%)
1	CSD	F	72	1	4,7,8	0.90	0	2,8,10	1.39	0
1	CSD	G	72	1	4,7,8	1.29	1 (25%)	2,8,10	1.77	1 (50%)
1	CSD	H	72	1	4,7,8	0.88	0	2,8,10	1.32	0
1	CSD	I	72	1	4,7,8	0.70	0	2,8,10	1.80	0
1	CSD	J	72	1	4,7,8	0.70	0	2,8,10	1.29	0
1	CSD	K	72	1	4,7,8	0.80	0	2,8,10	1.33	0
1	CSD	L	72	1	4,7,8	1.17	0	2,8,10	2.71	1 (50%)
1	CSD	M	72	1	4,7,8	0.88	0	2,8,10	1.49	1 (50%)
1	CSD	N	72	1	4,7,8	0.96	0	2,8,10	1.97	1 (50%)
1	CSD	O	72	1	4,7,8	0.97	0	2,8,10	1.35	0
1	CSD	P	72	1	4,7,8	0.97	0	2,8,10	1.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	72	1	-	0/2/6/8	0/0/0/0
1	CSD	B	72	1	-	0/2/6/8	0/0/0/0
1	CSD	C	72	1	-	0/2/6/8	0/0/0/0
1	CSD	D	72	1	-	0/2/6/8	0/0/0/0
1	CSD	E	72	1	-	0/2/6/8	0/0/0/0
1	CSD	F	72	1	-	0/2/6/8	0/0/0/0
1	CSD	G	72	1	-	0/2/6/8	0/0/0/0
1	CSD	H	72	1	-	0/2/6/8	0/0/0/0
1	CSD	I	72	1	-	0/2/6/8	0/0/0/0
1	CSD	J	72	1	-	0/2/6/8	0/0/0/0
1	CSD	K	72	1	-	0/2/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	L	72	1	-	0/2/6/8	0/0/0/0
1	CSD	M	72	1	-	0/2/6/8	0/0/0/0
1	CSD	N	72	1	-	0/2/6/8	0/0/0/0
1	CSD	O	72	1	-	0/2/6/8	0/0/0/0
1	CSD	P	72	1	-	0/2/6/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	72	CSD	CA-N	-2.00	1.41	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	CSD	O-C-CA	-2.15	119.07	125.02
1	M	72	CSD	O-C-CA	-2.06	119.32	125.02
1	G	72	CSD	OD1-SG-CB	2.11	109.56	105.61
1	N	72	CSD	OD1-SG-CB	2.13	109.61	105.61
1	E	72	CSD	OD1-SG-CB	2.90	111.04	105.61
1	D	72	CSD	OD1-SG-CB	3.01	111.25	105.61
1	L	72	CSD	OD1-SG-CB	3.55	112.26	105.61
1	C	72	CSD	OD1-SG-CB	5.01	114.99	105.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	72	CSD	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

69 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	EDO	A	213	-	3,3,3	0.31	0	2,2,2	0.50	0
2	EDO	A	214	-	3,3,3	0.54	0	2,2,2	0.47	0
2	EDO	A	215	-	3,3,3	0.39	0	2,2,2	0.52	0
2	EDO	A	216	-	3,3,3	0.69	0	2,2,2	0.67	0
2	EDO	A	217	-	3,3,3	0.28	0	2,2,2	0.49	0
2	EDO	A	218	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	A	219	-	3,3,3	0.42	0	2,2,2	0.48	0
2	EDO	A	220	-	3,3,3	0.60	0	2,2,2	0.32	0
2	EDO	B	213	-	3,3,3	0.16	0	2,2,2	0.81	0
2	EDO	B	214	-	3,3,3	0.42	0	2,2,2	0.46	0
2	EDO	B	215	-	3,3,3	0.60	0	2,2,2	0.31	0
2	EDO	B	216	-	3,3,3	0.45	0	2,2,2	0.38	0
2	EDO	B	217	-	3,3,3	0.43	0	2,2,2	0.16	0
2	EDO	B	218	-	3,3,3	0.60	0	2,2,2	0.18	0
2	EDO	C	213	-	3,3,3	0.45	0	2,2,2	0.71	0
2	EDO	C	214	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	D	213	-	3,3,3	0.64	0	2,2,2	0.40	0
2	EDO	D	214	-	3,3,3	0.41	0	2,2,2	0.51	0
2	EDO	E	213	-	3,3,3	0.40	0	2,2,2	0.48	0
2	EDO	E	214	-	3,3,3	0.36	0	2,2,2	0.56	0
2	EDO	E	215	-	3,3,3	0.26	0	2,2,2	0.84	0
2	EDO	E	216	-	3,3,3	0.48	0	2,2,2	0.38	0
2	EDO	E	217	-	3,3,3	0.42	0	2,2,2	0.40	0
3	NO3	F	213	-	1,3,3	3.66	1 (100%)	0,3,3	0.00	-
3	NO3	F	214	-	1,3,3	4.55	1 (100%)	0,3,3	0.00	-
3	NO3	F	215	-	1,3,3	2.78	1 (100%)	0,3,3	0.00	-
3	NO3	F	216	-	1,3,3	4.70	1 (100%)	0,3,3	0.00	-
2	EDO	F	217	-	3,3,3	0.36	0	2,2,2	0.32	0
2	EDO	F	218	-	3,3,3	0.28	0	2,2,2	0.66	0
2	EDO	F	219	-	3,3,3	0.38	0	2,2,2	0.53	0
2	EDO	F	220	-	3,3,3	0.47	0	2,2,2	0.03	0
2	EDO	F	221	-	3,3,3	0.50	0	2,2,2	0.37	0
2	EDO	F	222	-	3,3,3	0.51	0	2,2,2	0.23	0
3	NO3	G	213	-	1,3,3	4.76	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NO3	G	214	-	1,3,3	3.31	1 (100%)	0,3,3	0.00	-
2	EDO	G	215	-	3,3,3	0.36	0	2,2,2	0.76	0
2	EDO	G	216	-	3,3,3	0.39	0	2,2,2	0.49	0
2	EDO	G	217	-	3,3,3	0.41	0	2,2,2	0.69	0
2	EDO	G	218	-	3,3,3	0.59	0	2,2,2	0.19	0
2	EDO	G	219	-	3,3,3	0.64	0	2,2,2	0.08	0
2	EDO	G	220	-	3,3,3	0.61	0	2,2,2	0.10	0
2	EDO	G	221	-	3,3,3	0.64	0	2,2,2	0.17	0
2	EDO	H	213	-	3,3,3	0.51	0	2,2,2	0.36	0
2	EDO	H	214	-	3,3,3	0.68	0	2,2,2	0.20	0
2	EDO	H	215	-	3,3,3	0.57	0	2,2,2	0.15	0
2	EDO	H	216	-	3,3,3	0.47	0	2,2,2	0.77	0
2	EDO	H	217	-	3,3,3	0.36	0	2,2,2	0.75	0
2	EDO	H	218	-	3,3,3	0.48	0	2,2,2	0.21	0
3	NO3	I	213	-	1,3,3	4.86	1 (100%)	0,3,3	0.00	-
2	EDO	I	214	-	3,3,3	0.31	0	2,2,2	0.08	0
2	EDO	I	215	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	I	216	-	3,3,3	0.39	0	2,2,2	0.20	0
2	EDO	I	217	-	3,3,3	0.33	0	2,2,2	0.67	0
2	EDO	J	213	-	3,3,3	0.49	0	2,2,2	0.34	0
2	EDO	J	214	-	3,3,3	0.45	0	2,2,2	0.24	0
2	EDO	J	215	-	3,3,3	0.50	0	2,2,2	0.05	0
2	EDO	K	213	-	3,3,3	0.36	0	2,2,2	0.36	0
2	EDO	K	214	-	3,3,3	0.50	0	2,2,2	0.42	0
2	EDO	K	215	-	3,3,3	0.44	0	2,2,2	0.23	0
2	EDO	L	213	-	3,3,3	0.38	0	2,2,2	0.55	0
2	EDO	M	213	-	3,3,3	0.48	0	2,2,2	0.29	0
2	EDO	M	214	-	3,3,3	0.41	0	2,2,2	0.49	0
2	EDO	M	215	-	3,3,3	0.58	0	2,2,2	0.08	0
2	EDO	M	216	-	3,3,3	0.69	0	2,2,2	0.03	0
2	EDO	N	213	-	3,3,3	0.42	0	2,2,2	0.54	0
2	EDO	N	214	-	3,3,3	0.35	0	2,2,2	0.59	0
2	EDO	N	215	-	3,3,3	0.55	0	2,2,2	0.27	0
3	NO3	P	213	-	1,3,3	4.43	1 (100%)	0,3,3	0.00	-
2	EDO	P	214	-	3,3,3	0.52	0	2,2,2	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	213	-	-	0/1/1/1	0/0/0/0
2	EDO	A	214	-	-	0/1/1/1	0/0/0/0
2	EDO	A	215	-	-	0/1/1/1	0/0/0/0
2	EDO	A	216	-	-	0/1/1/1	0/0/0/0
2	EDO	A	217	-	-	0/1/1/1	0/0/0/0
2	EDO	A	218	-	-	0/1/1/1	0/0/0/0
2	EDO	A	219	-	-	0/1/1/1	0/0/0/0
2	EDO	A	220	-	-	0/1/1/1	0/0/0/0
2	EDO	B	213	-	-	0/1/1/1	0/0/0/0
2	EDO	B	214	-	-	0/1/1/1	0/0/0/0
2	EDO	B	215	-	-	0/1/1/1	0/0/0/0
2	EDO	B	216	-	-	0/1/1/1	0/0/0/0
2	EDO	B	217	-	-	0/1/1/1	0/0/0/0
2	EDO	B	218	-	-	0/1/1/1	0/0/0/0
2	EDO	C	213	-	-	0/1/1/1	0/0/0/0
2	EDO	C	214	-	-	0/1/1/1	0/0/0/0
2	EDO	D	213	-	-	0/1/1/1	0/0/0/0
2	EDO	D	214	-	-	0/1/1/1	0/0/0/0
2	EDO	E	213	-	-	0/1/1/1	0/0/0/0
2	EDO	E	214	-	-	0/1/1/1	0/0/0/0
2	EDO	E	215	-	-	0/1/1/1	0/0/0/0
2	EDO	E	216	-	-	0/1/1/1	0/0/0/0
2	EDO	E	217	-	-	0/1/1/1	0/0/0/0
3	NO3	F	213	-	-	0/0/0/0	0/0/0/0
3	NO3	F	214	-	-	0/0/0/0	0/0/0/0
3	NO3	F	215	-	-	0/0/0/0	0/0/0/0
3	NO3	F	216	-	-	0/0/0/0	0/0/0/0
2	EDO	F	217	-	-	0/1/1/1	0/0/0/0
2	EDO	F	218	-	-	0/1/1/1	0/0/0/0
2	EDO	F	219	-	-	0/1/1/1	0/0/0/0
2	EDO	F	220	-	-	0/1/1/1	0/0/0/0
2	EDO	F	221	-	-	0/1/1/1	0/0/0/0
2	EDO	F	222	-	-	0/1/1/1	0/0/0/0
3	NO3	G	213	-	-	0/0/0/0	0/0/0/0
3	NO3	G	214	-	-	0/0/0/0	0/0/0/0
2	EDO	G	215	-	-	0/1/1/1	0/0/0/0
2	EDO	G	216	-	-	0/1/1/1	0/0/0/0
2	EDO	G	217	-	-	0/1/1/1	0/0/0/0
2	EDO	G	218	-	-	0/1/1/1	0/0/0/0
2	EDO	G	219	-	-	0/1/1/1	0/0/0/0
2	EDO	G	220	-	-	0/1/1/1	0/0/0/0
2	EDO	G	221	-	-	0/1/1/1	0/0/0/0
2	EDO	H	213	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	H	214	-	-	0/1/1/1	0/0/0/0
2	EDO	H	215	-	-	0/1/1/1	0/0/0/0
2	EDO	H	216	-	-	0/1/1/1	0/0/0/0
2	EDO	H	217	-	-	0/1/1/1	0/0/0/0
2	EDO	H	218	-	-	0/1/1/1	0/0/0/0
3	NO3	I	213	-	-	0/0/0/0	0/0/0/0
2	EDO	I	214	-	-	0/1/1/1	0/0/0/0
2	EDO	I	215	-	-	0/1/1/1	0/0/0/0
2	EDO	I	216	-	-	0/1/1/1	0/0/0/0
2	EDO	I	217	-	-	0/1/1/1	0/0/0/0
2	EDO	J	213	-	-	0/1/1/1	0/0/0/0
2	EDO	J	214	-	-	0/1/1/1	0/0/0/0
2	EDO	J	215	-	-	0/1/1/1	0/0/0/0
2	EDO	K	213	-	-	0/1/1/1	0/0/0/0
2	EDO	K	214	-	-	0/1/1/1	0/0/0/0
2	EDO	K	215	-	-	0/1/1/1	0/0/0/0
2	EDO	L	213	-	-	0/1/1/1	0/0/0/0
2	EDO	M	213	-	-	0/1/1/1	0/0/0/0
2	EDO	M	214	-	-	0/1/1/1	0/0/0/0
2	EDO	M	215	-	-	0/1/1/1	0/0/0/0
2	EDO	M	216	-	-	0/1/1/1	0/0/0/0
2	EDO	N	213	-	-	0/1/1/1	0/0/0/0
2	EDO	N	214	-	-	0/1/1/1	0/0/0/0
2	EDO	N	215	-	-	0/1/1/1	0/0/0/0
3	NO3	P	213	-	-	0/0/0/0	0/0/0/0
2	EDO	P	214	-	-	0/1/1/1	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	215	NO3	O1-N	2.78	1.34	1.23
3	G	214	NO3	O1-N	3.31	1.36	1.23
3	F	213	NO3	O1-N	3.66	1.37	1.23
3	P	213	NO3	O1-N	4.43	1.40	1.23
3	F	214	NO3	O1-N	4.55	1.40	1.23
3	F	216	NO3	O1-N	4.70	1.41	1.23
3	G	213	NO3	O1-N	4.76	1.41	1.23
3	I	213	NO3	O1-N	4.86	1.42	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	215	EDO	2	0
2	A	216	EDO	2	0
2	A	217	EDO	3	0
2	B	217	EDO	2	0
2	C	214	EDO	3	0
2	E	215	EDO	4	0
2	F	219	EDO	3	0
2	F	220	EDO	2	0
2	G	219	EDO	3	0
2	G	220	EDO	1	0
2	J	214	EDO	1	0
2	N	215	EDO	1	0

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	201/231 (87%)	-0.73	0 100 100	17, 25, 40, 58	0
1	B	202/231 (87%)	-0.47	1 (0%) 90 89	19, 27, 50, 69	0
1	C	202/231 (87%)	-0.47	0 100 100	23, 33, 50, 60	0
1	D	201/231 (87%)	-0.29	1 (0%) 90 89	24, 36, 55, 70	0
1	E	205/231 (88%)	-0.72	2 (0%) 82 80	14, 23, 37, 57	0
1	F	203/231 (87%)	-0.33	4 (1%) 65 62	14, 25, 51, 70	0
1	G	201/231 (87%)	-0.73	0 100 100	17, 24, 38, 64	0
1	H	204/231 (88%)	-0.48	1 (0%) 90 89	18, 28, 45, 66	0
1	I	202/231 (87%)	-0.69	0 100 100	19, 27, 42, 59	0
1	J	202/231 (87%)	-0.45	3 (1%) 74 70	20, 28, 56, 76	0
1	K	202/231 (87%)	-0.46	0 100 100	23, 33, 49, 62	0
1	L	203/231 (87%)	-0.49	2 (0%) 82 80	22, 31, 47, 71	0
1	M	202/231 (87%)	-0.61	1 (0%) 90 89	18, 27, 45, 57	0
1	N	202/231 (87%)	-0.30	5 (2%) 58 53	24, 35, 61, 86	0
1	O	201/231 (87%)	-0.02	11 (5%) 26 21	27, 41, 63, 90	0
1	P	201/231 (87%)	-0.15	1 (0%) 90 89	26, 40, 58, 68	0
All	All	3234/3696 (87%)	-0.46	32 (0%) 82 80	14, 30, 53, 90	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	146	GLU	6.1
1	L	212	ALA	5.9
1	N	145	ARG	5.0
1	O	144	PRO	4.9
1	O	150	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	N	146	GLU	4.6
1	F	144	PRO	4.2
1	O	145	ARG	3.8
1	O	148	ALA	3.8
1	B	148	ALA	3.8
1	O	147	ARG	3.6
1	H	-3	TYR	3.4
1	F	146	GLU	3.0
1	N	121	TRP	2.8
1	N	144	PRO	2.7
1	J	146	GLU	2.6
1	J	150	ILE	2.6
1	N	211	ASP	2.6
1	J	144	PRO	2.5
1	E	-2	PHE	2.4
1	O	0	GLY	2.3
1	M	211	ASP	2.3
1	E	212	ALA	2.3
1	O	141	LEU	2.3
1	O	41	ALA	2.2
1	D	191	ALA	2.2
1	F	150	ILE	2.2
1	F	145	ARG	2.2
1	O	143	TYR	2.2
1	L	150	ILE	2.1
1	O	121	TRP	2.0
1	P	43	ASP	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	N	72	8/9	0.97	0.08	-	26,29,41,45	0
1	CSD	P	72	8/9	0.97	0.11	-	34,35,52,55	0
1	CSD	I	72	8/9	0.98	0.07	-	21,23,36,43	0
1	CSD	F	72	8/9	0.98	0.08	-	16,18,32,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	CSD	K	72	8/9	0.98	0.08	-	26,29,43,45	0
1	CSD	H	72	8/9	0.98	0.07	-	18,21,31,40	0
1	CSD	M	72	8/9	0.98	0.07	-	22,25,43,44	0
1	CSD	J	72	8/9	0.97	0.08	-	18,22,41,42	0
1	CSD	O	72	8/9	0.98	0.07	-	27,31,45,48	0
1	CSD	L	72	8/9	0.98	0.07	-	23,26,37,39	0
1	CSD	A	72	8/9	0.98	0.08	-	18,22,32,39	0
1	CSD	C	72	8/9	0.98	0.08	-	23,27,47,57	0
1	CSD	E	72	8/9	0.97	0.08	-	15,19,36,39	0
1	CSD	B	72	8/9	0.96	0.10	-	16,20,40,40	0
1	CSD	G	72	8/9	0.98	0.09	-	20,21,32,41	0
1	CSD	D	72	8/9	0.98	0.07	-	24,27,41,45	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	EDO	B	218	4/4	0.54	0.29	17.29	55,72,72,72	0
2	EDO	I	217	4/4	0.92	0.11	14.11	48,49,56,61	0
2	EDO	A	215	4/4	0.81	0.17	13.97	49,51,55,56	0
2	EDO	A	217	4/4	0.61	0.26	11.82	53,56,57,72	0
3	NO3	G	213	4/4	0.90	0.17	10.22	40,42,43,43	0
3	NO3	P	213	4/4	0.88	0.23	9.17	66,66,67,70	0
2	EDO	N	215	4/4	0.77	0.20	8.99	52,56,56,62	0
2	EDO	B	217	4/4	0.84	0.17	8.84	49,56,57,57	0
3	NO3	F	213	4/4	0.93	0.15	8.73	39,40,44,44	0
2	EDO	F	220	4/4	0.89	0.21	7.18	45,45,52,60	0
2	EDO	H	216	4/4	0.89	0.18	6.99	36,54,54,55	0
2	EDO	F	219	4/4	0.88	0.19	6.96	33,39,51,57	0
2	EDO	G	216	4/4	0.93	0.12	6.96	41,46,49,51	0
2	EDO	M	216	4/4	0.81	0.15	4.95	42,47,49,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	EDO	G	218	4/4	0.85	0.12	4.57	46,47,51,55	0
2	EDO	B	216	4/4	0.92	0.14	4.54	32,37,42,45	0
3	NO3	G	214	4/4	0.98	0.10	4.51	28,31,32,35	0
2	EDO	H	217	4/4	0.88	0.13	4.36	40,48,54,56	0
2	EDO	D	214	4/4	0.83	0.17	3.76	49,56,56,69	0
2	EDO	A	213	4/4	0.96	0.08	3.42	24,25,31,33	0
3	NO3	F	215	4/4	0.96	0.11	3.41	27,30,34,35	0
2	EDO	A	220	4/4	0.84	0.12	3.40	51,53,53,56	0
2	EDO	G	221	4/4	0.82	0.14	3.33	48,50,57,60	0
2	EDO	E	215	4/4	0.89	0.13	3.02	21,33,41,46	0
2	EDO	H	218	4/4	0.74	0.22	2.97	69,78,82,87	0
2	EDO	F	217	4/4	0.92	0.09	2.74	33,39,40,42	0
2	EDO	A	219	4/4	0.89	0.16	2.71	57,61,61,66	0
2	EDO	E	216	4/4	0.94	0.16	2.59	48,59,59,65	0
2	EDO	B	215	4/4	0.88	0.10	1.97	46,46,47,54	0
2	EDO	P	214	4/4	0.93	0.10	1.56	34,36,39,39	0
2	EDO	H	215	4/4	0.89	0.13	1.38	40,40,45,45	0
2	EDO	A	218	4/4	0.87	0.09	1.35	60,61,64,65	0
2	EDO	D	213	4/4	0.93	0.10	1.22	33,34,34,40	0
2	EDO	G	217	4/4	0.94	0.12	1.12	37,54,56,63	0
2	EDO	K	215	4/4	0.90	0.12	1.09	45,48,50,52	0
2	EDO	E	214	4/4	0.96	0.09	1.02	22,33,42,49	0
3	NO3	I	213	4/4	0.58	0.14	0.98	55,56,57,59	0
2	EDO	M	215	4/4	0.92	0.10	0.91	38,45,51,58	0
2	EDO	B	213	4/4	0.96	0.08	0.82	22,26,30,31	0
2	EDO	H	213	4/4	0.98	0.11	0.77	20,22,26,30	0
2	EDO	A	214	4/4	0.94	0.09	0.47	28,40,43,49	0
2	EDO	K	213	4/4	0.97	0.08	0.46	27,28,32,33	0
3	NO3	F	216	4/4	0.75	0.13	0.42	62,63,64,65	0
2	EDO	I	214	4/4	0.98	0.09	0.36	22,25,27,28	0
2	EDO	H	214	4/4	0.91	0.09	0.01	34,42,44,53	0
2	EDO	F	218	4/4	0.97	0.07	-0.16	28,28,31,33	0
2	EDO	E	213	4/4	0.99	0.07	-0.32	17,18,21,24	0
2	EDO	N	213	4/4	0.98	0.06	-0.83	25,29,30,30	0
2	EDO	G	215	4/4	0.99	0.06	-0.85	24,27,27,27	0
2	EDO	M	213	4/4	0.97	0.07	-0.86	25,30,32,35	0
2	EDO	L	213	4/4	0.98	0.06	-0.94	27,29,31,38	0
2	EDO	B	214	4/4	0.98	0.07	-1.19	43,46,46,48	0
2	EDO	J	213	4/4	0.98	0.06	-1.37	19,29,30,31	0
2	EDO	C	213	4/4	0.97	0.06	-1.48	29,30,32,34	0
2	EDO	N	214	4/4	0.94	0.11	-	45,49,52,52	0
2	EDO	J	215	4/4	0.85	0.14	-	55,60,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	EDO	C	214	4/4	0.89	0.13	-	48,49,52,53	0
2	EDO	A	216	4/4	0.84	0.17	-	43,50,51,53	0
2	EDO	K	214	4/4	0.92	0.09	-	39,39,41,41	0
3	NO3	F	214	4/4	0.80	0.13	-	54,54,54,54	0
2	EDO	E	217	4/4	0.94	0.11	-	42,52,53,63	0
2	EDO	M	214	4/4	0.92	0.12	-	46,48,56,60	0
2	EDO	I	216	4/4	0.87	0.13	-	51,52,56,57	0
2	EDO	G	219	4/4	0.90	0.19	-	31,40,49,52	0
2	EDO	J	214	4/4	0.76	0.23	-	60,60,61,61	0
2	EDO	F	221	4/4	0.91	0.13	-	39,42,48,55	0
2	EDO	F	222	4/4	0.88	0.09	-	56,59,60,61	0
2	EDO	I	215	4/4	0.80	0.14	-	46,51,53,56	0
2	EDO	G	220	4/4	0.83	0.20	-	48,52,54,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.