



# Full wwPDB X-ray Structure Validation Report

Nov 3, 2014 – 11:02 AM EST

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 : 2008-02-01  
Resolution : 1.81 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

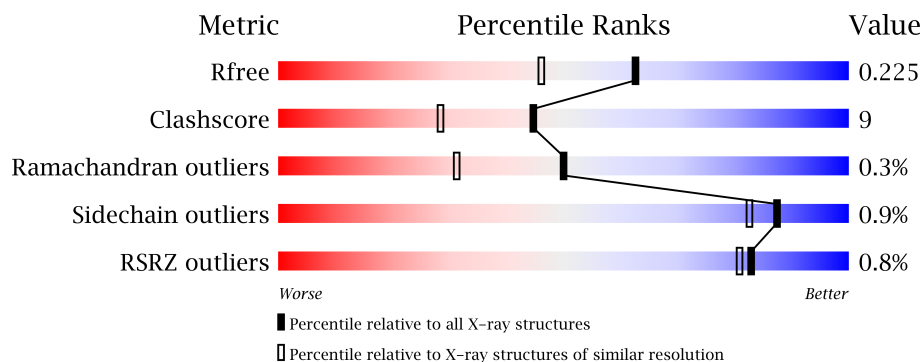
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

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))
$R_{free}$	66092	4101 (1.84-1.80)
Clashscore	79885	5140 (1.84-1.80)
Ramachandran outliers	78287	5077 (1.84-1.80)
Sidechain outliers	78261	5077 (1.84-1.80)
RSRZ outliers	66119	4103 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	231	
1	B	231	
1	C	231	
1	D	231	
1	E	231	
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	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	O	231	
1	P	231	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NO3	F	213	X	X
2	NO3	F	214	X	X
2	NO3	F	215	X	X
2	NO3	F	216	X	-
2	NO3	G	213	X	X
2	NO3	G	214	X	X
2	NO3	I	213	X	-
2	NO3	P	213	X	X
3	EDO	A	213	-	X
3	EDO	A	215	-	X
3	EDO	A	216	-	X
3	EDO	A	217	-	X
3	EDO	A	219	-	X
3	EDO	A	220	-	X
3	EDO	B	216	-	X
3	EDO	B	217	-	X
3	EDO	B	218	-	X
3	EDO	C	214	-	X
3	EDO	D	214	-	X
3	EDO	E	215	-	X
3	EDO	E	216	-	X
3	EDO	F	219	-	X
3	EDO	F	220	-	X
3	EDO	F	221	-	X
3	EDO	F	222	-	X
3	EDO	G	216	-	X
3	EDO	G	218	-	X
3	EDO	G	219	-	X
3	EDO	G	220	-	X
3	EDO	G	221	-	X
3	EDO	H	216	-	X
3	EDO	H	217	-	X
3	EDO	H	218	-	X
3	EDO	I	215	-	X
3	EDO	I	216	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	I	217	-	X
3	EDO	J	214	-	X
3	EDO	J	215	-	X
3	EDO	M	214	-	X
3	EDO	M	216	-	X
3	EDO	N	215	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28863 atoms, of which 0 are hydrogen and 0 are deuterium.

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

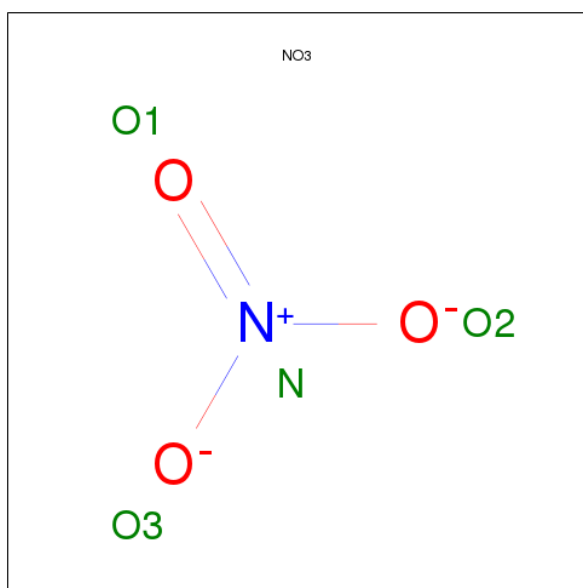
Chain	Residue	Modelled	Actual	Comment	Reference
N	-13	ILE	-	LEADER SEQUENCE	UNP A4XEL3
N	-12	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-11	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-10	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-9	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-8	HIS	-	LEADER SEQUENCE	UNP A4XEL3
N	-7	HIS	-	LEADER SEQUENCE	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

*Continued on next page...*

Continued from previous page...

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 NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



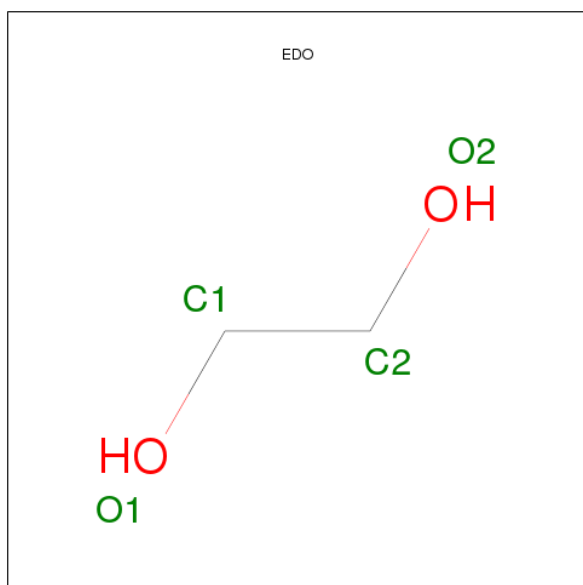
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total N O 4 1 3	0	0
2	F	1	Total N O 4 1 3	0	0
2	F	1	Total N O 4 1 3	0	0
2	F	1	Total N O 4 1 3	0	0
2	G	1	Total N O 4 1 3	0	0
2	G	1	Total N O 4 1 3	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	192	Total O 192 192	0	0
4	B	210	Total O 211 211	0	1
4	C	120	Total O 120 120	0	0
4	D	74	Total O 74 74	0	0
4	E	233	Total O 235 235	0	2
4	F	210	Total O 212 212	0	2
4	G	223	Total O 223 223	0	0
4	H	203	Total O 204 204	0	1
4	I	186	Total O 187 187	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ribose/galactose isomerase

Chain A:

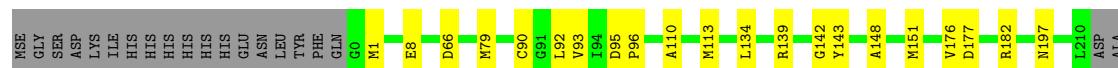


Chain F: 



- Molecule 1: Ribose/galactose isomerase

Chain G: 



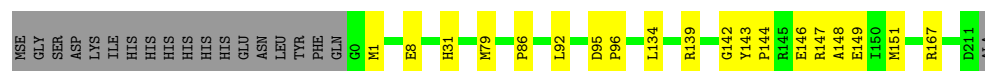
- Molecule 1: Ribose/galactose isomerase

Chain H: 



- Molecule 1: Ribose/galactose isomerase

Chain I: 



- Molecule 1: Ribose/galactose isomerase

Chain J: 



- Molecule 1: Ribose/galactose isomerase

Chain K: 

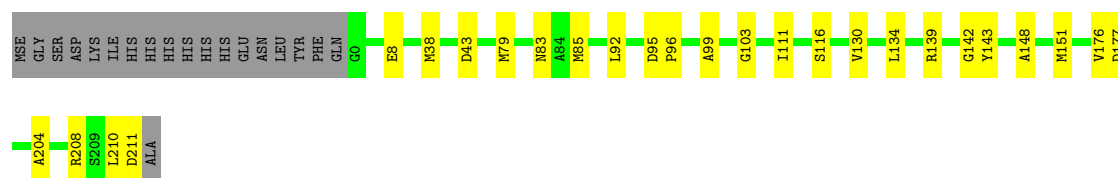


- Molecule 1: Ribose/galactose isomerase

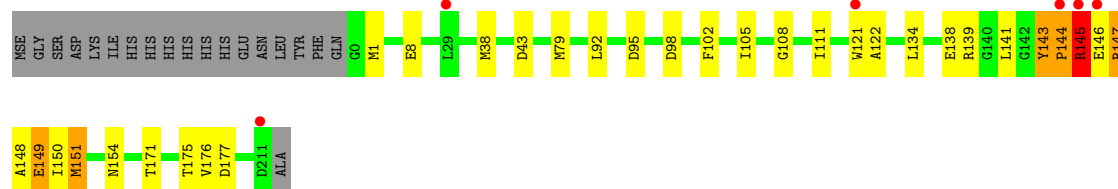
Chain L: 



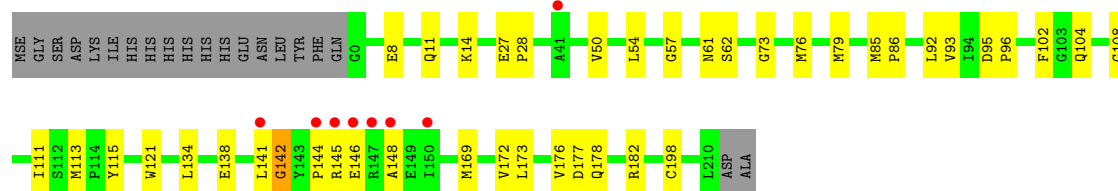
- Molecule 1: Ribose/galactose isomerase

Chain M: 

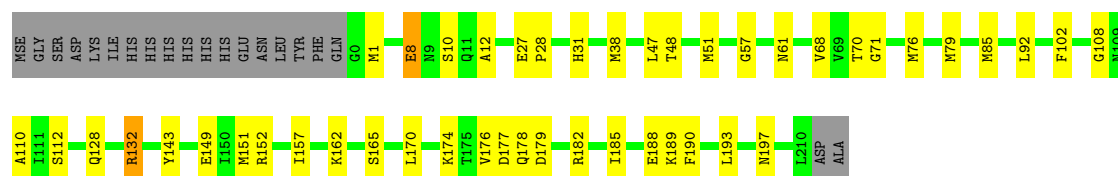
- Molecule 1: Ribose/galactose isomerase

Chain N: 

- Molecule 1: Ribose/galactose isomerase

Chain O: 

- Molecule 1: Ribose/galactose isomerase

Chain P: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, $R_{free}$	0.170 , 0.220 0.178 , 0.225	Depositor DCC
$R_{free}$ test set	16707 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 330786 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	28863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1618	0	1617	25	0
1	K	1615	0	1617	19	0
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	F	16	0	0	0	0
2	G	8	0	0	0	0
2	I	4	0	0	0	0
2	P	4	0	0	0	0
3	A	32	0	48	7	0
3	B	24	0	36	2	0
3	C	8	0	12	3	0
3	D	8	0	12	0	0
3	E	20	0	30	4	0
3	F	24	0	36	5	0
3	G	28	0	42	4	0
3	H	24	0	36	0	0
3	I	16	0	24	0	0
3	J	12	0	18	1	0
3	K	12	0	18	0	0
3	L	4	0	6	0	0
3	M	16	0	24	0	0
3	N	12	0	18	1	0
3	P	4	0	6	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	28863	0	26334	448	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (448) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
3: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	3: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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
3: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
3: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
3: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	3:E:215:EDO:H12	1.56	0.70
1:M:176:VAL:HG22	1:M:177:ASP:N	2.06	0.70
3:E:215:EDO:H21	3: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:142:GLY:HA2	1:I:151[B]:MSE:CE	2.13	0.68
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
3: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	3: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	3: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
3: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(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	3: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	3: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
3: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
1:L:142:GLY:HA3	1:L:151[B]:MSE:HE2	1.88	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	3:G:219:EDO:C2	2.23	0.52
1:J:138:GLU:OE1	1:J:141:LEU:HD11	2.09	0.52
3: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
3: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
3:A:217:EDO:H12	4:B:250:HOH:O	2.11	0.50
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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3: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	3: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
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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:A:217:EDO:H11	4:B:278:HOH:O	2.16	0.46
1:A:147:ARG:HE	3: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
1:E:151:MSE:HE2	3: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	3: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	3: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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	3: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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	38	19
1	C	215/231 (93%)	211 (98%)	4 (2%)	0	100	100
1	D	212/231 (92%)	206 (97%)	4 (2%)	2 (1%)	25	8
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%)	38	19
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%)	16	4
1	O	211/231 (91%)	206 (98%)	3 (1%)	2 (1%)	25	8
1	P	210/231 (91%)	204 (97%)	6 (3%)	0	100	100
All	All	3410/3696 (92%)	3342 (98%)	59 (2%)	9 (0%)	50	31

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
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%)	92	90
1	B	164/171 (96%)	163 (99%)	1 (1%)	92	90
1	C	166/171 (97%)	164 (99%)	2 (1%)	82	74
1	D	162/171 (95%)	161 (99%)	1 (1%)	92	90
1	E	168/171 (98%)	167 (99%)	1 (1%)	92	90
1	F	167/171 (98%)	165 (99%)	2 (1%)	82	74
1	G	166/171 (97%)	165 (99%)	1 (1%)	92	90
1	H	170/171 (99%)	169 (99%)	1 (1%)	92	90
1	I	167/171 (98%)	165 (99%)	2 (1%)	82	74
1	J	164/171 (96%)	163 (99%)	1 (1%)	92	90
1	K	163/171 (95%)	162 (99%)	1 (1%)	92	90
1	L	163/171 (95%)	162 (99%)	1 (1%)	92	90
1	M	165/171 (96%)	164 (99%)	1 (1%)	92	90
1	N	165/171 (96%)	160 (97%)	5 (3%)	53	34
1	O	155/171 (91%)	154 (99%)	1 (1%)	92	90
1	P	162/171 (95%)	161 (99%)	1 (1%)	92	90
All	All	2635/2736 (96%)	2612 (99%)	23 (1%)	87	82

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

Mol	Chain	Res	Type
1	A	8	GLU
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains in this entry.

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

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	7,7,8	6.94	2 (28%)	6,8,10	3.79	3 (50%)
1	CSD	B	72	1	7,7,8	5.17	2 (28%)	6,8,10	3.53	4 (66%)
1	CSD	C	72	1	7,7,8	7.24	1 (14%)	6,8,10	4.33	4 (66%)
1	CSD	D	72	1	7,7,8	6.97	2 (28%)	6,8,10	3.56	5 (83%)
1	CSD	E	72	1	7,7,8	7.20	2 (28%)	6,8,10	3.84	4 (66%)
1	CSD	F	72	1	7,7,8	4.97	2 (28%)	6,8,10	3.58	3 (50%)
1	CSD	G	72	1	7,7,8	5.18	4 (57%)	6,8,10	2.59	3 (50%)
1	CSD	H	72	1	7,7,8	7.41	2 (28%)	6,8,10	3.44	3 (50%)
1	CSD	I	72	1	7,7,8	4.04	3 (42%)	6,8,10	3.56	3 (50%)
1	CSD	J	72	1	7,7,8	6.41	2 (28%)	6,8,10	3.36	3 (50%)
1	CSD	K	72	1	7,7,8	6.42	2 (28%)	6,8,10	3.48	3 (50%)
1	CSD	L	72	1	7,7,8	7.41	2 (28%)	6,8,10	3.82	4 (66%)
1	CSD	M	72	1	7,7,8	6.24	2 (28%)	6,8,10	4.14	3 (50%)
1	CSD	N	72	1	7,7,8	6.45	2 (28%)	6,8,10	3.69	4 (66%)
1	CSD	O	72	1	7,7,8	5.94	2 (28%)	6,8,10	3.25	3 (50%)
1	CSD	P	72	1	7,7,8	5.70	2 (28%)	6,8,10	3.17	3 (50%)

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	-	0/3/6/8	0/0/0/0
1	CSD	B	72	1	-	0/3/6/8	0/0/0/0
1	CSD	C	72	1	-	0/3/6/8	0/0/0/0
1	CSD	D	72	1	-	0/3/6/8	0/0/0/0
1	CSD	E	72	1	-	0/3/6/8	0/0/0/0
1	CSD	F	72	1	-	0/3/6/8	0/0/0/0
1	CSD	G	72	1	-	0/3/6/8	0/0/0/0
1	CSD	H	72	1	-	0/3/6/8	0/0/0/0
1	CSD	I	72	1	-	0/3/6/8	0/0/0/0
1	CSD	J	72	1	-	0/3/6/8	0/0/0/0
1	CSD	K	72	1	-	0/3/6/8	0/0/0/0
1	CSD	L	72	1	-	0/3/6/8	0/0/0/0
1	CSD	M	72	1	-	0/3/6/8	0/0/0/0
1	CSD	N	72	1	-	0/3/6/8	0/0/0/0
1	CSD	O	72	1	-	0/3/6/8	0/0/0/0
1	CSD	P	72	1	-	0/3/6/8	0/0/0/0



All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	72	CSD	O-C	19.24	1.24	1.11
1	L	72	CSD	O-C	19.10	1.24	1.11
1	C	72	CSD	O-C	18.92	1.24	1.11
1	D	72	CSD	O-C	17.96	1.23	1.11
1	E	72	CSD	O-C	17.53	1.23	1.11
1	N	72	CSD	O-C	16.47	1.22	1.11
1	K	72	CSD	O-C	16.45	1.22	1.11
1	J	72	CSD	O-C	16.13	1.22	1.11
1	M	72	CSD	O-C	15.94	1.22	1.11
1	A	72	CSD	O-C	15.40	1.22	1.11
1	O	72	CSD	O-C	15.23	1.21	1.11
1	P	72	CSD	O-C	14.35	1.21	1.11
1	B	72	CSD	O-C	13.30	1.20	1.11
1	G	72	CSD	O-C	12.64	1.20	1.11
1	F	72	CSD	O-C	11.85	1.19	1.11
1	I	72	CSD	O-C	9.74	1.18	1.11
1	A	72	CSD	OD1-SG	-9.56	1.37	1.47
1	E	72	CSD	OD1-SG	-7.21	1.39	1.47
1	F	72	CSD	OD1-SG	-5.16	1.42	1.47
1	J	72	CSD	OD1-SG	-4.65	1.42	1.47
1	N	72	CSD	OD1-SG	-3.77	1.43	1.47
1	P	72	CSD	OD1-SG	-3.71	1.43	1.47
1	I	72	CSD	OD1-SG	-3.63	1.43	1.47
1	L	72	CSD	OD1-SG	-3.51	1.43	1.47
1	M	72	CSD	OD1-SG	-3.49	1.43	1.47
1	K	72	CSD	OD1-SG	-3.42	1.43	1.47
1	G	72	CSD	OD1-SG	-3.27	1.44	1.47
1	D	72	CSD	OD1-SG	-3.19	1.44	1.47
1	H	72	CSD	OD1-SG	-2.90	1.44	1.47
1	O	72	CSD	OD1-SG	-2.81	1.44	1.47
1	G	72	CSD	CB-CA	2.40	1.57	1.53
1	G	72	CSD	CA-N	-2.12	1.41	1.47
1	B	72	CSD	OD1-SG	-2.07	1.45	1.47
1	I	72	CSD	OD2-SG	-2.01	1.41	1.55

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	CSD	CA-CB-SG	7.80	121.94	110.82
1	A	72	CSD	C-CA-N	-7.29	106.54	113.83
1	I	72	CSD	CA-CB-SG	6.43	120.00	110.82
1	J	72	CSD	C-CA-N	-6.40	107.44	113.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	72	CSD	CA-CB-SG	6.39	119.93	110.82
1	H	72	CSD	C-CA-N	-6.29	107.54	113.83
1	M	72	CSD	C-CA-N	-6.29	107.55	113.83
1	M	72	CSD	CA-CB-SG	6.12	119.55	110.82
1	D	72	CSD	CA-CB-SG	6.04	119.43	110.82
1	N	72	CSD	C-CA-N	-5.86	107.98	113.83
1	B	72	CSD	CA-CB-SG	5.79	119.08	110.82
1	E	72	CSD	C-CA-N	-5.78	108.06	113.83
1	K	72	CSD	C-CA-N	-5.74	108.10	113.83
1	N	72	CSD	CA-CB-SG	5.71	118.96	110.82
1	E	72	CSD	CA-CB-SG	5.70	118.94	110.82
1	F	72	CSD	C-CA-N	-5.65	108.19	113.83
1	C	72	CSD	OD1-SG-CB	5.61	114.99	105.29
1	P	72	CSD	CA-CB-SG	5.53	118.70	110.82
1	F	72	CSD	CA-CB-SG	5.35	118.45	110.82
1	G	72	CSD	CA-CB-SG	4.96	117.89	110.82
1	A	72	CSD	CA-CB-SG	4.94	117.86	110.82
1	O	72	CSD	CA-CB-SG	4.86	117.75	110.82
1	O	72	CSD	C-CA-N	-4.78	109.05	113.83
1	K	72	CSD	CA-CB-SG	4.74	117.58	110.82
1	B	72	CSD	C-CA-N	-4.72	109.12	113.83
1	I	72	CSD	C-CA-N	-4.64	109.20	113.83
1	M	72	CSD	OD2-SG-CB	4.62	115.28	98.82
1	L	72	CSD	OD1-SG-CB	4.03	112.26	105.29
1	P	72	CSD	OD2-SG-CB	4.01	113.10	98.82
1	L	72	CSD	C-CA-N	-3.95	109.89	113.83
1	D	72	CSD	C-CA-N	-3.93	109.90	113.83
1	H	72	CSD	CA-CB-SG	3.76	116.18	110.82
1	J	72	CSD	CA-CB-SG	3.73	116.14	110.82
1	L	72	CSD	OD2-SG-CB	3.70	112.00	98.82
1	O	72	CSD	OD2-SG-CB	3.69	111.97	98.82
1	F	72	CSD	OD2-SG-CB	3.60	111.65	98.82
1	K	72	CSD	OD2-SG-CB	3.53	111.40	98.82
1	B	72	CSD	OD2-SG-CB	3.48	111.22	98.82
1	D	72	CSD	OD1-SG-CB	3.44	111.25	105.29
1	H	72	CSD	OD2-SG-OD1	3.40	116.18	109.75
1	E	72	CSD	OD1-SG-CB	3.32	111.04	105.29
1	C	72	CSD	OD2-SG-CB	3.20	110.22	98.82
1	E	72	CSD	OD2-SG-CB	2.84	108.94	98.82
1	J	72	CSD	OD2-SG-CB	2.83	108.89	98.82
1	P	72	CSD	C-CA-N	-2.79	111.04	113.83
1	D	72	CSD	OD2-SG-OD1	2.58	114.62	109.75

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	72	CSD	OD1-SG-CB	2.50	109.61	105.29
1	C	72	CSD	OD2-SG-OD1	2.48	114.44	109.75
1	G	72	CSD	OD1-SG-CB	2.47	109.56	105.29
1	G	72	CSD	OD2-SG-CB	2.42	107.44	98.82
1	D	72	CSD	OD2-SG-CB	2.40	107.35	98.82
1	I	72	CSD	OD2-SG-OD1	2.36	114.21	109.75
1	N	72	CSD	OD2-SG-CB	2.35	107.20	98.82
1	B	72	CSD	OD2-SG-OD1	2.29	114.08	109.75
1	A	72	CSD	OD2-SG-CB	2.02	106.02	98.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	$\# Z  > 2$
3	EDO	A	213	-	3,3,3	0.35	0	2,2,2	0.53	0
3	EDO	A	214	-	3,3,3	0.59	0	2,2,2	0.51	0
3	EDO	A	215	-	3,3,3	0.44	0	2,2,2	0.56	0
3	EDO	A	216	-	3,3,3	0.73	0	2,2,2	0.66	0
3	EDO	A	217	-	3,3,3	0.33	0	2,2,2	0.51	0
3	EDO	A	218	-	3,3,3	0.49	0	2,2,2	0.41	0
3	EDO	A	219	-	3,3,3	0.47	0	2,2,2	0.52	0
3	EDO	A	220	-	3,3,3	0.65	0	2,2,2	0.33	0
3	EDO	B	213	-	3,3,3	0.21	0	2,2,2	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	B	214	-	3,3,3	0.47	0	2,2,2	0.50	0
3	EDO	B	215	-	3,3,3	0.64	0	2,2,2	0.33	0
3	EDO	B	216	-	3,3,3	0.50	0	2,2,2	0.40	0
3	EDO	B	217	-	3,3,3	0.48	0	2,2,2	0.17	0
3	EDO	B	218	-	3,3,3	0.65	0	2,2,2	0.17	0
3	EDO	C	213	-	3,3,3	0.49	0	2,2,2	0.76	0
3	EDO	C	214	-	3,3,3	0.49	0	2,2,2	0.40	0
3	EDO	D	213	-	3,3,3	0.69	0	2,2,2	0.44	0
3	EDO	D	214	-	3,3,3	0.46	0	2,2,2	0.55	0
3	EDO	E	213	-	3,3,3	0.45	0	2,2,2	0.50	0
3	EDO	E	214	-	3,3,3	0.41	0	2,2,2	0.59	0
3	EDO	E	215	-	3,3,3	0.31	0	2,2,2	0.88	0
3	EDO	E	216	-	3,3,3	0.53	0	2,2,2	0.42	0
3	EDO	E	217	-	3,3,3	0.48	0	2,2,2	0.44	0
2	NO3	F	213	-	3,3,3	2.85	3 (100%)	3,3,3	0.78	0
2	NO3	F	214	-	3,3,3	3.37	3 (100%)	3,3,3	0.43	0
2	NO3	F	215	-	3,3,3	2.31	3 (100%)	3,3,3	0.29	0
2	NO3	F	216	-	3,3,3	3.32	3 (100%)	3,3,3	0.15	0
3	EDO	F	217	-	3,3,3	0.41	0	2,2,2	0.36	0
3	EDO	F	218	-	3,3,3	0.33	0	2,2,2	0.70	0
3	EDO	F	219	-	3,3,3	0.43	0	2,2,2	0.56	0
3	EDO	F	220	-	3,3,3	0.52	0	2,2,2	0.05	0
3	EDO	F	221	-	3,3,3	0.55	0	2,2,2	0.38	0
3	EDO	F	222	-	3,3,3	0.56	0	2,2,2	0.27	0
2	NO3	G	213	-	3,3,3	3.09	3 (100%)	3,3,3	0.58	0
2	NO3	G	214	-	3,3,3	2.61	3 (100%)	3,3,3	0.94	0
3	EDO	G	215	-	3,3,3	0.41	0	2,2,2	0.81	0
3	EDO	G	216	-	3,3,3	0.44	0	2,2,2	0.53	0
3	EDO	G	217	-	3,3,3	0.46	0	2,2,2	0.73	0
3	EDO	G	218	-	3,3,3	0.63	0	2,2,2	0.20	0
3	EDO	G	219	-	3,3,3	0.69	0	2,2,2	0.05	0
3	EDO	G	220	-	3,3,3	0.66	0	2,2,2	0.14	0
3	EDO	G	221	-	3,3,3	0.68	0	2,2,2	0.15	0
3	EDO	H	213	-	3,3,3	0.56	0	2,2,2	0.40	0
3	EDO	H	214	-	3,3,3	0.72	0	2,2,2	0.21	0
3	EDO	H	215	-	3,3,3	0.61	0	2,2,2	0.16	0
3	EDO	H	216	-	3,3,3	0.51	0	2,2,2	0.81	0
3	EDO	H	217	-	3,3,3	0.41	0	2,2,2	0.80	0
3	EDO	H	218	-	3,3,3	0.53	0	2,2,2	0.25	0
2	NO3	I	213	-	3,3,3	3.51	3 (100%)	3,3,3	0.13	0
3	EDO	I	214	-	3,3,3	0.34	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	I	215	-	3,3,3	0.48	0	2,2,2	0.39	0
3	EDO	I	216	-	3,3,3	0.44	0	2,2,2	0.24	0
3	EDO	I	217	-	3,3,3	0.38	0	2,2,2	0.71	0
3	EDO	J	213	-	3,3,3	0.53	0	2,2,2	0.38	0
3	EDO	J	214	-	3,3,3	0.49	0	2,2,2	0.26	0
3	EDO	J	215	-	3,3,3	0.55	0	2,2,2	0.08	0
3	EDO	K	213	-	3,3,3	0.41	0	2,2,2	0.39	0
3	EDO	K	214	-	3,3,3	0.55	0	2,2,2	0.46	0
3	EDO	K	215	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	L	213	-	3,3,3	0.42	0	2,2,2	0.59	0
3	EDO	M	213	-	3,3,3	0.53	0	2,2,2	0.33	0
3	EDO	M	214	-	3,3,3	0.46	0	2,2,2	0.53	0
3	EDO	M	215	-	3,3,3	0.63	0	2,2,2	0.07	0
3	EDO	M	216	-	3,3,3	0.74	0	2,2,2	0.03	0
3	EDO	N	213	-	3,3,3	0.47	0	2,2,2	0.58	0
3	EDO	N	214	-	3,3,3	0.41	0	2,2,2	0.64	0
3	EDO	N	215	-	3,3,3	0.60	0	2,2,2	0.29	0
2	NO3	P	213	-	3,3,3	3.19	3 (100%)	3,3,3	0.29	0
3	EDO	P	214	-	3,3,3	0.56	0	2,2,2	0.17	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
3	EDO	A	213	-	-	0/1/1/1	0/0/0/0
3	EDO	A	214	-	-	0/1/1/1	0/0/0/0
3	EDO	A	215	-	-	0/1/1/1	0/0/0/0
3	EDO	A	216	-	-	0/1/1/1	0/0/0/0
3	EDO	A	217	-	-	0/1/1/1	0/0/0/0
3	EDO	A	218	-	-	0/1/1/1	0/0/0/0
3	EDO	A	219	-	-	0/1/1/1	0/0/0/0
3	EDO	A	220	-	-	0/1/1/1	0/0/0/0
3	EDO	B	213	-	-	0/1/1/1	0/0/0/0
3	EDO	B	214	-	-	0/1/1/1	0/0/0/0
3	EDO	B	215	-	-	0/1/1/1	0/0/0/0
3	EDO	B	216	-	-	0/1/1/1	0/0/0/0
3	EDO	B	217	-	-	0/1/1/1	0/0/0/0
3	EDO	B	218	-	-	0/1/1/1	0/0/0/0
3	EDO	C	213	-	-	0/1/1/1	0/0/0/0
3	EDO	C	214	-	-	0/1/1/1	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	213	NO3	O1-N	4.22	1.42	1.24
2	G	213	NO3	O1-N	4.13	1.41	1.24
2	F	216	NO3	O1-N	4.09	1.41	1.24
2	F	214	NO3	O1-N	3.95	1.40	1.24
2	P	213	NO3	O1-N	3.84	1.40	1.24
2	F	213	NO3	O1-N	3.17	1.37	1.24
2	F	214	NO3	O2-N	3.14	1.41	1.25
2	I	213	NO3	O2-N	3.12	1.41	1.25
2	I	213	NO3	O3-N	3.05	1.41	1.25
2	F	216	NO3	O2-N	2.95	1.40	1.25
2	F	214	NO3	O3-N	2.93	1.40	1.25
2	P	213	NO3	O3-N	2.92	1.40	1.25
2	F	213	NO3	O3-N	2.88	1.40	1.25
2	G	214	NO3	O1-N	2.85	1.36	1.24
2	F	216	NO3	O3-N	2.75	1.39	1.25
2	G	214	NO3	O2-N	2.74	1.39	1.25
2	P	213	NO3	O2-N	2.71	1.39	1.25
2	G	213	NO3	O3-N	2.53	1.38	1.25
2	F	213	NO3	O2-N	2.47	1.38	1.25
2	F	215	NO3	O1-N	2.38	1.34	1.24
2	F	215	NO3	O2-N	2.34	1.37	1.25
2	G	213	NO3	O2-N	2.27	1.37	1.25
2	F	215	NO3	O3-N	2.21	1.36	1.25
2	G	214	NO3	O3-N	2.19	1.36	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	211/231 (91%)	-0.66	0 100 100	17, 25, 40, 58	0
1	B	212/231 (91%)	-0.42	1 (0%) 88 87	19, 27, 50, 69	0
1	C	212/231 (91%)	-0.41	0 100 100	23, 33, 50, 60	0
1	D	211/231 (91%)	-0.24	0 100 100	24, 36, 55, 70	0
1	E	215/231 (93%)	-0.65	2 (0%) 81 78	14, 23, 37, 57	0
1	F	213/231 (92%)	-0.31	3 (1%) 72 68	14, 25, 51, 70	0
1	G	211/231 (91%)	-0.66	0 100 100	17, 24, 38, 64	0
1	H	214/231 (92%)	-0.42	1 (0%) 88 87	18, 27, 45, 66	0
1	I	212/231 (91%)	-0.62	0 100 100	19, 26, 42, 59	0
1	J	212/231 (91%)	-0.43	3 (1%) 72 68	20, 28, 56, 76	0
1	K	212/231 (91%)	-0.41	0 100 100	23, 33, 49, 62	0
1	L	213/231 (92%)	-0.43	2 (0%) 81 78	22, 30, 47, 71	0
1	M	212/231 (91%)	-0.55	0 100 100	18, 27, 45, 57	0
1	N	212/231 (91%)	-0.24	6 (2%) 50 43	24, 35, 61, 86	0
1	O	211/231 (91%)	-0.02	8 (3%) 38 31	27, 40, 64, 90	0
1	P	211/231 (91%)	-0.12	0 100 100	26, 40, 58, 68	0
All	All	3394/3696 (91%)	-0.41	26 (0%) 83 81	14, 30, 52, 90	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	146	GLU	5.2
1	L	212	ALA	4.8
1	N	145	ARG	4.6
1	N	146	GLU	4.3
1	F	144	PRO	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	-3	TYR	3.7
1	O	150	ILE	3.6
1	O	144	PRO	3.3
1	O	145	ARG	3.0
1	F	146	GLU	3.0
1	O	147	ARG	2.8
1	O	148	ALA	2.7
1	B	148	ALA	2.7
1	F	150	ILE	2.6
1	N	144	PRO	2.6
1	N	121	TRP	2.5
1	N	211	ASP	2.4
1	J	150	ILE	2.4
1	O	41	ALA	2.3
1	E	212	ALA	2.3
1	E	-2	PHE	2.2
1	N	29	LEU	2.2
1	J	144	PRO	2.2
1	O	141	LEU	2.1
1	L	150	ILE	2.1
1	J	146	GLU	2.1

## 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSD	P	72	8/9	0.10	2.42	34,35,52,55	0
1	CSD	A	72	8/9	0.08	2.20	18,22,32,39	0
1	CSD	B	72	8/9	0.10	2.17	16,20,40,40	0
1	CSD	C	72	8/9	0.07	0.96	23,27,47,57	0
1	CSD	J	72	8/9	0.08	0.87	18,22,41,42	0
1	CSD	G	72	8/9	0.09	0.85	20,21,32,41	0
1	CSD	E	72	8/9	0.08	0.75	15,19,36,39	0
1	CSD	K	72	8/9	0.08	0.59	26,29,43,45	0
1	CSD	I	72	8/9	0.07	0.43	21,23,36,43	0
1	CSD	D	72	8/9	0.07	0.39	24,27,41,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSD	N	72	8/9	0.07	0.11	26,29,41,45	0
1	CSD	M	72	8/9	0.07	0.09	22,25,43,44	0
1	CSD	H	72	8/9	0.07	-0.13	18,21,31,40	0
1	CSD	L	72	8/9	0.06	-0.48	23,26,37,39	0
1	CSD	O	72	8/9	0.06	-0.58	27,31,45,48	0
1	CSD	F	72	8/9	0.07	-1.70	16,18,32,34	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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	218	4/4	0.28	16.78	55,72,72,72	0
3	EDO	G	219	4/4	0.21	16.00	31,40,49,52	0
2	NO3	F	214	4/4	0.13	13.81	54,54,54,54	0
2	NO3	G	213	4/4	0.17	12.98	40,42,43,43	0
3	EDO	I	217	4/4	0.10	12.76	48,49,56,61	0
2	NO3	P	213	4/4	0.26	12.47	66,66,67,70	0
3	EDO	A	215	4/4	0.17	12.43	49,51,55,56	0
3	EDO	N	215	4/4	0.21	11.21	52,56,56,62	0
3	EDO	A	217	4/4	0.29	10.74	53,56,57,72	0
3	EDO	J	214	4/4	0.22	10.52	60,60,61,61	0
3	EDO	A	216	4/4	0.15	9.44	43,50,51,53	0
3	EDO	M	216	4/4	0.20	9.24	42,47,49,58	0
3	EDO	G	216	4/4	0.13	8.52	41,46,49,51	0
3	EDO	F	220	4/4	0.22	8.25	45,45,52,60	0
3	EDO	B	217	4/4	0.15	7.09	49,56,57,57	0
3	EDO	I	216	4/4	0.13	7.00	51,52,56,57	0
3	EDO	H	216	4/4	0.18	6.75	36,54,54,55	0
3	EDO	F	219	4/4	0.18	6.42	33,39,51,57	0
3	EDO	I	215	4/4	0.13	5.74	46,51,53,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	J	215	4/4	0.12	5.23	55,60,61,61	0
3	EDO	C	214	4/4	0.14	5.13	48,49,52,53	0
3	EDO	G	218	4/4	0.14	4.88	46,47,51,55	0
2	NO3	F	213	4/4	0.14	4.40	39,40,44,44	0
3	EDO	D	214	4/4	0.16	3.91	49,56,56,69	0
3	EDO	F	221	4/4	0.13	3.61	39,42,48,55	0
3	EDO	A	220	4/4	0.13	3.61	51,53,53,56	0
3	EDO	F	222	4/4	0.10	3.39	56,59,60,61	0
2	NO3	G	214	4/4	0.09	3.39	28,31,32,35	0
3	EDO	G	221	4/4	0.13	3.01	48,50,57,60	0
3	EDO	E	216	4/4	0.18	2.94	48,59,59,65	0
3	EDO	H	217	4/4	0.11	2.93	40,48,54,56	0
3	EDO	E	215	4/4	0.13	2.92	21,33,41,46	0
3	EDO	B	216	4/4	0.12	2.85	32,37,42,45	0
3	EDO	A	219	4/4	0.17	2.71	57,61,61,66	0
3	EDO	H	218	4/4	0.21	2.61	69,78,82,87	0
3	EDO	A	213	4/4	0.08	2.55	24,25,31,33	0
3	EDO	M	214	4/4	0.12	2.40	46,48,56,60	0
2	NO3	F	215	4/4	0.11	2.13	27,30,34,35	0
3	EDO	G	220	4/4	0.20	2.11	48,52,54,56	0
3	EDO	F	217	4/4	0.09	1.85	33,39,40,42	0
3	EDO	B	215	4/4	0.10	1.60	46,46,47,54	0
3	EDO	G	217	4/4	0.12	1.57	37,54,56,63	0
3	EDO	H	215	4/4	0.13	1.51	40,40,45,45	0
3	EDO	D	213	4/4	0.09	1.39	33,34,34,40	0
3	EDO	A	218	4/4	0.09	1.21	60,61,64,65	0
3	EDO	B	213	4/4	0.08	1.10	22,26,30,31	0
3	EDO	M	215	4/4	0.10	1.06	38,45,51,58	0
2	NO3	I	213	4/4	0.15	1.02	55,56,57,59	0
3	EDO	P	214	4/4	0.09	0.98	34,36,39,39	0
3	EDO	N	214	4/4	0.10	0.95	45,49,52,52	0
3	EDO	E	214	4/4	0.09	0.94	22,33,42,49	0
3	EDO	K	215	4/4	0.11	0.89	45,48,50,52	0
3	EDO	A	214	4/4	0.09	0.74	28,40,43,49	0
2	NO3	F	216	4/4	0.15	0.73	62,63,64,65	0
3	EDO	E	217	4/4	0.12	0.52	42,52,53,63	0
3	EDO	H	213	4/4	0.10	0.37	20,22,26,30	0
3	EDO	K	214	4/4	0.09	0.20	39,39,41,41	0
3	EDO	F	218	4/4	0.07	0.20	28,28,31,33	0
3	EDO	I	214	4/4	0.08	0.17	22,25,27,28	0
3	EDO	M	213	4/4	0.09	0.02	25,30,32,35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	L	213	4/4	0.07	-0.33	27,29,31,38	0
3	EDO	K	213	4/4	0.07	-0.35	27,28,32,33	0
3	EDO	E	213	4/4	0.07	-0.39	17,18,21,24	0
3	EDO	H	214	4/4	0.09	-0.50	34,42,44,53	0
3	EDO	N	213	4/4	0.06	-0.73	25,29,30,30	0
3	EDO	C	213	4/4	0.06	-1.13	29,30,32,34	0
3	EDO	G	215	4/4	0.06	-1.17	24,27,27,27	0
3	EDO	B	214	4/4	0.07	-1.32	43,46,46,48	0
3	EDO	J	213	4/4	0.06	-1.51	19,29,30,31	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.