



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:47 AM UTC

PDB ID : 4V1Y / pdb_00004v1y
Title : The structure of the hexameric atrazine chlorohydrolase, AtzA
Authors : Peat, T.S.; Newman, J.; Balotra, S.; Lucent, D.; Warden, A.C.; Scott, C.
Deposited on : 2014-10-04
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

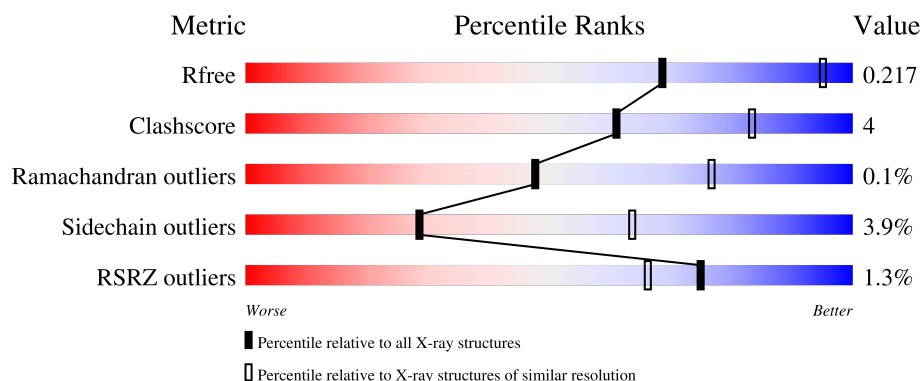
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



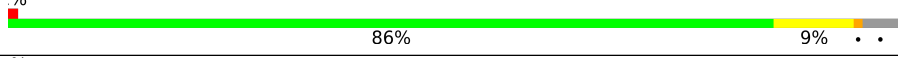
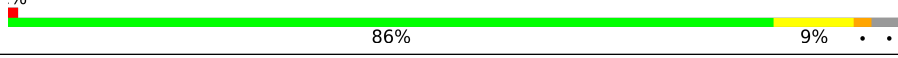
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	494	2% 86% 8% • •
1	B	494	2% 83% 11% • •
1	C	494	2% 86% 9% • •
1	D	494	2% 87% 8% • •
1	E	494	2% 87% 8% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	F	494		%
1	G	494		%
1	H	494		%
1	I	494		%
1	J	494		%
1	K	494		%
1	L	494		%

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
3	EDO	B	1475	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 44883 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 ATRAZINE CHLOROXYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	5	0
			3725	2323	687	691	24			
1	B	474	Total	C	N	O	S	0	5	0
			3735	2329	690	691	25			
1	C	473	Total	C	N	O	S	0	2	0
			3695	2308	680	683	24			
1	D	474	Total	C	N	O	S	0	2	0
			3704	2312	681	686	25			
1	E	474	Total	C	N	O	S	0	5	0
			3732	2329	688	690	25			
1	F	474	Total	C	N	O	S	0	3	0
			3710	2315	683	688	24			
1	G	474	Total	C	N	O	S	0	4	0
			3719	2320	683	690	26			
1	H	472	Total	C	N	O	S	0	4	0
			3707	2313	683	687	24			
1	I	474	Total	C	N	O	S	0	3	0
			3712	2318	683	686	25			
1	J	473	Total	C	N	O	S	0	3	0
			3705	2312	682	687	24			
1	K	474	Total	C	N	O	S	0	7	0
			3749	2338	692	693	26			
1	L	474	Total	C	N	O	S	0	4	0
			3719	2320	685	690	24			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P72156
A	-18	GLY	-	expression tag	UNP P72156
A	-17	SER	-	expression tag	UNP P72156
A	-16	SER	-	expression tag	UNP P72156
A	-15	HIS	-	expression tag	UNP P72156

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P72156
A	-13	HIS	-	expression tag	UNP P72156
A	-12	HIS	-	expression tag	UNP P72156
A	-11	HIS	-	expression tag	UNP P72156
A	-10	HIS	-	expression tag	UNP P72156
A	-9	SER	-	expression tag	UNP P72156
A	-8	SER	-	expression tag	UNP P72156
A	-7	GLY	-	expression tag	UNP P72156
A	-6	LEU	-	expression tag	UNP P72156
A	-5	VAL	-	expression tag	UNP P72156
A	-4	PRO	-	expression tag	UNP P72156
A	-3	ARG	-	expression tag	UNP P72156
A	-2	GLY	-	expression tag	UNP P72156
A	-1	SER	-	expression tag	UNP P72156
A	0	HIS	-	expression tag	UNP P72156
B	-19	MET	-	expression tag	UNP P72156
B	-18	GLY	-	expression tag	UNP P72156
B	-17	SER	-	expression tag	UNP P72156
B	-16	SER	-	expression tag	UNP P72156
B	-15	HIS	-	expression tag	UNP P72156
B	-14	HIS	-	expression tag	UNP P72156
B	-13	HIS	-	expression tag	UNP P72156
B	-12	HIS	-	expression tag	UNP P72156
B	-11	HIS	-	expression tag	UNP P72156
B	-10	HIS	-	expression tag	UNP P72156
B	-9	SER	-	expression tag	UNP P72156
B	-8	SER	-	expression tag	UNP P72156
B	-7	GLY	-	expression tag	UNP P72156
B	-6	LEU	-	expression tag	UNP P72156
B	-5	VAL	-	expression tag	UNP P72156
B	-4	PRO	-	expression tag	UNP P72156
B	-3	ARG	-	expression tag	UNP P72156
B	-2	GLY	-	expression tag	UNP P72156
B	-1	SER	-	expression tag	UNP P72156
B	0	HIS	-	expression tag	UNP P72156
C	-19	MET	-	expression tag	UNP P72156
C	-18	GLY	-	expression tag	UNP P72156
C	-17	SER	-	expression tag	UNP P72156
C	-16	SER	-	expression tag	UNP P72156
C	-15	HIS	-	expression tag	UNP P72156
C	-14	HIS	-	expression tag	UNP P72156
C	-13	HIS	-	expression tag	UNP P72156

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP P72156
C	-11	HIS	-	expression tag	UNP P72156
C	-10	HIS	-	expression tag	UNP P72156
C	-9	SER	-	expression tag	UNP P72156
C	-8	SER	-	expression tag	UNP P72156
C	-7	GLY	-	expression tag	UNP P72156
C	-6	LEU	-	expression tag	UNP P72156
C	-5	VAL	-	expression tag	UNP P72156
C	-4	PRO	-	expression tag	UNP P72156
C	-3	ARG	-	expression tag	UNP P72156
C	-2	GLY	-	expression tag	UNP P72156
C	-1	SER	-	expression tag	UNP P72156
C	0	HIS	-	expression tag	UNP P72156
D	-19	MET	-	expression tag	UNP P72156
D	-18	GLY	-	expression tag	UNP P72156
D	-17	SER	-	expression tag	UNP P72156
D	-16	SER	-	expression tag	UNP P72156
D	-15	HIS	-	expression tag	UNP P72156
D	-14	HIS	-	expression tag	UNP P72156
D	-13	HIS	-	expression tag	UNP P72156
D	-12	HIS	-	expression tag	UNP P72156
D	-11	HIS	-	expression tag	UNP P72156
D	-10	HIS	-	expression tag	UNP P72156
D	-9	SER	-	expression tag	UNP P72156
D	-8	SER	-	expression tag	UNP P72156
D	-7	GLY	-	expression tag	UNP P72156
D	-6	LEU	-	expression tag	UNP P72156
D	-5	VAL	-	expression tag	UNP P72156
D	-4	PRO	-	expression tag	UNP P72156
D	-3	ARG	-	expression tag	UNP P72156
D	-2	GLY	-	expression tag	UNP P72156
D	-1	SER	-	expression tag	UNP P72156
D	0	HIS	-	expression tag	UNP P72156
E	-19	MET	-	expression tag	UNP P72156
E	-18	GLY	-	expression tag	UNP P72156
E	-17	SER	-	expression tag	UNP P72156
E	-16	SER	-	expression tag	UNP P72156
E	-15	HIS	-	expression tag	UNP P72156
E	-14	HIS	-	expression tag	UNP P72156
E	-13	HIS	-	expression tag	UNP P72156
E	-12	HIS	-	expression tag	UNP P72156
E	-11	HIS	-	expression tag	UNP P72156

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP P72156
E	-9	SER	-	expression tag	UNP P72156
E	-8	SER	-	expression tag	UNP P72156
E	-7	GLY	-	expression tag	UNP P72156
E	-6	LEU	-	expression tag	UNP P72156
E	-5	VAL	-	expression tag	UNP P72156
E	-4	PRO	-	expression tag	UNP P72156
E	-3	ARG	-	expression tag	UNP P72156
E	-2	GLY	-	expression tag	UNP P72156
E	-1	SER	-	expression tag	UNP P72156
E	0	HIS	-	expression tag	UNP P72156
F	-19	MET	-	expression tag	UNP P72156
F	-18	GLY	-	expression tag	UNP P72156
F	-17	SER	-	expression tag	UNP P72156
F	-16	SER	-	expression tag	UNP P72156
F	-15	HIS	-	expression tag	UNP P72156
F	-14	HIS	-	expression tag	UNP P72156
F	-13	HIS	-	expression tag	UNP P72156
F	-12	HIS	-	expression tag	UNP P72156
F	-11	HIS	-	expression tag	UNP P72156
F	-10	HIS	-	expression tag	UNP P72156
F	-9	SER	-	expression tag	UNP P72156
F	-8	SER	-	expression tag	UNP P72156
F	-7	GLY	-	expression tag	UNP P72156
F	-6	LEU	-	expression tag	UNP P72156
F	-5	VAL	-	expression tag	UNP P72156
F	-4	PRO	-	expression tag	UNP P72156
F	-3	ARG	-	expression tag	UNP P72156
F	-2	GLY	-	expression tag	UNP P72156
F	-1	SER	-	expression tag	UNP P72156
F	0	HIS	-	expression tag	UNP P72156
G	-19	MET	-	expression tag	UNP P72156
G	-18	GLY	-	expression tag	UNP P72156
G	-17	SER	-	expression tag	UNP P72156
G	-16	SER	-	expression tag	UNP P72156
G	-15	HIS	-	expression tag	UNP P72156
G	-14	HIS	-	expression tag	UNP P72156
G	-13	HIS	-	expression tag	UNP P72156
G	-12	HIS	-	expression tag	UNP P72156
G	-11	HIS	-	expression tag	UNP P72156
G	-10	HIS	-	expression tag	UNP P72156
G	-9	SER	-	expression tag	UNP P72156

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	expression tag	UNP P72156
G	-7	GLY	-	expression tag	UNP P72156
G	-6	LEU	-	expression tag	UNP P72156
G	-5	VAL	-	expression tag	UNP P72156
G	-4	PRO	-	expression tag	UNP P72156
G	-3	ARG	-	expression tag	UNP P72156
G	-2	GLY	-	expression tag	UNP P72156
G	-1	SER	-	expression tag	UNP P72156
G	0	HIS	-	expression tag	UNP P72156
H	-19	MET	-	expression tag	UNP P72156
H	-18	GLY	-	expression tag	UNP P72156
H	-17	SER	-	expression tag	UNP P72156
H	-16	SER	-	expression tag	UNP P72156
H	-15	HIS	-	expression tag	UNP P72156
H	-14	HIS	-	expression tag	UNP P72156
H	-13	HIS	-	expression tag	UNP P72156
H	-12	HIS	-	expression tag	UNP P72156
H	-11	HIS	-	expression tag	UNP P72156
H	-10	HIS	-	expression tag	UNP P72156
H	-9	SER	-	expression tag	UNP P72156
H	-8	SER	-	expression tag	UNP P72156
H	-7	GLY	-	expression tag	UNP P72156
H	-6	LEU	-	expression tag	UNP P72156
H	-5	VAL	-	expression tag	UNP P72156
H	-4	PRO	-	expression tag	UNP P72156
H	-3	ARG	-	expression tag	UNP P72156
H	-2	GLY	-	expression tag	UNP P72156
H	-1	SER	-	expression tag	UNP P72156
H	0	HIS	-	expression tag	UNP P72156
I	-19	MET	-	expression tag	UNP P72156
I	-18	GLY	-	expression tag	UNP P72156
I	-17	SER	-	expression tag	UNP P72156
I	-16	SER	-	expression tag	UNP P72156
I	-15	HIS	-	expression tag	UNP P72156
I	-14	HIS	-	expression tag	UNP P72156
I	-13	HIS	-	expression tag	UNP P72156
I	-12	HIS	-	expression tag	UNP P72156
I	-11	HIS	-	expression tag	UNP P72156
I	-10	HIS	-	expression tag	UNP P72156
I	-9	SER	-	expression tag	UNP P72156
I	-8	SER	-	expression tag	UNP P72156
I	-7	GLY	-	expression tag	UNP P72156

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP P72156
I	-5	VAL	-	expression tag	UNP P72156
I	-4	PRO	-	expression tag	UNP P72156
I	-3	ARG	-	expression tag	UNP P72156
I	-2	GLY	-	expression tag	UNP P72156
I	-1	SER	-	expression tag	UNP P72156
I	0	HIS	-	expression tag	UNP P72156
J	-19	MET	-	expression tag	UNP P72156
J	-18	GLY	-	expression tag	UNP P72156
J	-17	SER	-	expression tag	UNP P72156
J	-16	SER	-	expression tag	UNP P72156
J	-15	HIS	-	expression tag	UNP P72156
J	-14	HIS	-	expression tag	UNP P72156
J	-13	HIS	-	expression tag	UNP P72156
J	-12	HIS	-	expression tag	UNP P72156
J	-11	HIS	-	expression tag	UNP P72156
J	-10	HIS	-	expression tag	UNP P72156
J	-9	SER	-	expression tag	UNP P72156
J	-8	SER	-	expression tag	UNP P72156
J	-7	GLY	-	expression tag	UNP P72156
J	-6	LEU	-	expression tag	UNP P72156
J	-5	VAL	-	expression tag	UNP P72156
J	-4	PRO	-	expression tag	UNP P72156
J	-3	ARG	-	expression tag	UNP P72156
J	-2	GLY	-	expression tag	UNP P72156
J	-1	SER	-	expression tag	UNP P72156
J	0	HIS	-	expression tag	UNP P72156
K	-19	MET	-	expression tag	UNP P72156
K	-18	GLY	-	expression tag	UNP P72156
K	-17	SER	-	expression tag	UNP P72156
K	-16	SER	-	expression tag	UNP P72156
K	-15	HIS	-	expression tag	UNP P72156
K	-14	HIS	-	expression tag	UNP P72156
K	-13	HIS	-	expression tag	UNP P72156
K	-12	HIS	-	expression tag	UNP P72156
K	-11	HIS	-	expression tag	UNP P72156
K	-10	HIS	-	expression tag	UNP P72156
K	-9	SER	-	expression tag	UNP P72156
K	-8	SER	-	expression tag	UNP P72156
K	-7	GLY	-	expression tag	UNP P72156
K	-6	LEU	-	expression tag	UNP P72156
K	-5	VAL	-	expression tag	UNP P72156

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP P72156
K	-3	ARG	-	expression tag	UNP P72156
K	-2	GLY	-	expression tag	UNP P72156
K	-1	SER	-	expression tag	UNP P72156
K	0	HIS	-	expression tag	UNP P72156
L	-19	MET	-	expression tag	UNP P72156
L	-18	GLY	-	expression tag	UNP P72156
L	-17	SER	-	expression tag	UNP P72156
L	-16	SER	-	expression tag	UNP P72156
L	-15	HIS	-	expression tag	UNP P72156
L	-14	HIS	-	expression tag	UNP P72156
L	-13	HIS	-	expression tag	UNP P72156
L	-12	HIS	-	expression tag	UNP P72156
L	-11	HIS	-	expression tag	UNP P72156
L	-10	HIS	-	expression tag	UNP P72156
L	-9	SER	-	expression tag	UNP P72156
L	-8	SER	-	expression tag	UNP P72156
L	-7	GLY	-	expression tag	UNP P72156
L	-6	LEU	-	expression tag	UNP P72156
L	-5	VAL	-	expression tag	UNP P72156
L	-4	PRO	-	expression tag	UNP P72156
L	-3	ARG	-	expression tag	UNP P72156
L	-2	GLY	-	expression tag	UNP P72156
L	-1	SER	-	expression tag	UNP P72156
L	0	HIS	-	expression tag	UNP P72156

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

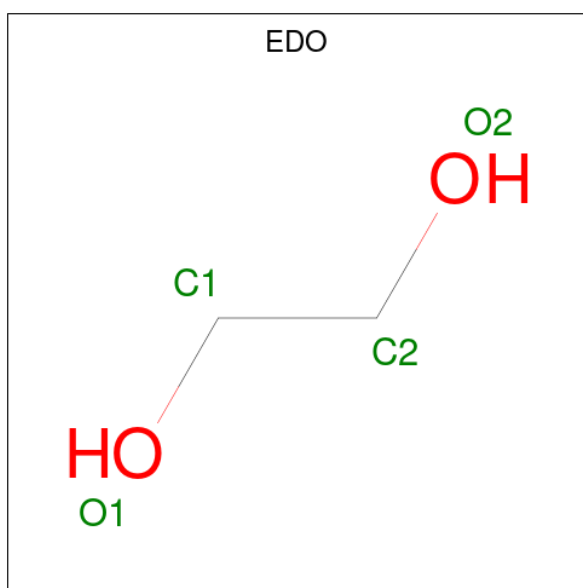
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total	Fe	0	0
			1	1		
2	I	1	Total	Fe	0	0
			1	1		
2	J	1	Total	Fe	0	0
			1	1		
2	K	1	Total	Fe	0	0
			1	1		
2	L	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



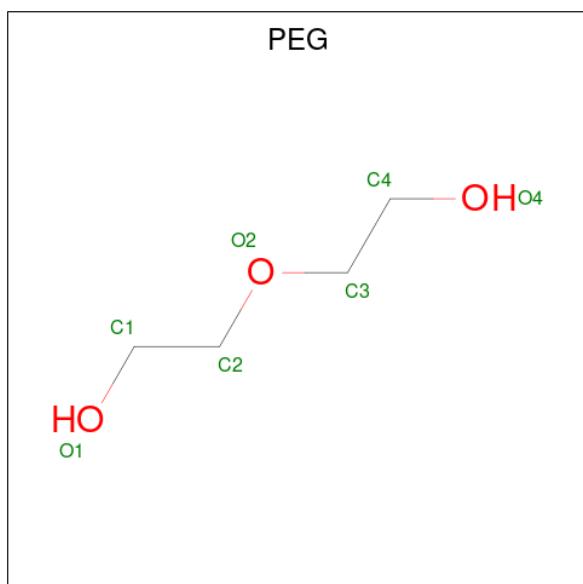
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	I	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	K	1	Total	C	O	0	0
			7	4	3		
4	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Cl	0	0
			1	1		

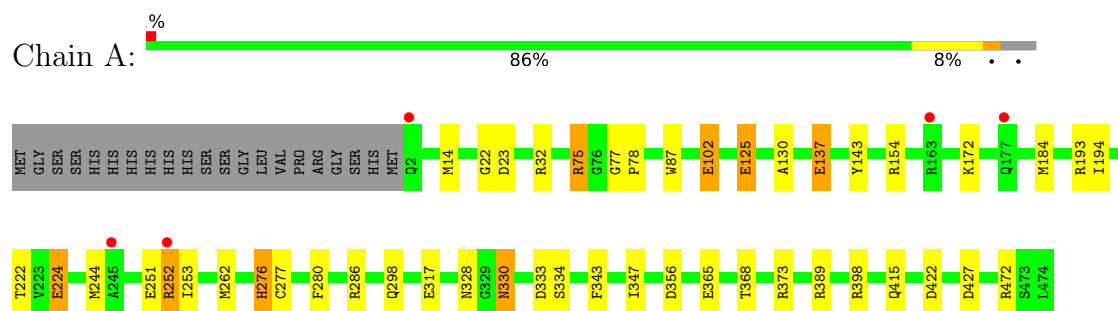
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	17	Total	O	0	0
			17	17		
6	C	11	Total	O	0	0
			11	11		
6	D	10	Total	O	0	0
			10	10		
6	E	15	Total	O	0	0
			15	15		
6	F	7	Total	O	0	0
			7	7		
6	G	11	Total	O	0	0
			11	11		
6	H	11	Total	O	0	0
			11	11		
6	I	25	Total	O	0	0
			25	25		
6	J	8	Total	O	0	0
			8	8		
6	K	20	Total	O	0	0
			20	20		
6	L	12	Total	O	0	0
			12	12		

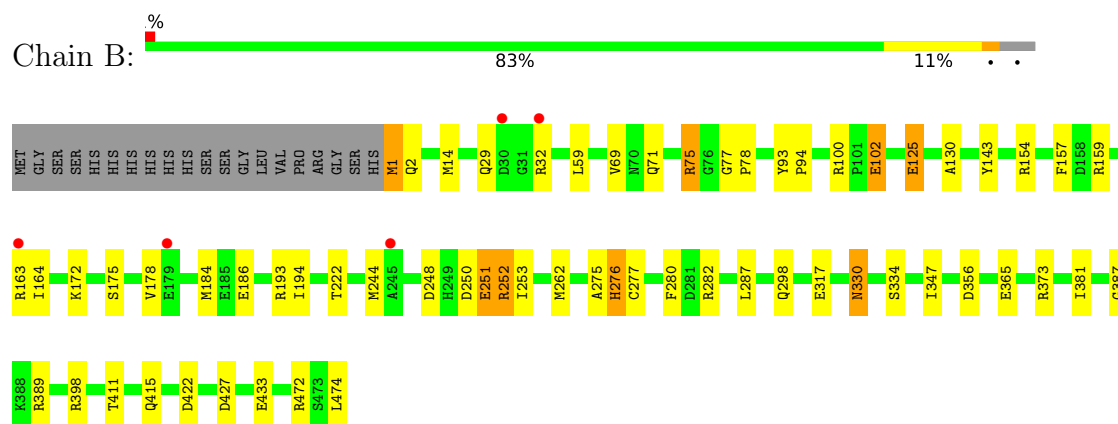
3 Residue-property plots [i](#)

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

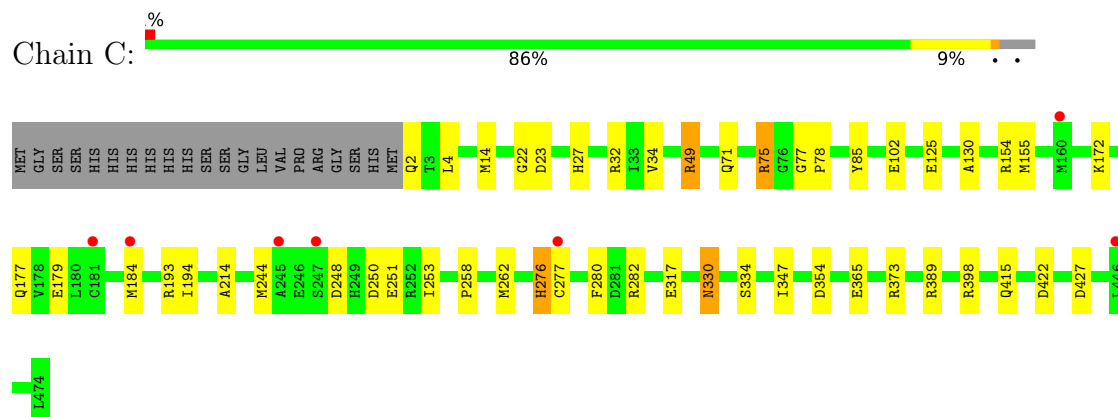
• Molecule 1: ATRAZINE CHLOROHYDROLASE



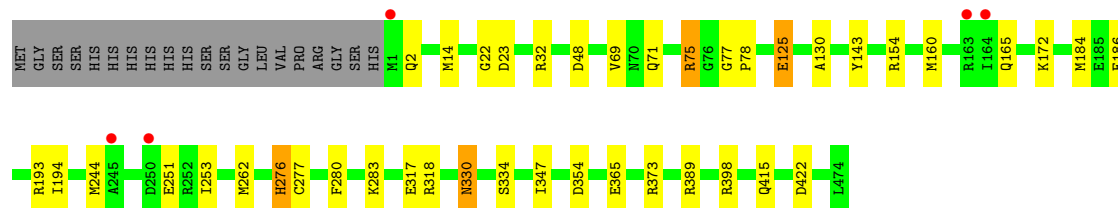
• Molecule 1: ATRAZINE CHLOROHYDROLASE



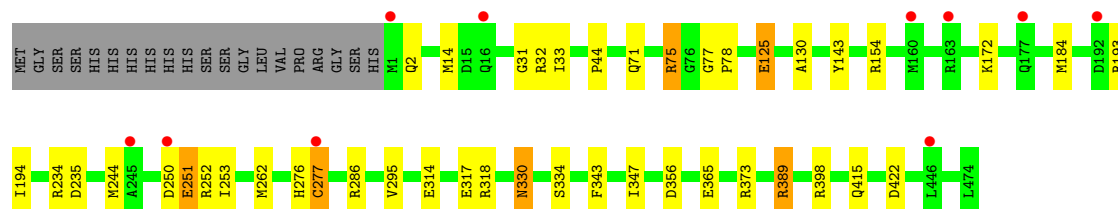
• Molecule 1: ATRAZINE CHLOROHYDROLASE



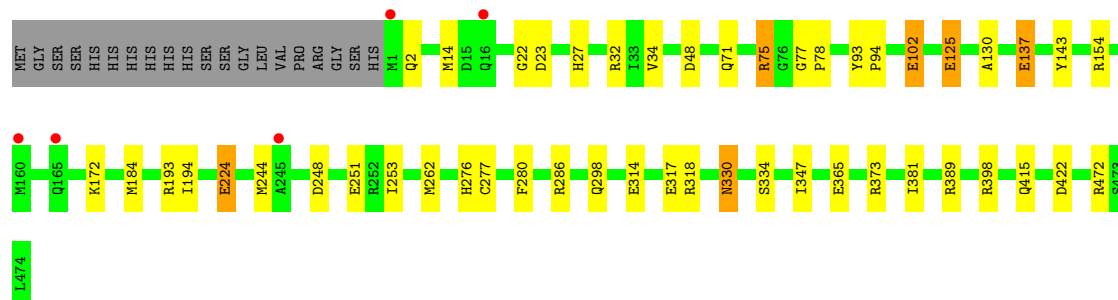
● Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain D: 

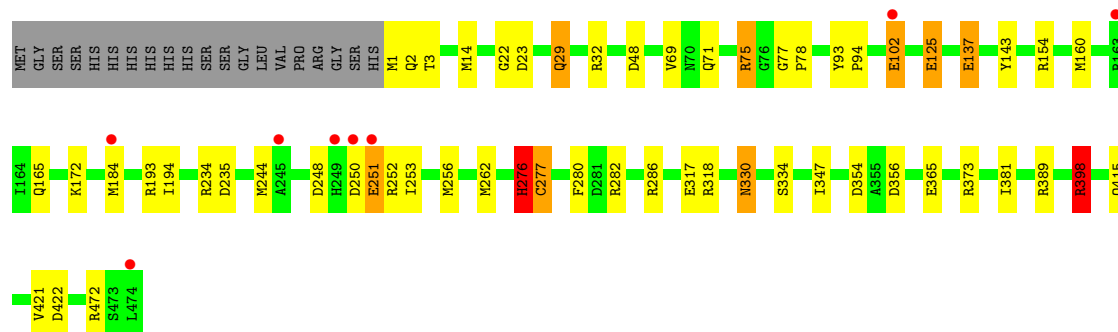
● Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain E: 

● Molecule 1: ATRAZINE CHLOROHYDROLASE

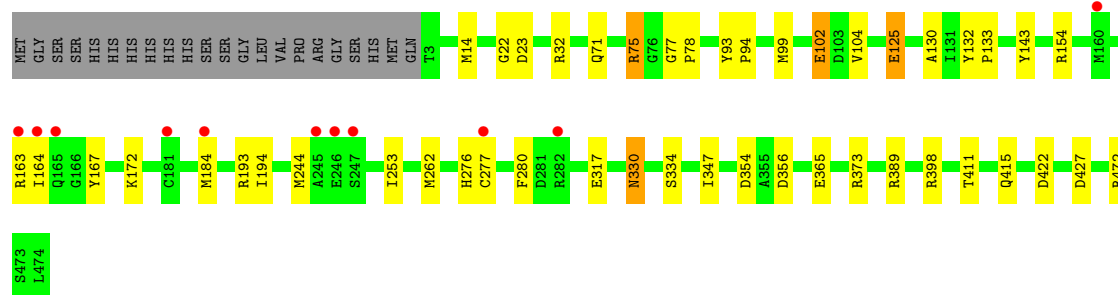
Chain F: 

● Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain G: 

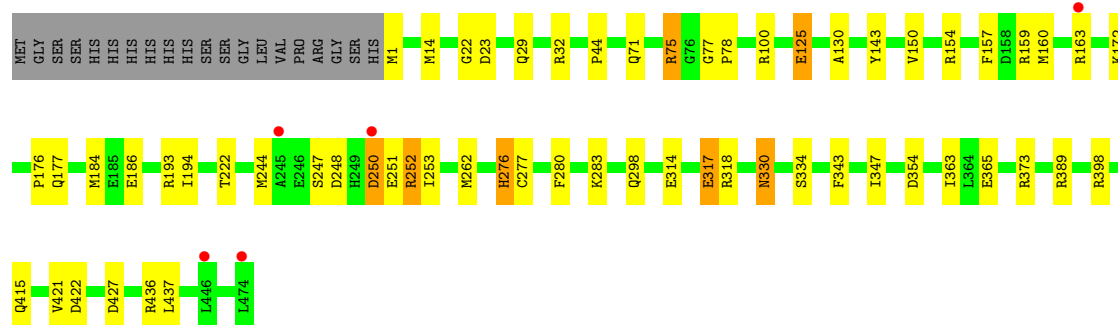
● Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain H:  2% 86% 9% . .



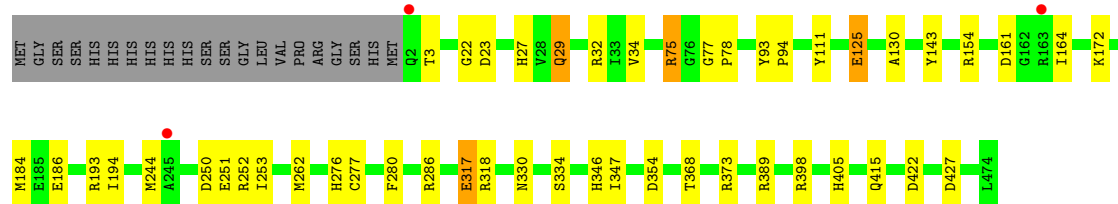
• Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain I:  84% 11% . .



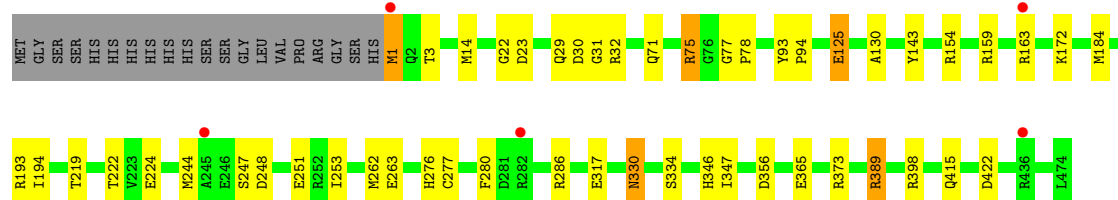
• Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain J:  86% 9% . .

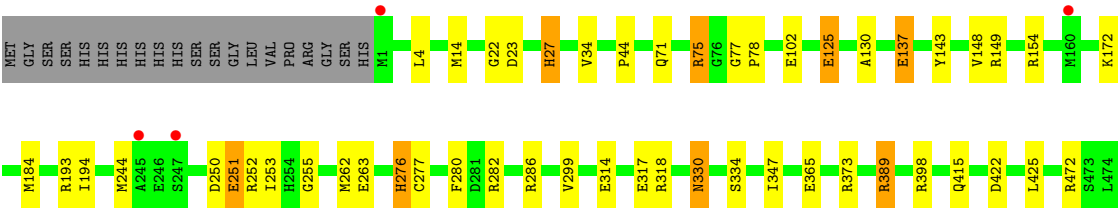
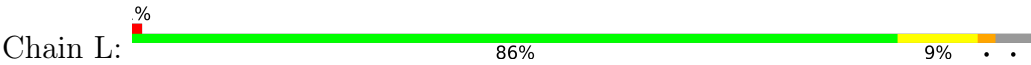


• Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain K:  86% 9% . .



• Molecule 1: ATRAZINE CHLOROHYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	117.49Å 195.56Å 283.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	161.05 – 2.80 161.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (161.05-2.80) 99.9 (161.05-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.187 , 0.218 0.190 , 0.217	Depositor DCC
R_{free} test set	7864 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 19.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	44883	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5597e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, FE, CL, EDO

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	0.99	1/3802 (0.0%)	0.99	3/5160 (0.1%)
1	B	1.07	3/3812 (0.1%)	1.03	7/5172 (0.1%)
1	C	0.94	0/3772	0.98	2/5121 (0.0%)
1	D	1.02	0/3781	1.01	3/5132 (0.1%)
1	E	1.03	0/3809	0.99	2/5169 (0.0%)
1	F	1.01	0/3787	1.00	2/5141 (0.0%)
1	G	1.02	3/3796 (0.1%)	0.99	6/5152 (0.1%)
1	H	0.96	0/3784	0.98	0/5136
1	I	1.06	3/3789 (0.1%)	1.02	5/5143 (0.1%)
1	J	1.00	2/3782 (0.1%)	1.02	1/5134 (0.0%)
1	K	1.02	0/3826	0.99	2/5191 (0.0%)
1	L	1.04	2/3796 (0.1%)	1.02	6/5153 (0.1%)
All	All	1.01	14/45536 (0.0%)	1.00	39/61804 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1	MET	C-N	13.43	1.51	1.33
1	A	368	THR	CA-C	6.93	1.55	1.52
1	I	421	VAL	C-O	-6.72	1.16	1.24
1	G	421	VAL	C-O	-6.42	1.16	1.24
1	I	437	LEU	C-O	-6.06	1.16	1.24
1	J	368	THR	CA-C	5.95	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	276	HIS	C-O	-5.85	1.16	1.24
1	L	27	HIS	C-O	-5.58	1.17	1.24
1	B	178	VAL	CA-C	-5.53	1.45	1.52
1	B	59	LEU	N-CA	5.38	1.50	1.45
1	I	436	ARG	C-O	-5.33	1.17	1.24
1	B	433	GLU	C-O	-5.28	1.18	1.23
1	L	44	PRO	C-O	-5.13	1.20	1.24
1	J	405	HIS	C-O	-5.13	1.18	1.23

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	VAL	N-CA-C	-9.63	94.04	108.97
1	D	69	VAL	N-CA-C	6.35	116.98	110.82
1	G	137	GLU	N-CA-CB	6.14	118.91	110.01
1	B	175	SER	CA-C-N	-6.08	113.70	120.45
1	B	175	SER	C-N-CA	-6.08	113.70	120.45
1	F	137	GLU	N-CA-CB	6.02	118.97	110.12
1	A	137	GLU	N-CA-CB	5.95	118.64	110.01
1	L	137	GLU	N-CA-CB	5.89	118.54	110.01
1	D	276	HIS	CA-C-N	-5.76	114.58	123.17
1	D	276	HIS	C-N-CA	-5.76	114.58	123.17
1	G	1	MET	CA-C-N	5.69	129.87	120.94
1	G	1	MET	C-N-CA	5.69	129.87	120.94
1	B	276	HIS	CA-C-N	-5.59	114.84	123.17
1	B	276	HIS	C-N-CA	-5.59	114.84	123.17
1	I	276	HIS	CA-C-N	-5.57	114.87	123.17
1	I	276	HIS	C-N-CA	-5.57	114.87	123.17
1	F	381	ILE	N-CA-C	5.56	115.60	108.82
1	L	299	VAL	N-CA-C	5.51	116.24	110.62
1	K	346	HIS	N-CA-C	5.48	118.43	111.69
1	I	363	ILE	CB-CA-C	-5.47	104.75	112.14
1	A	276	HIS	CA-C-N	-5.47	115.02	123.17
1	A	276	HIS	C-N-CA	-5.47	115.02	123.17
1	K	389	ARG	CB-CG-CD	5.45	123.84	111.30
1	I	150	VAL	CB-CA-C	-5.37	102.50	110.33
1	J	346	HIS	N-CA-C	5.34	118.26	111.69
1	G	381	ILE	N-CA-C	5.34	115.33	108.82
1	G	69	VAL	N-CA-C	5.31	115.97	110.82
1	E	44	PRO	O-C-N	5.31	123.65	121.15
1	G	398	ARG	CG-CD-NE	5.29	123.63	112.00
1	L	276	HIS	CA-C-N	-5.19	115.43	123.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	276	HIS	C-N-CA	-5.19	115.43	123.17
1	L	44	PRO	O-C-N	5.18	123.59	121.15
1	C	276	HIS	CA-C-N	-5.16	115.48	123.17
1	C	276	HIS	C-N-CA	-5.16	115.48	123.17
1	B	69	VAL	N-CA-C	5.12	115.79	110.82
1	I	44	PRO	O-C-N	5.05	123.52	121.15
1	L	148	VAL	CB-CA-C	-5.03	106.05	111.59
1	B	381	ILE	N-CA-C	5.01	114.94	108.82
1	E	389	ARG	CB-CG-CD	5.01	122.82	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	276	HIS	Peptide,Mainchain

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	3725	0	3656	43	0
1	B	3735	0	3673	55	0
1	C	3695	0	3637	28	0
1	D	3704	0	3644	33	0
1	E	3732	0	3673	31	0
1	F	3710	0	3644	34	0
1	G	3719	0	3653	44	0
1	H	3707	0	3641	30	0
1	I	3712	0	3656	46	0
1	J	3705	0	3639	31	0
1	K	3749	0	3687	31	0
1	L	3719	0	3649	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	8	0	12	0	0
3	B	4	0	6	6	0
3	C	4	0	6	2	0
3	E	4	0	6	0	0
3	F	4	0	6	0	0
3	G	4	0	6	0	0
3	H	4	0	6	0	0
3	J	8	0	12	3	0
3	L	8	0	12	3	0
4	B	7	0	10	1	0
4	C	7	0	10	0	0
4	D	7	0	10	2	0
4	F	7	0	10	0	0
4	I	7	0	10	2	0
4	K	7	0	10	1	0
4	L	7	0	10	1	0
5	H	1	0	0	0	0
6	A	14	0	0	0	0
6	B	17	0	0	4	0
6	C	11	0	0	0	0
6	D	10	0	0	0	0
6	E	15	0	0	0	0
6	F	7	0	0	0	0
6	G	11	0	0	0	0
6	H	11	0	0	1	0
6	I	25	0	0	1	0
6	J	8	0	0	0	0
6	K	20	0	0	1	0
6	L	12	0	0	0	0
All	All	44883	0	43994	375	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 4.

All (375) 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:G:234:ARG:NH2	1:G:235:ASP:OD1	1.86	1.07
1:G:3:THR:HG22	1:G:29:GLN:HG3	1.36	1.04
1:B:186:GLU:HG2	1:I:222:THR:HG22	1.39	1.03
1:G:3:THR:CG2	1:G:29:GLN:HG3	1.98	0.94
1:K:277[A]:CYS:SG	1:K:280:PHE:CZ	2.62	0.93
1:F:224:GLU:N	1:F:224:GLU:OE1	2.01	0.92
1:B:222:THR:HG22	1:I:186:GLU:HG2	1.50	0.91
1:J:161:ASP:O	1:J:164:ILE:HG22	1.71	0.90
1:I:1:MET:HE3	1:I:29:GLN:CD	1.97	0.90
1:I:252:ARG:HG2	1:I:252:ARG:HH11	1.34	0.88
1:G:277[B]:CYS:SG	1:G:280:PHE:CZ	2.67	0.88
1:F:277:CYS:SG	1:F:280:PHE:CZ	2.66	0.87
1:I:277:CYS:SG	1:I:280:PHE:CZ	2.68	0.86
1:C:277:CYS:SG	1:C:280:PHE:CZ	2.68	0.86
1:B:1:MET:HE2	1:B:29:GLN:NE2	1.91	0.86
1:A:277:CYS:SG	1:A:280:PHE:CZ	2.69	0.85
1:J:277:CYS:SG	1:J:280:PHE:CZ	2.70	0.84
1:L:277:CYS:SG	1:L:280:PHE:CZ	2.70	0.83
1:H:277:CYS:SG	1:H:280:PHE:CZ	2.71	0.83
1:B:282[B]:ARG:NH1	3:B:1475:EDO:H22	1.94	0.83
1:G:2:GLN:NE2	1:G:48:ASP:OD2	2.11	0.83
1:B:282[B]:ARG:NH1	3:B:1475:EDO:O2	2.13	0.82
1:J:3:THR:HG22	1:J:29:GLN:HG3	1.60	0.81
1:B:282[B]:ARG:NH1	3:B:1475:EDO:C2	2.43	0.81
1:B:277:CYS:SG	1:B:280:PHE:CZ	2.74	0.81
1:D:277:CYS:SG	1:D:280:PHE:CZ	2.72	0.81
1:C:282:ARG:HH22	1:F:314:GLU:HG3	1.45	0.80
1:E:234:ARG:NH1	1:E:235:ASP:OD1	2.14	0.80
1:I:163:ARG:NH2	6:I:2015:HOH:O	1.69	0.79
1:K:3:THR:HG22	1:K:29:GLN:HG3	1.64	0.78
1:C:251:GLU:O	1:C:258:PRO:HD3	1.82	0.78
1:G:398:ARG:HH11	1:G:398:ARG:HB2	1.49	0.77
1:J:318:ARG:HH22	3:J:1476:EDO:H11	1.49	0.77
1:B:317[A]:GLU:HG2	1:E:318:ARG:HE	1.51	0.76
1:F:2:GLN:HG2	1:F:48:ASP:OD2	1.84	0.76
1:I:252:ARG:HG2	1:I:252:ARG:NH1	2.01	0.76
3:B:1475:EDO:H11	1:E:318:ARG:HH22	1.50	0.76
1:I:1:MET:HE3	1:I:29:GLN:NE2	2.01	0.75
3:C:1475:EDO:H12	1:F:318:ARG:HH22	1.48	0.75
1:B:282[B]:ARG:HH12	3:B:1475:EDO:C2	1.99	0.75
1:G:251:GLU:O	1:G:252:ARG:HG2	1.87	0.74
1:G:398:ARG:HH11	1:G:398:ARG:CB	2.02	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1475:EDO:C1	1:F:318:ARG:HH22	2.02	0.73
1:L:389:ARG:NH1	1:L:389:ARG:HG3	2.04	0.72
1:D:2:GLN:NE2	1:D:48:ASP:OD2	2.22	0.72
1:K:248:ASP:HA	1:K:251:GLU:HG3	1.69	0.72
1:E:356:ASP:OD2	1:F:472:ARG:NH2	2.22	0.72
1:A:356:ASP:OD2	1:B:472:ARG:NH2	2.24	0.71
1:K:277[A]:CYS:SG	1:K:280:PHE:CE2	2.83	0.71
1:H:163:ARG:NH2	6:H:2004:HOH:O	1.97	0.71
1:G:277[B]:CYS:SG	1:G:280:PHE:CE2	2.84	0.70
1:G:3:THR:HG22	1:G:29:GLN:CG	2.19	0.66
1:G:244:MET:O	1:G:276:HIS:O	2.12	0.66
1:C:4:LEU:HD12	1:C:49:ARG:HB3	1.77	0.66
1:A:317[A]:GLU:HG2	1:D:318:ARG:HE	1.60	0.66
1:H:354:ASP:OD2	1:K:286:ARG:NH1	2.25	0.66
1:B:317[A]:GLU:HG2	1:E:318:ARG:NE	2.10	0.65
1:I:277:CYS:SG	1:I:280:PHE:CE2	2.90	0.65
1:K:163:ARG:NH2	6:K:2013:HOH:O	2.12	0.65
1:A:317[A]:GLU:HG2	1:D:318:ARG:NE	2.12	0.65
1:L:252:ARG:HE	1:L:255:GLY:HA2	1.62	0.65
1:J:318:ARG:HH22	3:J:1476:EDO:C1	2.09	0.64
1:A:286:ARG:NH1	1:D:354:ASP:OD2	2.25	0.64
1:B:102[A]:GLU:HG3	6:B:2006:HOH:O	1.97	0.63
1:C:277:CYS:SG	1:C:280:PHE:CE2	2.90	0.63
1:L:250:ASP:C	1:L:252:ARG:H	2.08	0.62
1:C:4:LEU:CD1	1:C:49:ARG:HB3	2.29	0.62
1:F:277:CYS:SG	1:F:280:PHE:CE2	2.90	0.62
1:B:102[A]:GLU:CG	6:B:2006:HOH:O	2.48	0.62
1:B:154:ARG:HG3	1:B:194:ILE:HG12	1.82	0.62
1:L:277:CYS:SG	1:L:280:PHE:CE2	2.90	0.61
1:G:154:ARG:HG3	1:G:194:ILE:HG12	1.83	0.61
1:D:283:LYS:NZ	4:D:1475:PEG:H21	2.14	0.61
1:G:472:ARG:NH2	1:H:356:ASP:OD2	2.33	0.60
1:B:100:ARG:NH2	1:G:165:GLN:HG2	2.17	0.60
1:B:277:CYS:SG	1:B:280:PHE:CE2	2.94	0.60
1:G:415:GLN:NE2	1:H:75:ARG:HD3	2.17	0.60
1:L:154:ARG:HG3	1:L:194:ILE:HG12	1.83	0.60
1:D:277:CYS:SG	1:D:280:PHE:CE2	2.93	0.60
1:H:277:CYS:SG	1:H:280:PHE:CE2	2.92	0.60
1:I:283:LYS:HZ1	4:I:1475:PEG:H21	1.66	0.59
1:A:277:CYS:SG	1:A:280:PHE:CE2	2.93	0.59
1:A:328:ASN:HB3	1:A:330:ASN:HD22	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:GLN:CD	1:D:48:ASP:OD2	2.46	0.59
1:L:250:ASP:O	1:L:252:ARG:N	2.34	0.59
1:G:154:ARG:CG	1:G:194:ILE:HG12	2.33	0.59
1:K:248:ASP:HA	1:K:251:GLU:CG	2.33	0.59
1:B:1:MET:CE	1:B:29:GLN:NE2	2.64	0.58
1:B:186:GLU:OE2	1:I:159:ARG:NE	2.32	0.58
1:I:154:ARG:HG3	1:I:194:ILE:HG12	1.84	0.58
1:L:154:ARG:CG	1:L:194:ILE:HG12	2.33	0.58
1:D:154:ARG:HG2	1:D:194:ILE:HG12	1.84	0.58
1:F:27:HIS:HD2	1:F:34:VAL:CG2	2.16	0.58
1:C:27:HIS:HD2	1:C:34:VAL:CG2	2.16	0.58
1:A:347:ILE:CD1	1:B:347:ILE:HD12	2.33	0.58
1:L:251:GLU:HG2	1:L:251:GLU:O	2.02	0.58
1:A:222:THR:OG1	1:A:224:GLU:HG2	2.03	0.58
1:B:154:ARG:CG	1:B:194:ILE:HG12	2.34	0.58
1:F:154:ARG:HG3	1:F:194:ILE:HG12	1.86	0.58
1:E:244:MET:O	1:E:276:HIS:O	2.22	0.58
1:A:347:ILE:HD12	1:B:347:ILE:CD1	2.34	0.57
1:I:247:SER:OG	1:I:250:ASP:OD2	2.22	0.57
1:A:251:GLU:O	1:A:252[A]:ARG:HD2	2.03	0.57
1:I:283:LYS:NZ	4:I:1475:PEG:H21	2.19	0.57
1:C:154:ARG:HG3	1:C:194:ILE:HG12	1.86	0.57
1:I:75:ARG:HD3	1:J:415:GLN:NE2	2.19	0.57
1:J:244:MET:O	1:J:276:HIS:O	2.23	0.57
1:K:356:ASP:OD2	1:L:472:ARG:NH2	2.37	0.57
1:E:154:ARG:HG3	1:E:194:ILE:HG12	1.85	0.57
1:E:250:ASP:O	1:E:252:ARG:N	2.37	0.57
1:C:244:MET:O	1:C:276:HIS:O	2.23	0.57
1:J:154:ARG:HG3	1:J:194:ILE:HG12	1.86	0.57
1:A:154:ARG:HG3	1:A:194:ILE:HG12	1.87	0.57
1:A:472:ARG:NH2	1:B:356:ASP:OD2	2.38	0.57
1:H:154:ARG:CG	1:H:194:ILE:HG12	2.35	0.57
1:H:154:ARG:HG3	1:H:194:ILE:HG12	1.86	0.57
1:A:244:MET:O	1:A:276:HIS:O	2.23	0.56
1:D:244:MET:O	1:D:276:HIS:O	2.23	0.56
1:F:244:MET:O	1:F:276:HIS:O	2.23	0.56
1:G:356:ASP:OD2	1:H:472:ARG:NH2	2.37	0.56
1:K:415:GLN:NE2	1:L:75:ARG:HD3	2.19	0.56
1:K:244:MET:O	1:K:276:HIS:O	2.22	0.56
1:E:75:ARG:HD3	1:F:415:GLN:NE2	2.20	0.56
1:K:154:ARG:HG3	1:K:194:ILE:HG12	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:NH2	6:B:2010:HOH:O	2.02	0.56
1:G:347:ILE:CD1	1:H:347:ILE:HD12	2.36	0.56
1:K:263:GLU:HG2	4:K:1475:PEG:H22	1.88	0.56
1:C:415:GLN:NE2	1:D:75:ARG:HD3	2.21	0.56
1:B:159:ARG:NE	1:I:186:GLU:OE2	2.37	0.56
1:E:154:ARG:CG	1:E:194:ILE:HG12	2.36	0.56
1:I:244:MET:O	1:I:276:HIS:O	2.23	0.56
1:J:154:ARG:CG	1:J:194:ILE:HG12	2.36	0.56
1:B:244:MET:O	1:B:276:HIS:O	2.22	0.55
1:A:328:ASN:HB3	1:A:330:ASN:ND2	2.21	0.55
1:G:2:GLN:CD	1:G:48:ASP:OD2	2.49	0.55
1:D:165:GLN:CD	1:I:100:ARG:HH22	2.14	0.55
1:I:154:ARG:CG	1:I:194:ILE:HG12	2.37	0.55
1:C:154:ARG:CG	1:C:194:ILE:HG12	2.36	0.55
1:H:244:MET:O	1:H:276:HIS:O	2.24	0.55
1:C:75:ARG:HD3	1:D:415:GLN:NE2	2.21	0.55
1:G:347:ILE:HD12	1:H:347:ILE:CD1	2.37	0.55
1:L:244:MET:O	1:L:276:HIS:O	2.23	0.55
1:I:1:MET:HE3	1:I:29:GLN:OE1	2.06	0.55
1:J:277:CYS:SG	1:J:280:PHE:CE2	2.97	0.55
1:J:318:ARG:NH2	3:J:1476:EDO:H11	2.21	0.55
1:L:149:ARG:NH2	1:L:389:ARG:HG2	2.21	0.55
1:A:154:ARG:CG	1:A:194:ILE:HG12	2.36	0.54
1:K:154:ARG:CG	1:K:194:ILE:HG12	2.37	0.54
1:E:415:GLN:NE2	1:F:75:ARG:HD3	2.23	0.54
1:F:154:ARG:CG	1:F:194:ILE:HG12	2.37	0.54
1:G:75:ARG:HD3	1:H:415:GLN:NE2	2.23	0.54
1:I:176:PRO:HD2	1:I:177:GLN:OE1	2.08	0.54
1:A:347:ILE:HD12	1:B:347:ILE:HD12	1.90	0.53
1:C:282:ARG:NH2	1:F:314:GLU:HG3	2.20	0.53
1:J:250:ASP:O	1:J:252:ARG:N	2.41	0.53
1:C:354:ASP:OD2	1:F:286:ARG:NH1	2.29	0.53
1:D:283:LYS:HZ3	4:D:1475:PEG:H21	1.72	0.53
1:A:330:ASN:C	1:A:333:ASP:OD1	2.52	0.53
1:B:100:ARG:HH22	1:G:165:GLN:HG2	1.73	0.53
1:G:251:GLU:O	1:G:252:ARG:CG	2.56	0.53
1:C:347:ILE:CD1	1:D:347:ILE:HD12	2.38	0.53
1:C:347:ILE:HD12	1:D:347:ILE:CD1	2.38	0.53
1:I:347:ILE:HD12	1:J:347:ILE:CD1	2.40	0.52
1:D:154:ARG:CG	1:D:194:ILE:HG12	2.39	0.52
1:A:252[A]:ARG:HH11	1:A:252[A]:ARG:CG	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:347:ILE:HD12	1:H:347:ILE:HD12	1.92	0.52
1:J:27:HIS:HD2	1:J:34:VAL:CG2	2.22	0.52
1:E:250:ASP:C	1:E:252:ARG:H	2.16	0.52
1:G:354:ASP:OD2	1:J:286:ARG:NH1	2.30	0.52
1:I:415:GLN:NE2	1:J:75:ARG:HD3	2.24	0.52
1:I:347:ILE:CD1	1:J:347:ILE:HD12	2.40	0.51
1:A:415:GLN:NE2	1:B:75:ARG:HD3	2.26	0.51
1:B:1:MET:HE2	1:B:29:GLN:CD	2.36	0.51
1:E:347:ILE:CD1	1:F:347:ILE:HD12	2.41	0.51
1:H:164:ILE:HG13	1:H:164:ILE:O	2.10	0.51
1:I:314:GLU:HG3	1:L:282:ARG:NH1	2.26	0.51
1:L:263:GLU:HG2	4:L:1477:PEG:H22	1.92	0.51
1:K:248:ASP:CB	1:K:251:GLU:OE2	2.59	0.50
1:A:75:ARG:HD3	1:B:415:GLN:NE2	2.26	0.50
1:G:286:ARG:NH1	1:J:354:ASP:OD2	2.31	0.50
1:B:164:ILE:HG13	1:B:164:ILE:O	2.11	0.50
1:E:347:ILE:HD12	1:F:347:ILE:CD1	2.41	0.50
1:F:248:ASP:HB2	1:F:251:GLU:OE2	2.11	0.50
1:B:248:ASP:HA	1:B:251:GLU:HG3	1.93	0.50
1:C:347:ILE:HD12	1:D:347:ILE:HD12	1.94	0.50
1:G:251:GLU:O	1:G:252:ARG:NH1	2.41	0.50
1:K:347:ILE:HD12	1:L:347:ILE:CD1	2.42	0.50
1:E:347:ILE:HD12	1:F:347:ILE:HD12	1.94	0.50
1:B:250:ASP:O	1:B:252[B]:ARG:N	2.45	0.49
1:K:347:ILE:CD1	1:L:347:ILE:HD12	2.42	0.49
1:I:1:MET:CE	1:I:29:GLN:NE2	2.74	0.49
1:A:330:ASN:HD22	1:A:330:ASN:H	1.61	0.49
1:A:330:ASN:O	1:A:333:ASP:OD1	2.30	0.49
1:I:347:ILE:HD12	1:J:347:ILE:HD12	1.95	0.48
1:L:389:ARG:NH1	1:L:389:ARG:CG	2.74	0.48
1:A:317[A]:GLU:OE1	1:B:474:LEU:HD11	2.14	0.48
1:L:27:HIS:HD2	1:L:34:VAL:CG2	2.26	0.48
1:L:77:GLY:N	1:L:78:PRO:CD	2.76	0.48
1:K:1:MET:HB2	1:K:30:ASP:OD2	2.14	0.48
1:G:252:ARG:HA	1:G:256:MET:O	2.14	0.47
1:J:22:GLY:O	1:J:23:ASP:C	2.57	0.47
1:A:87:TRP:HZ2	1:A:330:ASN:HD21	1.62	0.47
1:F:224:GLU:H	1:F:224:GLU:CD	2.18	0.47
1:B:287:LEU:HD21	4:B:1476:PEG:H42	1.96	0.47
1:B:32:ARG:HD2	1:B:387:GLY:HA2	1.96	0.47
1:E:14:MET:HE1	1:E:365:GLU:HG3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:250:ASP:C	1:L:252:ARG:N	2.73	0.47
1:G:318:ARG:HE	1:J:317[A]:GLU:CD	2.23	0.46
1:J:250:ASP:C	1:J:252:ARG:H	2.21	0.46
1:K:71:GLN:HB3	1:K:330:ASN:ND2	2.31	0.46
1:A:317[A]:GLU:CG	1:D:318:ARG:NE	2.77	0.46
1:B:102[A]:GLU:HG2	6:B:2006:HOH:O	2.15	0.46
1:E:244:MET:CE	1:E:262:MET:SD	3.04	0.46
1:F:77:GLY:N	1:F:78:PRO:CD	2.78	0.46
1:C:248:ASP:HA	1:C:251:GLU:HG3	1.96	0.46
1:H:77:GLY:N	1:H:78:PRO:CD	2.79	0.46
1:J:250:ASP:C	1:J:252:ARG:N	2.74	0.46
1:J:244:MET:CE	1:J:262:MET:SD	3.04	0.46
1:B:71:GLN:HB3	1:B:330:ASN:ND2	2.31	0.46
1:F:130:ALA:HB3	1:F:154:ARG:HD3	1.98	0.46
1:H:244:MET:CE	1:H:262:MET:SD	3.04	0.46
1:L:14:MET:HE1	1:L:365:GLU:HG3	1.98	0.46
1:F:14:MET:HE1	1:F:365:GLU:HG3	1.98	0.46
1:G:14:MET:HE1	1:G:365:GLU:HG3	1.99	0.45
1:K:347:ILE:HD12	1:L:347:ILE:HD12	1.97	0.45
1:A:32:ARG:HG3	1:A:389:ARG:NH2	2.30	0.45
1:K:75:ARG:HD3	1:L:415:GLN:NE2	2.30	0.45
1:A:125:GLU:HG2	1:A:143:TYR:OH	2.16	0.45
1:B:282[A]:ARG:NH1	1:E:314:GLU:HG3	2.31	0.45
1:E:77:GLY:N	1:E:78:PRO:CD	2.80	0.45
1:C:22:GLY:O	1:C:23:ASP:C	2.59	0.45
1:E:250:ASP:C	1:E:252:ARG:N	2.73	0.45
1:B:77:GLY:N	1:B:78:PRO:CD	2.80	0.45
1:F:32:ARG:HG3	1:F:389:ARG:NH2	2.32	0.45
1:G:77:GLY:N	1:G:78:PRO:CD	2.80	0.45
1:H:14:MET:HE1	1:H:365:GLU:HG3	1.99	0.45
1:A:244:MET:CE	1:A:262:MET:SD	3.05	0.45
1:K:14:MET:HE1	1:K:365:GLU:HG3	1.99	0.45
1:B:130:ALA:HB3	1:B:154:ARG:HD3	1.99	0.45
1:C:244:MET:CE	1:C:262:MET:SD	3.05	0.45
1:E:31:GLY:HA3	1:E:389:ARG:HH21	1.82	0.45
1:E:71:GLN:HB3	1:E:330:ASN:ND2	2.32	0.45
1:G:22:GLY:O	1:G:23:ASP:C	2.60	0.45
1:G:244:MET:CE	1:G:262:MET:SD	3.05	0.44
1:D:14:MET:HE1	1:D:365:GLU:HG3	1.98	0.44
1:G:125:GLU:HG2	1:G:143:TYR:OH	2.17	0.44
1:C:85:TYR:OH	1:C:250:ASP:OD1	2.23	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ARG:HG3	1:D:389:ARG:NH2	2.31	0.44
1:I:71:GLN:HB3	1:I:330:ASN:ND2	2.32	0.44
1:K:77:GLY:N	1:K:78:PRO:CD	2.80	0.44
1:A:317[A]:GLU:CG	1:D:318:ARG:HE	2.28	0.44
1:F:248:ASP:O	1:F:251:GLU:HG2	2.17	0.44
1:C:14:MET:HE1	1:C:365:GLU:HG3	1.98	0.44
1:F:71:GLN:HB3	1:F:330:ASN:ND2	2.32	0.44
1:J:77:GLY:N	1:J:78:PRO:CD	2.81	0.44
1:D:165:GLN:CG	1:I:100:ARG:HH22	2.31	0.44
1:G:248:ASP:N	1:G:248:ASP:OD1	2.37	0.44
1:L:244:MET:CE	1:L:262:MET:SD	3.05	0.44
1:B:14:MET:HE1	1:B:365:GLU:HG3	2.00	0.44
1:K:248:ASP:CA	1:K:251:GLU:HG3	2.42	0.44
1:E:130:ALA:HB3	1:E:154:ARG:HD3	2.00	0.44
1:K:244:MET:CE	1:K:262:MET:SD	3.06	0.44
1:B:102[A]:GLU:CD	1:B:102[A]:GLU:H	2.26	0.43
1:H:102[A]:GLU:CD	1:H:102[A]:GLU:H	2.25	0.43
1:I:244:MET:CE	1:I:262:MET:SD	3.06	0.43
1:L:130:ALA:HB3	1:L:154:ARG:HD3	2.00	0.43
1:A:298:GLN:N	1:A:298:GLN:CD	2.77	0.43
1:F:93:TYR:HB2	1:F:94:PRO:HD3	2.00	0.43
1:L:318:ARG:HH22	3:L:1476:EDO:H11	1.83	0.43
1:C:130:ALA:HB3	1:C:154:ARG:HD3	2.00	0.43
1:D:71:GLN:HB3	1:D:330:ASN:ND2	2.33	0.43
1:F:93:TYR:N	1:F:94:PRO:CD	2.82	0.43
1:H:22:GLY:O	1:H:23:ASP:C	2.61	0.43
1:K:130:ALA:HB3	1:K:154:ARG:HD3	1.99	0.43
1:K:222:THR:HB	1:K:224[B]:GLU:OE1	2.18	0.43
1:A:77:GLY:N	1:A:78:PRO:CD	2.81	0.43
1:A:22:GLY:O	1:A:23:ASP:C	2.62	0.43
1:A:102[A]:GLU:CD	1:A:102[A]:GLU:H	2.26	0.43
1:D:22:GLY:O	1:D:23:ASP:C	2.61	0.43
1:D:77:GLY:N	1:D:78:PRO:CD	2.81	0.43
1:D:244:MET:CE	1:D:262:MET:SD	3.06	0.43
1:G:248:ASP:HA	1:G:251:GLU:OE2	2.19	0.43
1:E:251:GLU:HG2	1:E:251:GLU:O	2.19	0.43
1:H:71:GLN:HB3	1:H:330:ASN:ND2	2.34	0.43
1:A:252[A]:ARG:CG	1:A:252[A]:ARG:NH1	2.79	0.43
1:H:93:TYR:N	1:H:94:PRO:CD	2.82	0.43
1:K:22:GLY:O	1:K:23:ASP:C	2.62	0.43
1:B:244:MET:CE	1:B:262:MET:SD	3.07	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLN:HB3	1:C:330:ASN:ND2	2.34	0.42
1:E:277:CYS:SG	1:E:295:VAL:HG13	2.59	0.42
1:H:389:ARG:HD3	1:H:427:ASP:OD1	2.19	0.42
1:I:130:ALA:HB3	1:I:154:ARG:HD3	2.01	0.42
1:L:125:GLU:HG2	1:L:143:TYR:OH	2.20	0.42
1:J:389:ARG:HD3	1:J:427:ASP:OD1	2.20	0.42
1:H:164:ILE:HD11	1:H:167:TYR:CD2	2.54	0.42
1:C:32:ARG:HG3	1:C:389:ARG:NH2	2.34	0.42
1:F:244:MET:CE	1:F:262:MET:SD	3.07	0.42
1:A:252[A]:ARG:HH11	1:A:252[A]:ARG:HG2	1.84	0.42
1:E:286:ARG:HH11	1:E:286:ARG:HD3	1.70	0.42
1:I:22:GLY:O	1:I:23:ASP:C	2.62	0.42
1:K:159:ARG:NH1	1:K:219:THR:O	2.43	0.42
1:B:250:ASP:O	1:B:252[A]:ARG:N	2.52	0.42
1:I:252:ARG:HH11	1:I:252:ARG:CG	2.15	0.42
1:L:4:LEU:HD23	1:L:425:LEU:HD21	2.00	0.42
1:D:2:GLN:NE2	1:D:48:ASP:CG	2.78	0.42
1:E:125:GLU:HG2	1:E:143:TYR:OH	2.18	0.42
1:G:250:ASP:C	1:G:252:ARG:H	2.28	0.42
1:H:125:GLU:HG2	1:H:143:TYR:OH	2.19	0.42
1:L:154:ARG:HG2	1:L:194:ILE:HG12	2.01	0.42
1:D:125:GLU:HG2	1:D:143:TYR:OH	2.20	0.42
1:F:102:GLU:CD	1:F:102:GLU:H	2.28	0.42
1:I:125:GLU:HG2	1:I:143:TYR:OH	2.20	0.42
1:K:125:GLU:HG2	1:K:143:TYR:OH	2.19	0.42
1:B:125:GLU:HG2	1:B:143:TYR:OH	2.20	0.41
1:B:298:GLN:CD	1:B:298:GLN:N	2.78	0.41
1:H:130:ALA:HB3	1:H:154:ARG:HD3	2.01	0.41
1:I:14:MET:HE1	1:I:365:GLU:HG3	2.02	0.41
1:J:32:ARG:HG3	1:J:389:ARG:NH2	2.35	0.41
1:B:389:ARG:HD3	1:B:427:ASP:OD1	2.20	0.41
1:B:282[B]:ARG:HH12	3:B:1475:EDO:H22	1.66	0.41
1:C:77:GLY:N	1:C:78:PRO:CD	2.83	0.41
1:E:32:ARG:HG2	1:E:33:ILE:N	2.34	0.41
1:J:130:ALA:HB3	1:J:154:ARG:HD3	2.02	0.41
1:A:224:GLU:H	1:A:224:GLU:CD	2.28	0.41
1:I:354:ASP:OD2	1:L:286:ARG:NH1	2.35	0.41
1:L:314:GLU:HG2	3:L:1476:EDO:H21	2.01	0.41
1:A:14:MET:HE1	1:A:365:GLU:HG3	2.03	0.41
1:A:389:ARG:HD3	1:A:427:ASP:OD1	2.21	0.41
1:F:125:GLU:HG2	1:F:143:TYR:OH	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:GLN:HB3	1:G:330:ASN:ND2	2.35	0.41
1:G:154:ARG:HG2	1:G:194:ILE:HG12	2.01	0.41
1:I:343:PHE:O	1:I:347:ILE:HG22	2.21	0.41
1:G:32:ARG:HG3	1:G:389:ARG:NH2	2.35	0.41
1:I:157:PHE:N	1:I:157:PHE:CD1	2.89	0.41
1:I:389:ARG:HD3	1:I:427:ASP:OD1	2.21	0.41
1:J:125:GLU:HG2	1:J:143:TYR:OH	2.21	0.41
1:L:22:GLY:O	1:L:23:ASP:C	2.63	0.41
1:B:317[A]:GLU:CG	1:E:318:ARG:HE	2.25	0.41
1:D:251:GLU:O	1:D:251:GLU:HG2	2.21	0.41
1:G:48:ASP:OD1	1:G:48:ASP:N	2.52	0.41
1:G:93:TYR:N	1:G:94:PRO:CD	2.83	0.41
1:H:99:MET:HE2	1:H:104:VAL:CG2	2.51	0.41
1:I:318:ARG:HH12	3:L:1476:EDO:H11	1.85	0.41
1:K:93:TYR:HB2	1:K:94:PRO:HD3	2.03	0.41
1:L:71:GLN:HB3	1:L:330:ASN:ND2	2.35	0.41
1:C:155:MET:HA	1:C:214:ALA:O	2.21	0.41
1:F:22:GLY:O	1:F:23:ASP:C	2.63	0.41
1:H:93:TYR:HB2	1:H:94:PRO:HD3	2.03	0.41
1:J:111:TYR:CD1	1:J:111:TYR:C	2.99	0.41
1:A:130:ALA:HB3	1:A:154:ARG:HD3	2.03	0.40
1:D:130:ALA:HB3	1:D:154:ARG:CD	2.51	0.40
1:D:165:GLN:HG2	1:I:100:ARG:HH22	1.85	0.40
1:I:317:GLU:CD	1:L:318:ARG:HE	2.29	0.40
1:A:32:ARG:CG	1:A:389:ARG:NH2	2.85	0.40
1:B:93:TYR:HB2	1:B:94:PRO:HD3	2.04	0.40
1:B:275:ALA:O	1:B:276:HIS:HB2	2.22	0.40
1:B:317[A]:GLU:CG	1:E:318:ARG:NE	2.80	0.40
1:I:32:ARG:HG3	1:I:389:ARG:NH2	2.36	0.40
1:B:157:PHE:CD1	1:B:157:PHE:N	2.89	0.40
1:C:389:ARG:HD3	1:C:427:ASP:OD1	2.21	0.40
1:E:343:PHE:O	1:E:347:ILE:HG22	2.22	0.40
1:F:298:GLN:N	1:F:298:GLN:CD	2.80	0.40
1:H:132:TYR:HA	1:H:133:PRO:HD3	1.97	0.40
1:I:248:ASP:HA	1:I:251:GLU:HG2	2.02	0.40
1:J:93:TYR:HB2	1:J:94:PRO:HD3	2.03	0.40
1:A:343:PHE:O	1:A:347:ILE:HG22	2.22	0.40
1:B:411:THR:O	1:B:415:GLN:HB2	2.22	0.40
1:D:32:ARG:CG	1:D:389:ARG:NH2	2.84	0.40
1:G:93:TYR:HB2	1:G:94:PRO:HD3	2.04	0.40
1:G:102[A]:GLU:H	1:G:102[A]:GLU:CD	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:411:THR:O	1:H:415:GLN:HB2	2.22	0.40
1:I:298:GLN:N	1:I:298:GLN:CD	2.79	0.40
1:K:31:GLY:HA3	1:K:389:ARG:HH21	1.87	0.40
1:A:154:ARG:HG2	1:A:194:ILE:HG12	2.03	0.40
1:I:77:GLY:N	1:I:78:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	476/494 (96%)	454 (95%)	22 (5%)	0	100	100
1	B	477/494 (97%)	454 (95%)	22 (5%)	1 (0%)	43	72
1	C	473/494 (96%)	454 (96%)	19 (4%)	0	100	100
1	D	474/494 (96%)	452 (95%)	22 (5%)	0	100	100
1	E	477/494 (97%)	457 (96%)	19 (4%)	1 (0%)	43	72
1	F	475/494 (96%)	456 (96%)	19 (4%)	0	100	100
1	G	476/494 (96%)	456 (96%)	19 (4%)	1 (0%)	43	72
1	H	474/494 (96%)	454 (96%)	20 (4%)	0	100	100
1	I	475/494 (96%)	456 (96%)	19 (4%)	0	100	100
1	J	474/494 (96%)	453 (96%)	20 (4%)	1 (0%)	43	72
1	K	479/494 (97%)	461 (96%)	18 (4%)	0	100	100
1	L	476/494 (96%)	457 (96%)	18 (4%)	1 (0%)	43	72
All	All	5706/5928 (96%)	5464 (96%)	237 (4%)	5 (0%)	48	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	GLU
1	L	251	GLU
1	E	251	GLU
1	J	251	GLU
1	G	251	GLU

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	391/404 (97%)	374 (96%)	17 (4%)	26	60
1	B	392/404 (97%)	375 (96%)	17 (4%)	26	60
1	C	388/404 (96%)	371 (96%)	17 (4%)	25	59
1	D	389/404 (96%)	374 (96%)	15 (4%)	28	64
1	E	392/404 (97%)	377 (96%)	15 (4%)	29	64
1	F	389/404 (96%)	373 (96%)	16 (4%)	27	62
1	G	391/404 (97%)	370 (95%)	21 (5%)	20	51
1	H	389/404 (96%)	373 (96%)	16 (4%)	27	62
1	I	390/404 (96%)	375 (96%)	15 (4%)	29	64
1	J	389/404 (96%)	374 (96%)	15 (4%)	28	64
1	K	394/404 (98%)	378 (96%)	16 (4%)	27	62
1	L	390/404 (96%)	374 (96%)	16 (4%)	27	62
All	All	4684/4848 (97%)	4488 (96%)	196 (4%)	28	61

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	102[A]	GLU
1	A	102[B]	GLU
1	A	125	GLU
1	A	137	GLU
1	A	172	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	184	MET
1	A	193	ARG
1	A	224	GLU
1	A	252[A]	ARG
1	A	252[B]	ARG
1	A	253	ILE
1	A	330	ASN
1	A	334	SER
1	A	373	ARG
1	A	398	ARG
1	A	422	ASP
1	B	1	MET
1	B	2	GLN
1	B	75	ARG
1	B	102[A]	GLU
1	B	102[B]	GLU
1	B	125	GLU
1	B	172	LYS
1	B	184	MET
1	B	193	ARG
1	B	252[A]	ARG
1	B	252[B]	ARG
1	B	253	ILE
1	B	330	ASN
1	B	334	SER
1	B	373	ARG
1	B	398	ARG
1	B	422	ASP
1	C	2	GLN
1	C	49	ARG
1	C	75	ARG
1	C	102	GLU
1	C	125	GLU
1	C	172	LYS
1	C	177	GLN
1	C	179	GLU
1	C	184	MET
1	C	193	ARG
1	C	253	ILE
1	C	317	GLU
1	C	330	ASN
1	C	334	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	373	ARG
1	C	398	ARG
1	C	422	ASP
1	D	75	ARG
1	D	125	GLU
1	D	160	MET
1	D	172	LYS
1	D	184	MET
1	D	186	GLU
1	D	193	ARG
1	D	253	ILE
1	D	317[A]	GLU
1	D	317[B]	GLU
1	D	330	ASN
1	D	334	SER
1	D	373	ARG
1	D	398	ARG
1	D	422	ASP
1	E	2	GLN
1	E	75	ARG
1	E	125	GLU
1	E	172	LYS
1	E	184	MET
1	E	193	ARG
1	E	253	ILE
1	E	277	CYS
1	E	317[A]	GLU
1	E	317[B]	GLU
1	E	330	ASN
1	E	334	SER
1	E	373	ARG
1	E	398	ARG
1	E	422	ASP
1	F	75	ARG
1	F	102	GLU
1	F	125	GLU
1	F	137	GLU
1	F	172	LYS
1	F	184	MET
1	F	193	ARG
1	F	224	GLU
1	F	253	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	317[A]	GLU
1	F	317[B]	GLU
1	F	330	ASN
1	F	334	SER
1	F	373	ARG
1	F	398	ARG
1	F	422	ASP
1	G	29	GLN
1	G	75	ARG
1	G	102[A]	GLU
1	G	102[B]	GLU
1	G	125	GLU
1	G	137	GLU
1	G	160	MET
1	G	172	LYS
1	G	184	MET
1	G	193	ARG
1	G	253	ILE
1	G	277[A]	CYS
1	G	277[B]	CYS
1	G	282	ARG
1	G	317[A]	GLU
1	G	317[B]	GLU
1	G	330	ASN
1	G	334	SER
1	G	373	ARG
1	G	398	ARG
1	G	422	ASP
1	H	32	ARG
1	H	75	ARG
1	H	102[A]	GLU
1	H	102[B]	GLU
1	H	125	GLU
1	H	172	LYS
1	H	184	MET
1	H	193	ARG
1	H	253	ILE
1	H	317[A]	GLU
1	H	317[B]	GLU
1	H	330	ASN
1	H	334	SER
1	H	373	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	398	ARG
1	H	422	ASP
1	I	75	ARG
1	I	125	GLU
1	I	160	MET
1	I	172	LYS
1	I	184	MET
1	I	193	ARG
1	I	250	ASP
1	I	252	ARG
1	I	253	ILE
1	I	317	GLU
1	I	330	ASN
1	I	334	SER
1	I	373	ARG
1	I	398	ARG
1	I	422	ASP
1	J	29	GLN
1	J	75	ARG
1	J	125	GLU
1	J	172	LYS
1	J	184	MET
1	J	186	GLU
1	J	193	ARG
1	J	253	ILE
1	J	317[A]	GLU
1	J	317[B]	GLU
1	J	330	ASN
1	J	334	SER
1	J	373	ARG
1	J	398	ARG
1	J	422	ASP
1	K	1	MET
1	K	32	ARG
1	K	75	ARG
1	K	125	GLU
1	K	172	LYS
1	K	184	MET
1	K	193	ARG
1	K	247	SER
1	K	253	ILE
1	K	317[A]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	317[B]	GLU
1	K	330	ASN
1	K	334	SER
1	K	373	ARG
1	K	398	ARG
1	K	422	ASP
1	L	75	ARG
1	L	102	GLU
1	L	125	GLU
1	L	137	GLU
1	L	172	LYS
1	L	184	MET
1	L	193	ARG
1	L	253	ILE
1	L	317[A]	GLU
1	L	317[B]	GLU
1	L	330	ASN
1	L	334	SER
1	L	373	ARG
1	L	389	ARG
1	L	398	ARG
1	L	422	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	292	ASN
1	A	302	ASN
1	A	328	ASN
1	A	330	ASN
1	B	29	GLN
1	B	70	ASN
1	B	200	GLN
1	B	249	HIS
1	B	292	ASN
1	B	302	ASN
1	B	328	ASN
1	B	330	ASN
1	B	399	HIS
1	C	27	HIS
1	C	70	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	200	GLN
1	C	292	ASN
1	C	328	ASN
1	C	330	ASN
1	C	406	HIS
1	D	2	GLN
1	D	27	HIS
1	D	70	ASN
1	D	292	ASN
1	D	302	ASN
1	D	328	ASN
1	D	330	ASN
1	D	346	HIS
1	E	70	ASN
1	E	200	GLN
1	E	292	ASN
1	E	302	ASN
1	E	328	ASN
1	E	330	ASN
1	E	434	ASN
1	F	27	HIS
1	F	70	ASN
1	F	165	GLN
1	F	292	ASN
1	F	302	ASN
1	F	328	ASN
1	F	330	ASN
1	G	2	GLN
1	G	70	ASN
1	G	200	GLN
1	G	276	HIS
1	G	292	ASN
1	G	302	ASN
1	G	328	ASN
1	G	330	ASN
1	H	70	ASN
1	H	200	GLN
1	H	254	HIS
1	H	292	ASN
1	H	302	ASN
1	H	328	ASN
1	H	330	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	406	HIS
1	I	29	GLN
1	I	70	ASN
1	I	165	GLN
1	I	200	GLN
1	I	273	GLN
1	I	292	ASN
1	I	302	ASN
1	I	328	ASN
1	I	330	ASN
1	I	434	ASN
1	J	27	HIS
1	J	70	ASN
1	J	200	GLN
1	J	292	ASN
1	J	302	ASN
1	J	328	ASN
1	J	330	ASN
1	K	29	GLN
1	K	70	ASN
1	K	249	HIS
1	K	292	ASN
1	K	302	ASN
1	K	328	ASN
1	K	330	ASN
1	L	70	ASN
1	L	249	HIS
1	L	292	ASN
1	L	302	ASN
1	L	328	ASN
1	L	330	ASN
1	L	352	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 13 are monoatomic - leaving 19 for Mogul analysis.

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	J	1476	-	3,3,3	0.37	0	2,2,2	0.18	0
3	EDO	J	1475	-	3,3,3	0.71	0	2,2,2	0.67	0
4	PEG	K	1475	-	6,6,6	0.55	0	5,5,5	0.59	0
4	PEG	D	1475	-	6,6,6	0.38	0	5,5,5	0.37	0
4	PEG	C	1476	-	6,6,6	0.34	0	5,5,5	0.32	0
4	PEG	L	1477	-	6,6,6	0.62	0	5,5,5	0.48	0
3	EDO	A	1476	-	3,3,3	0.37	0	2,2,2	0.63	0
3	EDO	B	1475	-	3,3,3	0.46	0	2,2,2	0.16	0
3	EDO	H	1475	-	3,3,3	0.65	0	2,2,2	0.15	0
3	EDO	G	1475	-	3,3,3	0.74	0	2,2,2	0.55	0
3	EDO	L	1476	-	3,3,3	0.26	0	2,2,2	0.77	0
3	EDO	A	1475	-	3,3,3	0.82	0	2,2,2	0.52	0
4	PEG	B	1476	-	6,6,6	0.53	0	5,5,5	0.79	0
3	EDO	F	1475	-	3,3,3	0.67	0	2,2,2	0.70	0
3	EDO	E	1475	-	3,3,3	0.91	0	2,2,2	0.60	0
3	EDO	L	1475	-	3,3,3	0.56	0	2,2,2	0.24	0
4	PEG	F	1476	-	6,6,6	0.47	0	5,5,5	0.66	0
4	PEG	I	1475	-	6,6,6	0.94	0	5,5,5	1.20	1 (20%)
3	EDO	C	1475	-	3,3,3	0.41	0	2,2,2	1.11	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	J	1476	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	J	1475	-	-	1/1/1/1	-
4	PEG	K	1475	-	-	0/4/4/4	-
4	PEG	D	1475	-	-	4/4/4/4	-
4	PEG	C	1476	-	-	3/4/4/4	-
4	PEG	L	1477	-	-	2/4/4/4	-
3	EDO	A	1476	-	-	0/1/1/1	-
3	EDO	B	1475	-	-	0/1/1/1	-
3	EDO	H	1475	-	-	1/1/1/1	-
3	EDO	G	1475	-	-	1/1/1/1	-
3	EDO	L	1476	-	-	1/1/1/1	-
3	EDO	A	1475	-	-	1/1/1/1	-
4	PEG	B	1476	-	-	1/4/4/4	-
3	EDO	F	1475	-	-	0/1/1/1	-
3	EDO	E	1475	-	-	1/1/1/1	-
3	EDO	L	1475	-	-	1/1/1/1	-
4	PEG	F	1476	-	-	2/4/4/4	-
4	PEG	I	1475	-	-	4/4/4/4	-
3	EDO	C	1475	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1475	PEG	O2-C2-C1	2.09	119.32	110.11

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1476	PEG	O1-C1-C2-O2
4	L	1477	PEG	O2-C3-C4-O4
4	C	1476	PEG	O1-C1-C2-O2
4	C	1476	PEG	O2-C3-C4-O4
3	A	1475	EDO	O1-C1-C2-O2
3	E	1475	EDO	O1-C1-C2-O2
3	G	1475	EDO	O1-C1-C2-O2
3	H	1475	EDO	O1-C1-C2-O2
3	L	1475	EDO	O1-C1-C2-O2
3	L	1476	EDO	O1-C1-C2-O2
4	D	1475	PEG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	1475	PEG	O2-C3-C4-O4
4	I	1475	PEG	O1-C1-C2-O2
3	C	1475	EDO	O1-C1-C2-O2
3	J	1475	EDO	O1-C1-C2-O2
4	F	1476	PEG	O2-C3-C4-O4
4	F	1476	PEG	C1-C2-O2-C3
4	I	1475	PEG	C1-C2-O2-C3
4	D	1475	PEG	C4-C3-O2-C2
4	I	1475	PEG	C4-C3-O2-C2
4	I	1475	PEG	O2-C3-C4-O4
4	L	1477	PEG	C1-C2-O2-C3
4	C	1476	PEG	C4-C3-O2-C2
4	D	1475	PEG	C1-C2-O2-C3
3	J	1476	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1476	EDO	3	0
4	K	1475	PEG	1	0
4	D	1475	PEG	2	0
4	L	1477	PEG	1	0
3	B	1475	EDO	6	0
3	L	1476	EDO	3	0
4	B	1476	PEG	1	0
4	I	1475	PEG	2	0
3	C	1475	EDO	2	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	473/494 (95%)	-0.24	5 (1%)	78	70	10, 27, 53, 92	5 (1%)
1	B	474/494 (95%)	-0.42	5 (1%)	78	70	8, 19, 44, 76	5 (1%)
1	C	473/494 (95%)	-0.07	7 (1%)	72	63	16, 35, 64, 97	2 (0%)
1	D	474/494 (95%)	-0.28	5 (1%)	78	70	9, 27, 52, 77	2 (0%)
1	E	474/494 (95%)	-0.34	10 (2%)	63	54	8, 25, 54, 79	5 (1%)
1	F	474/494 (95%)	-0.29	5 (1%)	78	70	13, 26, 50, 79	3 (0%)
1	G	474/494 (95%)	-0.20	8 (1%)	69	60	10, 30, 59, 89	4 (0%)
1	H	472/494 (95%)	-0.09	11 (2%)	61	51	12, 35, 63, 90	4 (0%)
1	I	474/494 (95%)	-0.44	5 (1%)	78	70	7, 19, 44, 79	3 (0%)
1	J	473/494 (95%)	-0.30	3 (0%)	85	80	9, 25, 52, 85	3 (0%)
1	K	474/494 (95%)	-0.32	5 (1%)	78	70	10, 25, 51, 86	7 (1%)
1	L	474/494 (95%)	-0.36	4 (0%)	82	75	7, 23, 49, 77	4 (0%)
All	All	5683/5928 (95%)	-0.28	73 (1%)	75	66	7, 26, 54, 97	47 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	163	ARG	4.0
1	C	160	MET	3.5
1	A	163	ARG	3.3
1	F	1	MET	3.2
1	L	1	MET	3.2
1	L	245	ALA	3.2
1	D	1	MET	3.0
1	F	16[A]	GLN	2.9
1	J	245	ALA	2.8
1	E	277	CYS	2.8
1	E	1	MET	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2	GLN	2.7
1	G	163	ARG	2.7
1	H	247	SER	2.7
1	A	252[A]	ARG	2.7
1	J	2	GLN	2.7
1	C	446[A]	LEU	2.7
1	B	32	ARG	2.7
1	I	250	ASP	2.7
1	I	163	ARG	2.6
1	C	181	CYS	2.6
1	A	177[A]	GLN	2.6
1	C	184	MET	2.6
1	E	446[A]	LEU	2.5
1	B	30	ASP	2.5
1	A	245	ALA	2.5
1	K	163	ARG	2.5
1	G	184	MET	2.4
1	F	160	MET	2.4
1	H	277	CYS	2.4
1	I	446[A]	LEU	2.4
1	H	246	GLU	2.4
1	L	247	SER	2.4
1	H	164	ILE	2.3
1	B	163	ARG	2.3
1	L	160	MET	2.3
1	H	165	GLN	2.3
1	F	165	GLN	2.3
1	J	163	ARG	2.3
1	G	245	ALA	2.2
1	D	245	ALA	2.2
1	E	245	ALA	2.2
1	F	245	ALA	2.2
1	K	245	ALA	2.2
1	H	163	ARG	2.2
1	E	250	ASP	2.2
1	C	277	CYS	2.2
1	K	1	MET	2.2
1	G	474	LEU	2.2
1	E	192	ASP	2.2
1	G	250	ASP	2.2
1	H	245	ALA	2.2
1	E	163	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	249	HIS	2.1
1	C	247	SER	2.1
1	H	181	CYS	2.1
1	G	102[A]	GLU	2.1
1	K	282[A]	ARG	2.1
1	E	16	GLN	2.1
1	H	282[A]	ARG	2.1
1	D	164	ILE	2.1
1	H	184	MET	2.1
1	I	474	LEU	2.1
1	K	436[A]	ARG	2.1
1	C	245	ALA	2.1
1	I	245	ALA	2.1
1	B	179	GLU	2.1
1	G	251	GLU	2.1
1	B	245	ALA	2.0
1	E	160	MET	2.0
1	E	177[A]	GLN	2.0
1	D	250	ASP	2.0
1	H	160	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	L	481	1/1	0.76	0.14	37,37,37,37	1
2	FE	C	481	1/1	0.79	0.13	38,38,38,38	1
2	FE	K	481	1/1	0.80	0.10	31,31,31,31	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	H	1476	1/1	0.80	0.23	48,48,48,48	0
2	FE	G	481	1/1	0.82	0.09	31,31,31,31	1
3	EDO	L	1476	4/4	0.83	0.24	32,33,34,36	0
3	EDO	J	1476	4/4	0.84	0.25	23,25,26,31	0
4	PEG	I	1475	7/7	0.85	0.19	33,37,41,42	0
3	EDO	A	1476	4/4	0.85	0.22	30,32,32,35	0
4	PEG	K	1475	7/7	0.86	0.13	26,30,36,36	0
4	PEG	L	1477	7/7	0.86	0.13	22,24,31,31	0
3	EDO	C	1475	4/4	0.86	0.20	29,31,32,35	0
4	PEG	D	1475	7/7	0.87	0.13	23,27,33,34	0
3	EDO	B	1475	4/4	0.88	0.20	29,29,30,30	0
4	PEG	B	1476	7/7	0.89	0.14	20,22,26,27	0
2	FE	E	481	1/1	0.89	0.09	33,33,33,33	1
3	EDO	A	1475	4/4	0.90	0.16	31,33,34,35	0
2	FE	F	481	1/1	0.91	0.07	27,27,27,27	1
3	EDO	H	1475	4/4	0.92	0.13	21,21,22,22	0
2	FE	I	481	1/1	0.92	0.06	35,35,35,35	1
2	FE	J	481	1/1	0.92	0.10	32,32,32,32	1
3	EDO	E	1475	4/4	0.92	0.13	24,26,28,28	0
4	PEG	C	1476	7/7	0.92	0.13	30,31,39,41	0
3	EDO	F	1475	4/4	0.93	0.10	23,23,24,24	0
4	PEG	F	1476	7/7	0.93	0.11	31,34,38,39	0
2	FE	D	481	1/1	0.93	0.05	26,26,26,26	1
3	EDO	G	1475	4/4	0.94	0.16	22,22,23,24	0
3	EDO	J	1475	4/4	0.94	0.13	23,25,26,27	0
2	FE	A	481	1/1	0.96	0.07	33,33,33,33	1
2	FE	H	481	1/1	0.96	0.11	29,29,29,29	1
3	EDO	L	1475	4/4	0.96	0.10	22,23,24,25	0
2	FE	B	481	1/1	0.97	0.05	27,27,27,27	1

6.5 Other polymers ⓘ

There are no such residues in this entry.