



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:04 PM UTC

PDB ID : 8UP3 / pdb_00008up3
Title : Structure of atypical asparaginase from *Rhodospirillum rubrum* (mutant Y21F)
Authors : Lubkowski, J.; Wlodawer, A.; Zhang, D.
Deposited on : 2023-10-20
Resolution : 1.76 Å(reported)

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

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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

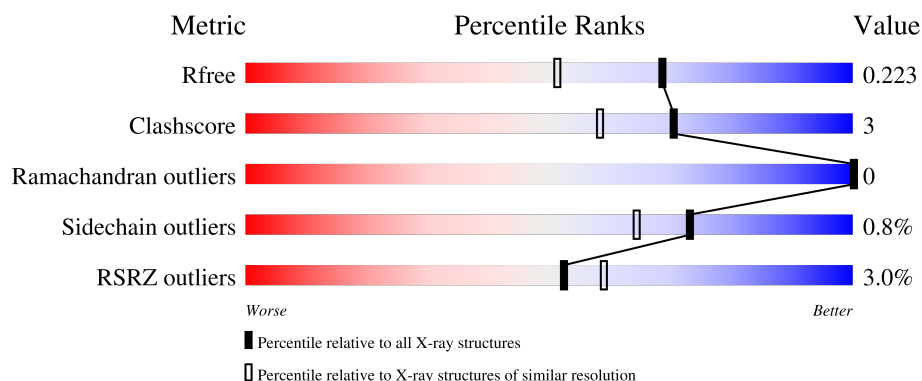
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	185	2% 80% 9% 11%
1	B	185	4% 84% 5% 11%
1	C	185	3% 82% 7% 11%
1	D	185	2% 88% . 11%
1	E	185	% 85% . . 11%

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Mol	Chain	Length	Quality of chain
1	F	185	
1	G	185	
1	H	185	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	205	-	-	X	-
2	EDO	B	202	-	-	X	-
4	ASP	F	201	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10920 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 Asparaginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	2	1
			1207	765	214	223	5			
1	B	165	Total	C	N	O	S	0	1	0
			1215	769	215	226	5			
1	C	164	Total	C	N	O	S	0	2	0
			1213	767	214	227	5			
1	D	165	Total	C	N	O	S	0	1	0
			1218	769	215	229	5			
1	E	164	Total	C	N	O	S	0	2	0
			1222	773	220	224	5			
1	F	163	Total	C	N	O	S	0	5	0
			1218	772	216	225	5			
1	G	163	Total	C	N	O	S	0	2	0
			1210	766	216	223	5			
1	H	161	Total	C	N	O	S	0	2	0
			1191	756	211	219	5			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q2RMX1
A	-11	HIS	-	expression tag	UNP Q2RMX1
A	-10	HIS	-	expression tag	UNP Q2RMX1
A	-9	HIS	-	expression tag	UNP Q2RMX1
A	-8	HIS	-	expression tag	UNP Q2RMX1
A	-7	HIS	-	expression tag	UNP Q2RMX1
A	-6	GLU	-	expression tag	UNP Q2RMX1
A	-5	ASN	-	expression tag	UNP Q2RMX1
A	-4	LEU	-	expression tag	UNP Q2RMX1
A	-3	TYR	-	expression tag	UNP Q2RMX1
A	-2	PHE	-	expression tag	UNP Q2RMX1
A	-1	GLN	-	expression tag	UNP Q2RMX1
A	0	GLY	-	expression tag	UNP Q2RMX1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	PHE	TYR	engineered mutation	UNP Q2RMX1
B	-12	HIS	-	expression tag	UNP Q2RMX1
B	-11	HIS	-	expression tag	UNP Q2RMX1
B	-10	HIS	-	expression tag	UNP Q2RMX1
B	-9	HIS	-	expression tag	UNP Q2RMX1
B	-8	HIS	-	expression tag	UNP Q2RMX1
B	-7	HIS	-	expression tag	UNP Q2RMX1
B	-6	GLU	-	expression tag	UNP Q2RMX1
B	-5	ASN	-	expression tag	UNP Q2RMX1
B	-4	LEU	-	expression tag	UNP Q2RMX1
B	-3	TYR	-	expression tag	UNP Q2RMX1
B	-2	PHE	-	expression tag	UNP Q2RMX1
B	-1	GLN	-	expression tag	UNP Q2RMX1
B	0	GLY	-	expression tag	UNP Q2RMX1
B	21	PHE	TYR	engineered mutation	UNP Q2RMX1
C	-12	HIS	-	expression tag	UNP Q2RMX1
C	-11	HIS	-	expression tag	UNP Q2RMX1
C	-10	HIS	-	expression tag	UNP Q2RMX1
C	-9	HIS	-	expression tag	UNP Q2RMX1
C	-8	HIS	-	expression tag	UNP Q2RMX1
C	-7	HIS	-	expression tag	UNP Q2RMX1
C	-6	GLU	-	expression tag	UNP Q2RMX1
C	-5	ASN	-	expression tag	UNP Q2RMX1
C	-4	LEU	-	expression tag	UNP Q2RMX1
C	-3	TYR	-	expression tag	UNP Q2RMX1
C	-2	PHE	-	expression tag	UNP Q2RMX1
C	-1	GLN	-	expression tag	UNP Q2RMX1
C	0	GLY	-	expression tag	UNP Q2RMX1
C	21	PHE	TYR	engineered mutation	UNP Q2RMX1
D	-12	HIS	-	expression tag	UNP Q2RMX1
D	-11	HIS	-	expression tag	UNP Q2RMX1
D	-10	HIS	-	expression tag	UNP Q2RMX1
D	-9	HIS	-	expression tag	UNP Q2RMX1
D	-8	HIS	-	expression tag	UNP Q2RMX1
D	-7	HIS	-	expression tag	UNP Q2RMX1
D	-6	GLU	-	expression tag	UNP Q2RMX1
D	-5	ASN	-	expression tag	UNP Q2RMX1
D	-4	LEU	-	expression tag	UNP Q2RMX1
D	-3	TYR	-	expression tag	UNP Q2RMX1
D	-2	PHE	-	expression tag	UNP Q2RMX1
D	-1	GLN	-	expression tag	UNP Q2RMX1
D	0	GLY	-	expression tag	UNP Q2RMX1

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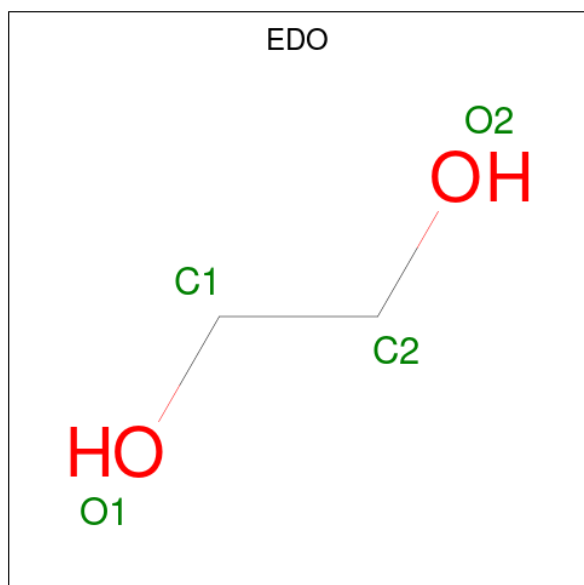
Chain	Residue	Modelled	Actual	Comment	Reference
D	21	PHE	TYR	engineered mutation	UNP Q2RMX1
E	-12	HIS	-	expression tag	UNP Q2RMX1
E	-11	HIS	-	expression tag	UNP Q2RMX1
E	-10	HIS	-	expression tag	UNP Q2RMX1
E	-9	HIS	-	expression tag	UNP Q2RMX1
E	-8	HIS	-	expression tag	UNP Q2RMX1
E	-7	HIS	-	expression tag	UNP Q2RMX1
E	-6	GLU	-	expression tag	UNP Q2RMX1
E	-5	ASN	-	expression tag	UNP Q2RMX1
E	-4	LEU	-	expression tag	UNP Q2RMX1
E	-3	TYR	-	expression tag	UNP Q2RMX1
E	-2	PHE	-	expression tag	UNP Q2RMX1
E	-1	GLN	-	expression tag	UNP Q2RMX1
E	0	GLY	-	expression tag	UNP Q2RMX1
E	21	PHE	TYR	engineered mutation	UNP Q2RMX1
F	-12	HIS	-	expression tag	UNP Q2RMX1
F	-11	HIS	-	expression tag	UNP Q2RMX1
F	-10	HIS	-	expression tag	UNP Q2RMX1
F	-9	HIS	-	expression tag	UNP Q2RMX1
F	-8	HIS	-	expression tag	UNP Q2RMX1
F	-7	HIS	-	expression tag	UNP Q2RMX1
F	-6	GLU	-	expression tag	UNP Q2RMX1
F	-5	ASN	-	expression tag	UNP Q2RMX1
F	-4	LEU	-	expression tag	UNP Q2RMX1
F	-3	TYR	-	expression tag	UNP Q2RMX1
F	-2	PHE	-	expression tag	UNP Q2RMX1
F	-1	GLN	-	expression tag	UNP Q2RMX1
F	0	GLY	-	expression tag	UNP Q2RMX1
F	21	PHE	TYR	engineered mutation	UNP Q2RMX1
G	-12	HIS	-	expression tag	UNP Q2RMX1
G	-11	HIS	-	expression tag	UNP Q2RMX1
G	-10	HIS	-	expression tag	UNP Q2RMX1
G	-9	HIS	-	expression tag	UNP Q2RMX1
G	-8	HIS	-	expression tag	UNP Q2RMX1
G	-7	HIS	-	expression tag	UNP Q2RMX1
G	-6	GLU	-	expression tag	UNP Q2RMX1
G	-5	ASN	-	expression tag	UNP Q2RMX1
G	-4	LEU	-	expression tag	UNP Q2RMX1
G	-3	TYR	-	expression tag	UNP Q2RMX1
G	-2	PHE	-	expression tag	UNP Q2RMX1
G	-1	GLN	-	expression tag	UNP Q2RMX1
G	0	GLY	-	expression tag	UNP Q2RMX1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	21	PHE	TYR	engineered mutation	UNP Q2RMX1
H	-12	HIS	-	expression tag	UNP Q2RMX1
H	-11	HIS	-	expression tag	UNP Q2RMX1
H	-10	HIS	-	expression tag	UNP Q2RMX1
H	-9	HIS	-	expression tag	UNP Q2RMX1
H	-8	HIS	-	expression tag	UNP Q2RMX1
H	-7	HIS	-	expression tag	UNP Q2RMX1
H	-6	GLU	-	expression tag	UNP Q2RMX1
H	-5	ASN	-	expression tag	UNP Q2RMX1
H	-4	LEU	-	expression tag	UNP Q2RMX1
H	-3	TYR	-	expression tag	UNP Q2RMX1
H	-2	PHE	-	expression tag	UNP Q2RMX1
H	-1	GLN	-	expression tag	UNP Q2RMX1
H	0	GLY	-	expression tag	UNP Q2RMX1
H	21	PHE	TYR	engineered mutation	UNP Q2RMX1

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			8	4	4		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	1
			8	4	4		
2	A	1	Total	C	O	0	0
			4	2	2		

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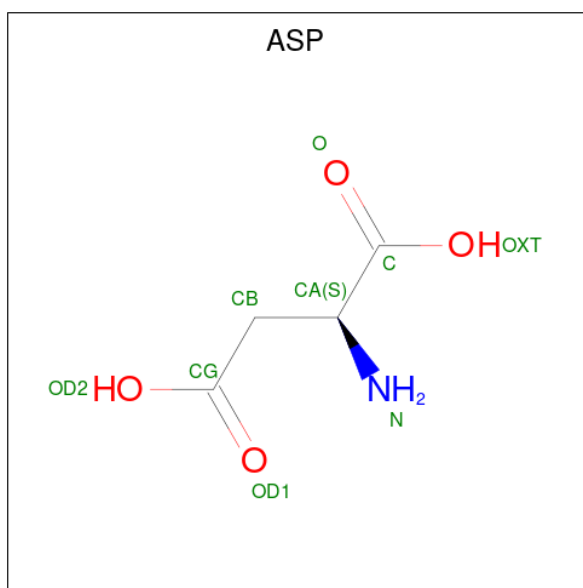
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 3	Cl 3	0	1
3	B	2	Total 2	Cl 2	0	0
3	C	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0
3	E	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0
3	G	1	Total 1	Cl 1	0	0
3	H	2	Total 2	Cl 2	0	0

- Molecule 4 is ASPARTIC ACID (CCD ID: ASP) (formula: C₄H₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total 9	C 4	N 1	O 4	0	0
4	F	1	Total 9	C 4	N 1	O 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	161	Total 163	O 163	0	2
5	B	132	Total 135	O 135	0	3
5	C	123	Total 125	O 125	0	2
5	D	143	Total 145	O 145	0	2
5	E	139	Total 139	O 139	0	0
5	F	129	Total 130	O 130	0	1
5	G	121	Total 122	O 122	0	1
5	H	128	Total 129	O 129	0	1

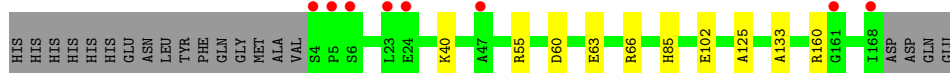
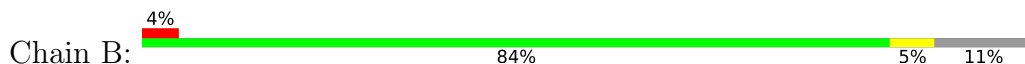
3 Residue-property plots

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.

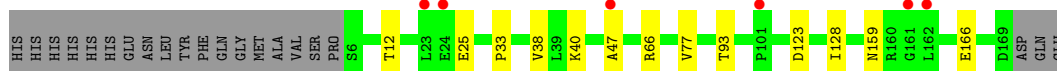
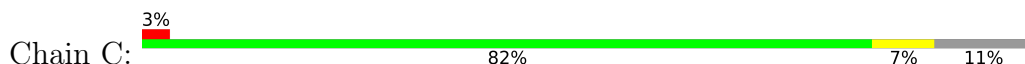
- Molecule 1: Asparaginase



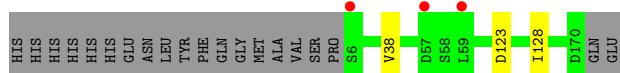
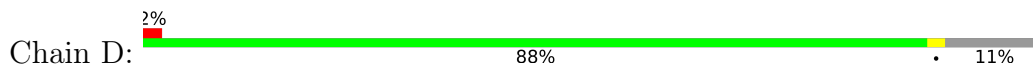
- Molecule 1: Asparaginase



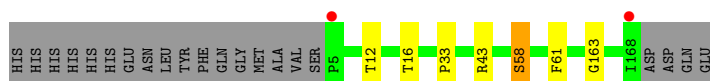
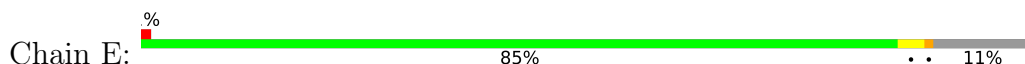
- Molecule 1: Asparaginase



- Molecule 1: Asparaginase

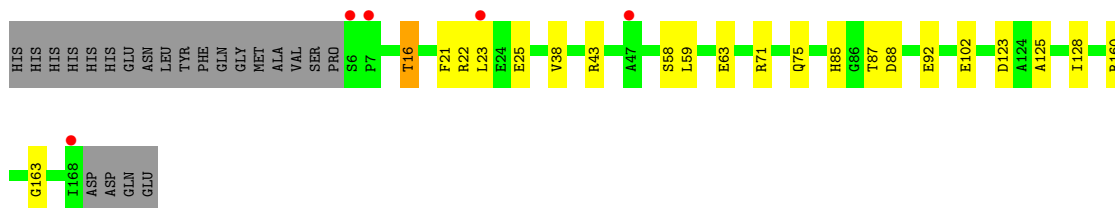


- Molecule 1: Asparaginase



- Molecule 1: Asparaginase

Chain F: 



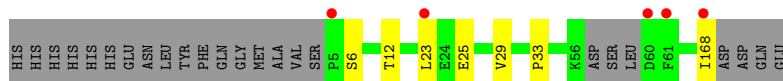
• Molecule 1: Asparaginase

Chain G: 



• Molecule 1: Asparaginase

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.64Å 63.19Å 92.97Å 90.00° 103.42° 90.00°	Depositor
Resolution (Å)	39.40 – 1.76 39.40 – 1.76	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.40-1.76) 94.3 (39.40-1.76)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.164 , 0.216 0.175 , 0.223	Depositor DCC
R_{free} test set	1657 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10920	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.86 % 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 1.4423e-03. 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: 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	1.14	0/1236	1.28	1/1672 (0.1%)
1	B	1.13	1/1241 (0.1%)	1.31	3/1679 (0.2%)
1	C	1.12	0/1241	1.32	1/1678 (0.1%)
1	D	1.13	0/1243	1.31	1/1681 (0.1%)
1	E	1.15	1/1249 (0.1%)	1.26	0/1687
1	F	1.16	0/1257	1.32	4/1699 (0.2%)
1	G	1.12	1/1238 (0.1%)	1.33	4/1673 (0.2%)
1	H	1.10	0/1217	1.34	0/1644
All	All	1.13	3/9922 (0.0%)	1.31	14/13413 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	HIS	CE1-NE2	7.41	1.40	1.32
1	E	58	SER	C-O	6.61	1.32	1.24
1	G	120	GLY	C-O	5.84	1.29	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	123	ASP	CA-CB-CG	6.64	119.24	112.60
1	F	85	HIS	CA-CB-CG	6.07	119.87	113.80
1	F	92	GLU	CB-CG-CD	6.07	122.92	112.60
1	C	123	ASP	CA-CB-CG	5.77	118.37	112.60
1	G	85	HIS	CA-CB-CG	5.65	119.45	113.80
1	B	160	ARG	CA-C-N	5.60	126.16	119.94
1	B	160	ARG	C-N-CA	5.60	126.16	119.94
1	F	16	THR	CA-CB-OG1	-5.55	101.28	109.60
1	D	123	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	32	ASP	CB-CA-C	5.48	118.17	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	ARG	CG-CD-NE	-5.38	100.16	112.00
1	F	123	ASP	CA-CB-CG	5.31	117.91	112.60
1	G	160	ARG	CA-C-N	5.06	125.60	119.98
1	G	160	ARG	C-N-CA	5.06	125.60	119.98

There are no chirality outliers.

There are no planarity outliers.

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	1207	0	1230	13	0
1	B	1215	0	1236	7	0
1	C	1213	0	1233	6	0
1	D	1218	0	1232	1	0
1	E	1222	0	1253	5	0
1	F	1218	0	1248	17	0
1	G	1210	0	1237	11	0
1	H	1191	0	1220	2	0
2	A	40	0	60	12	0
2	B	16	0	24	5	0
2	C	8	0	12	0	0
2	D	20	0	29	0	0
2	E	8	0	12	1	0
2	F	4	0	6	0	0
2	G	8	0	12	0	0
2	H	4	0	6	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	2	0	0	1	0
4	E	9	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	9	0	3	4	0
5	A	163	0	0	6	0
5	B	135	0	0	5	0
5	C	125	0	0	2	1
5	D	145	0	0	0	0
5	E	139	0	0	0	0
5	F	130	0	0	5	0
5	G	122	0	0	3	1
5	H	129	0	0	1	0
All	All	10920	0	10056	67	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (67) 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)
4:F:201:ASP:N	5:F:301:HOH:O	1.99	0.95
1:F:59:LEU:CD1	5:F:301:HOH:O	2.42	0.67
2:A:205:EDO:O1	2:B:202:EDO:O1	2.10	0.67
5:A:372:HOH:O	2:B:202:EDO:H12	1.93	0.66
1:C:159:ASN:HB2	1:C:166:GLU:OE2	1.96	0.65
2:A:205:EDO:H12	5:B:336:HOH:O	1.98	0.64
1:A:92:GLU:CD	5:A:331:HOH:O	2.42	0.63
2:A:204:EDO:O1	5:A:301:HOH:O	2.16	0.60
1:G:92:GLU:CD	5:G:301:HOH:O	2.44	0.60
1:F:59:LEU:HD11	5:F:301:HOH:O	2.03	0.59
1:A:125:ALA:HB2	2:A:205:EDO:H21	1.84	0.59
1:A:168:ILE:HD11	5:A:456:HOH:O	2.02	0.58
1:B:125:ALA:CB	2:B:202:EDO:H21	2.33	0.58
2:A:206:EDO:H21	5:A:364:HOH:O	2.04	0.56
1:C:77:VAL:HG22	5:C:335:HOH:O	2.06	0.56
1:E:163:GLY:O	1:F:43[A]:ARG:NH1	2.38	0.56
1:G:38:VAL:HG21	1:G:128[B]:ILE:CD1	2.37	0.55
1:A:125:ALA:CB	2:A:205:EDO:H21	2.37	0.55
1:F:163:GLY:HA3	1:G:23:LEU:HD23	1.88	0.55
1:A:89:THR:OG1	2:A:201[A]:EDO:H12	2.06	0.54
1:F:63:GLU:OE2	5:F:302:HOH:O	2.18	0.54
1:B:125:ALA:HB2	2:B:202:EDO:H21	1.90	0.54
1:E:12:THR:HG21	1:E:33:PRO:HB3	1.90	0.53
1:F:58:SER:OG	4:F:201:ASP:OXT	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:202:CL:CL	5:H:390:HOH:O	2.55	0.53
1:G:32:ASP:OD1	1:G:55:ARG:NH2	2.27	0.53
1:A:101:PRO:HD2	5:A:374:HOH:O	2.09	0.52
1:F:102:GLU:HB2	5:F:332:HOH:O	2.09	0.52
1:A:85:HIS:CE1	2:A:201[B]:EDO:H22	2.45	0.52
1:C:38:VAL:HG21	1:C:128[B]:ILE:HD12	1.91	0.52
1:A:38:VAL:HG21	1:A:128[B]:ILE:HD12	1.92	0.52
1:B:63:GLU:HG3	1:B:66:ARG:HH21	1.75	0.52
2:E:203:EDO:H21	1:F:125:ALA:HB3	1.93	0.51
1:B:102:GLU:OE2	5:B:302:HOH:O	2.19	0.50
1:F:22:ARG:HH11	1:F:25:GLU:HG3	1.75	0.50
1:E:16:THR:OG1	4:E:201:ASP:CG	2.55	0.49
1:B:60:ASP:OD1	5:B:301:HOH:O	2.19	0.49
1:D:38:VAL:HG21	1:D:128[A]:ILE:HD12	1.94	0.49
1:E:43[A]:ARG:NH1	1:F:163:GLY:O	2.46	0.48
1:C:66:ARG:HD3	1:C:93:THR:OG1	2.15	0.47
1:A:6:SER:HB3	1:A:7:PRO:HD3	1.98	0.46
1:A:48:VAL:CG2	2:A:206:EDO:H12	2.46	0.46
1:G:38:VAL:HG21	1:G:128[B]:ILE:HD13	1.98	0.46
1:C:47:ALA:HA	5:C:306:HOH:O	2.15	0.45
1:F:22:ARG:HD3	1:F:25:GLU:OE2	2.16	0.45
1:E:58:SER:OG	4:E:201:ASP:O	2.30	0.45
1:G:22[B]:ARG:HG3	1:G:29:VAL:HG21	1.97	0.45
1:H:12:THR:HG21	1:H:33:PRO:HB3	1.99	0.45
1:F:16:THR:OG1	4:F:201:ASP:HA	2.18	0.43
1:F:88:ASP:OD1	1:F:160:ARG:HD3	2.18	0.43
1:G:63:GLU:HG2	5:G:345:HOH:O	2.18	0.43
1:C:12:THR:HG21	1:C:33:PRO:HB3	1.99	0.43
1:A:72:ALA:HB1	2:A:204:EDO:H12	2.01	0.43
1:A:22:ARG:HH11	1:A:25:GLU:CG	2.30	0.43
1:G:23:LEU:HD13	5:G:384:HOH:O	2.18	0.43
2:A:205:EDO:H11	5:B:391:HOH:O	2.19	0.43
2:A:205:EDO:C1	5:B:336:HOH:O	2.63	0.42
1:G:38:VAL:HG21	1:G:128[B]:ILE:HD12	2.00	0.42
1:F:21:PHE:CE2	1:F:23:LEU:HA	2.55	0.42
1:F:38:VAL:HG21	1:F:128[B]:ILE:HD12	2.02	0.42
1:F:71:ARG:O	1:F:75:GLN:HG3	2.19	0.42
1:H:25:GLU:HG3	1:H:29:VAL:CG1	2.50	0.42
1:G:6:SER:N	1:G:7:PRO:CD	2.83	0.42
1:B:125:ALA:HB1	2:B:202:EDO:H21	2.01	0.41
1:A:133:ALA:HB3	1:B:133:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:THR:H	4:F:201:ASP:CG	2.28	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:390:HOH:O	5:G:368:HOH:O[4_546]	2.18	0.02

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	164/185 (89%)	164 (100%)	0	0	100	100
1	B	164/185 (89%)	163 (99%)	1 (1%)	0	100	100
1	C	164/185 (89%)	163 (99%)	1 (1%)	0	100	100
1	D	164/185 (89%)	164 (100%)	0	0	100	100
1	E	164/185 (89%)	162 (99%)	2 (1%)	0	100	100
1	F	166/185 (90%)	166 (100%)	0	0	100	100
1	G	163/185 (88%)	162 (99%)	1 (1%)	0	100	100
1	H	159/185 (86%)	158 (99%)	1 (1%)	0	100	100
All	All	1308/1480 (88%)	1302 (100%)	6 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	123/141 (87%)	123 (100%)	0	100	100
1	B	124/141 (88%)	123 (99%)	1 (1%)	73	64
1	C	124/141 (88%)	122 (98%)	2 (2%)	55	38
1	D	124/141 (88%)	124 (100%)	0	100	100
1	E	124/141 (88%)	123 (99%)	1 (1%)	73	64
1	F	126/141 (89%)	126 (100%)	0	100	100
1	G	123/141 (87%)	122 (99%)	1 (1%)	73	64
1	H	121/141 (86%)	118 (98%)	3 (2%)	42	22
All	All	989/1128 (88%)	981 (99%)	8 (1%)	73	64

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
1	C	25	GLU
1	C	40	LYS
1	E	61	PHE
1	G	160	ARG
1	H	6	SER
1	H	23	LEU
1	H	168	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 41 ligands modelled in this entry, 12 are monoatomic - leaving 29 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	$\# Z > 2$
2	EDO	A	208	-	3,3,3	0.14	0	2,2,2	0.03	0
2	EDO	B	203	-	3,3,3	0.04	0	2,2,2	0.23	0
2	EDO	H	201	-	3,3,3	0.17	0	2,2,2	0.22	0
2	EDO	A	204	-	3,3,3	0.35	0	2,2,2	0.48	0
2	EDO	A	207	-	3,3,3	0.24	0	2,2,2	0.42	0
2	EDO	F	202	-	3,3,3	0.53	0	2,2,2	0.31	0
4	ASP	F	201	-	7,8,8	0.90	0	6,10,10	0.94	0
2	EDO	A	201[B]	-	3,3,3	0.22	0	2,2,2	0.11	0
2	EDO	D	201	-	3,3,3	0.22	0	2,2,2	0.11	0
2	EDO	A	203[A]	-	3,3,3	0.19	0	2,2,2	0.33	0
2	EDO	E	202	-	3,3,3	0.32	0	2,2,2	0.25	0
2	EDO	D	204	-	3,3,3	0.08	0	2,2,2	0.14	0
2	EDO	B	204	-	3,3,3	0.26	0	2,2,2	0.21	0
2	EDO	A	202	-	3,3,3	0.28	0	2,2,2	0.31	0
2	EDO	A	203[B]	-	3,3,3	0.17	0	2,2,2	0.26	0
2	EDO	B	202	-	3,3,3	0.34	0	2,2,2	0.84	0
2	EDO	A	206	-	3,3,3	0.30	0	2,2,2	0.49	0
2	EDO	A	205	-	3,3,3	0.28	0	2,2,2	0.74	0
2	EDO	G	202	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	G	201	-	3,3,3	0.29	0	2,2,2	0.39	0
2	EDO	D	202	-	3,3,3	0.16	0	2,2,2	0.46	0
2	EDO	C	201	-	3,3,3	0.19	0	2,2,2	0.42	0
2	EDO	D	203	-	3,3,3	0.75	0	2,2,2	0.34	0
2	EDO	B	201	-	3,3,3	0.14	0	2,2,2	0.21	0
2	EDO	E	203	-	3,3,3	0.33	0	2,2,2	0.69	0
4	ASP	E	201	-	7,8,8	2.09	1 (14%)	6,10,10	0.78	0
2	EDO	D	205	-	3,3,3	0.23	0	2,2,2	0.21	0
2	EDO	A	201[A]	-	3,3,3	0.11	0	2,2,2	0.30	0
2	EDO	C	202	-	3,3,3	0.07	0	2,2,2	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	208	-	-	0/1/1/1	-
2	EDO	B	203	-	-	0/1/1/1	-
2	EDO	H	201	-	-	0/1/1/1	-
2	EDO	A	204	-	-	1/1/1/1	-
2	EDO	A	207	-	-	1/1/1/1	-
2	EDO	F	202	-	-	0/1/1/1	-
4	ASP	F	201	-	-	2/8/8/8	-
2	EDO	A	201[B]	-	-	0/1/1/1	-
2	EDO	D	201	-	-	0/1/1/1	-
2	EDO	A	203[A]	-	-	0/1/1/1	-
2	EDO	E	202	-	-	0/1/1/1	-
2	EDO	D	204	-	-	1/1/1/1	-
2	EDO	B	204	-	-	1/1/1/1	-
2	EDO	A	202	-	-	1/1/1/1	-
2	EDO	A	203[B]	-	-	1/1/1/1	-
2	EDO	B	202	-	-	1/1/1/1	-
2	EDO	A	206	-	-	1/1/1/1	-
2	EDO	A	205	-	-	1/1/1/1	-
2	EDO	G	202	-	-	0/1/1/1	-
2	EDO	G	201	-	-	1/1/1/1	-
2	EDO	D	202	-	-	1/1/1/1	-
2	EDO	C	201	-	-	0/1/1/1	-
2	EDO	D	203	-	-	1/1/1/1	-
2	EDO	B	201	-	-	0/1/1/1	-
2	EDO	E	203	-	-	1/1/1/1	-
4	ASP	E	201	-	-	4/8/8/8	-
2	EDO	D	205	-	-	1/1/1/1	-
2	EDO	A	201[A]	-	-	0/1/1/1	-
2	EDO	C	202	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	201	ASP	OXT-C	-4.72	1.15	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	201	ASP	O-C-CA-N
4	E	201	ASP	OXT-C-CA-N
4	F	201	ASP	OXT-C-CA-N
2	D	203	EDO	O1-C1-C2-O2
2	A	202	EDO	O1-C1-C2-O2
2	A	204	EDO	O1-C1-C2-O2
2	D	202	EDO	O1-C1-C2-O2
2	E	203	EDO	O1-C1-C2-O2
4	E	201	ASP	O-C-CA-N
2	D	205	EDO	O1-C1-C2-O2
2	A	206	EDO	O1-C1-C2-O2
2	A	205	EDO	O1-C1-C2-O2
2	A	207	EDO	O1-C1-C2-O2
2	B	204	EDO	O1-C1-C2-O2
4	E	201	ASP	OXT-C-CA-CB
2	G	201	EDO	O1-C1-C2-O2
2	A	203[B]	EDO	O1-C1-C2-O2
2	B	202	EDO	O1-C1-C2-O2
2	D	204	EDO	O1-C1-C2-O2
4	E	201	ASP	O-C-CA-CB

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	204	EDO	2	0
4	F	201	ASP	4	0
2	A	201[B]	EDO	1	0
2	B	202	EDO	5	0
2	A	206	EDO	2	0
2	A	205	EDO	6	0
2	E	203	EDO	1	0
4	E	201	ASP	2	0
2	A	201[A]	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	164/185 (88%)	-0.06	4 (2%)	59	66	9, 19, 33, 53	2 (1%)
1	B	165/185 (89%)	0.09	8 (4%)	35	41	10, 21, 41, 56	1 (0%)
1	C	164/185 (88%)	0.15	6 (3%)	45	51	11, 21, 42, 70	2 (1%)
1	D	165/185 (89%)	0.02	3 (1%)	67	74	10, 19, 36, 52	1 (0%)
1	E	164/185 (88%)	-0.12	2 (1%)	76	82	11, 17, 36, 53	2 (1%)
1	F	163/185 (88%)	0.17	5 (3%)	51	58	11, 22, 38, 54	5 (3%)
1	G	163/185 (88%)	0.08	6 (3%)	45	51	10, 21, 40, 60	2 (1%)
1	H	161/185 (87%)	0.11	5 (3%)	51	58	11, 20, 43, 56	2 (1%)
All	All	1309/1480 (88%)	0.05	39 (2%)	52	59	9, 20, 41, 70	17 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	ALA	4.7
1	F	168	ILE	4.3
1	A	169	ASP	4.0
1	H	168	ILE	3.9
1	B	168	ILE	3.8
1	E	168	ILE	3.7
1	C	23	LEU	3.4
1	F	23	LEU	3.3
1	C	162	LEU	3.2
1	G	47	ALA	3.1
1	G	6	SER	3.0
1	D	59	LEU	3.0
1	B	5	PRO	3.0
1	E	5	PRO	3.0
1	B	4	SER	2.9
1	F	7	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	47	ALA	2.7
1	H	5	PRO	2.7
1	A	6	SER	2.7
1	G	168	ILE	2.6
1	D	6	SER	2.6
1	B	24	GLU	2.6
1	B	161	GLY	2.5
1	H	60	ASP	2.5
1	C	24	GLU	2.5
1	C	161	GLY	2.4
1	H	61	PHE	2.4
1	D	57	ASP	2.3
1	G	104	ALA	2.3
1	B	6	SER	2.3
1	B	23	LEU	2.3
1	B	47	ALA	2.3
1	C	101	PRO	2.2
1	H	23	LEU	2.1
1	G	7	PRO	2.1
1	G	63	GLU	2.1
1	F	6	SER	2.1
1	A	7	PRO	2.1
1	A	101	PRO	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	D	202	4/4	0.76	0.17	42,44,45,48	0
2	EDO	A	208	4/4	0.81	0.14	42,43,43,44	0
2	EDO	A	202	4/4	0.83	0.18	44,47,49,51	0
3	CL	H	203	1/1	0.83	0.18	46,46,46,46	0
2	EDO	D	205	4/4	0.85	0.14	41,43,45,47	0
2	EDO	A	206	4/4	0.85	0.23	41,41,42,43	0
2	EDO	A	204	4/4	0.86	0.22	36,37,41,46	0
2	EDO	E	203	4/4	0.88	0.14	32,37,38,43	0
2	EDO	A	207	4/4	0.89	0.13	37,39,40,41	0
4	ASP	F	201	9/9	0.90	0.11	15,29,34,38	0
2	EDO	B	202	4/4	0.91	0.16	31,34,34,44	0
3	CL	B	206	1/1	0.91	0.18	51,51,51,51	0
2	EDO	D	204	4/4	0.91	0.10	33,34,39,40	0
2	EDO	B	204	4/4	0.91	0.13	37,43,44,46	0
2	EDO	B	203	4/4	0.92	0.10	33,38,44,46	0
2	EDO	A	203[B]	4/4	0.92	0.09	23,24,24,24	4
4	ASP	E	201	9/9	0.92	0.10	16,24,29,31	0
2	EDO	A	203[A]	4/4	0.92	0.09	17,24,27,29	4
3	CL	F	203	1/1	0.93	0.10	33,33,33,33	0
2	EDO	C	202	4/4	0.93	0.11	32,35,37,41	0
2	EDO	G	201	4/4	0.93	0.11	22,30,34,39	0
2	EDO	C	201	4/4	0.93	0.09	21,23,23,23	0
2	EDO	D	201	4/4	0.94	0.09	22,25,26,26	0
2	EDO	H	201	4/4	0.94	0.10	30,30,31,32	0
3	CL	B	205	1/1	0.94	0.08	24,24,24,24	0
2	EDO	A	201[B]	4/4	0.94	0.10	14,16,16,16	4
2	EDO	A	205	4/4	0.94	0.18	34,35,38,39	0
2	EDO	B	201	4/4	0.94	0.10	27,32,33,38	0
2	EDO	E	202	4/4	0.94	0.09	29,29,30,31	0
2	EDO	A	201[A]	4/4	0.94	0.10	20,22,23,26	4
2	EDO	F	202	4/4	0.95	0.08	19,20,21,23	0
3	CL	E	204	1/1	0.95	0.07	31,31,31,31	0
2	EDO	D	203	4/4	0.95	0.09	30,34,37,42	0
3	CL	A	210[A]	1/1	0.96	0.08	25,25,25,25	1
3	CL	A	210[B]	1/1	0.96	0.08	26,26,26,26	1
2	EDO	G	202	4/4	0.96	0.06	22,22,23,24	0
3	CL	D	206	1/1	0.98	0.07	25,25,25,25	0
3	CL	A	209	1/1	0.98	0.05	21,21,21,21	0
3	CL	H	202	1/1	0.99	0.07	40,40,40,40	0
3	CL	C	203	1/1	1.00	0.03	19,19,19,19	0
3	CL	G	203	1/1	1.00	0.08	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.