



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:13 AM UTC

PDB ID : 4V1X / pdb_00004v1x
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 : 2.20 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

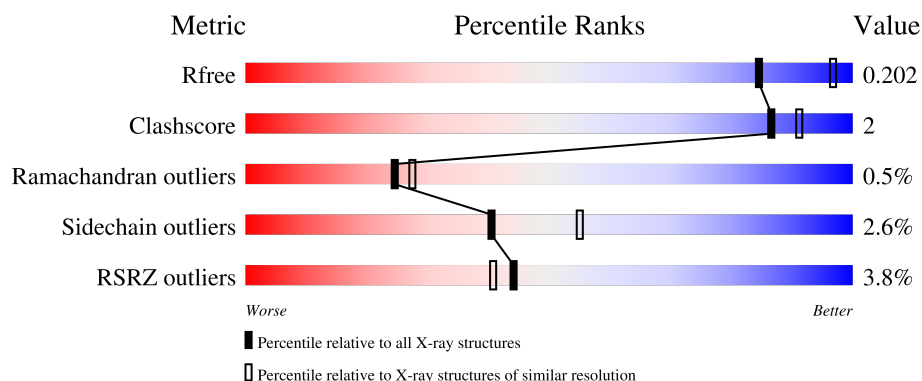
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	4% 88% 6% . .
1	B	494	4% 89% 6% . .
1	C	494	3% 90% 5% . .
1	D	494	4% 90% . . .
1	E	494	3% 90% 5% . .

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Mol	Chain	Length	Quality of chain
1	F	494	4% 89% 6% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23156 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	3	0
			3704	2311	682	687	24			
1	B	472	Total	C	N	O	S	0	4	0
			3707	2313	683	687	24			
1	C	473	Total	C	N	O	S	0	3	0
			3704	2313	682	685	24			
1	D	473	Total	C	N	O	S	0	2	0
			3696	2307	680	685	24			
1	E	474	Total	C	N	O	S	0	3	0
			3714	2319	685	685	25			
1	F	472	Total	C	N	O	S	0	3	0
			3696	2307	680	685	24			

There are 120 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

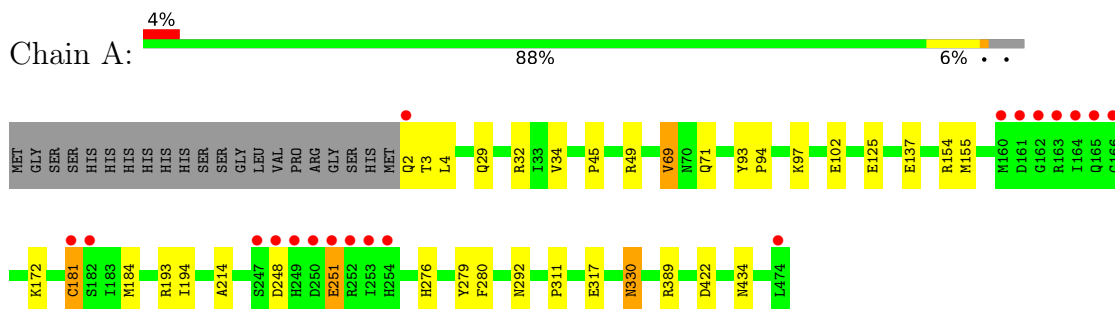
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	127	Total	O	0	0
			127	127		
4	C	185	Total	O	0	0
			185	185		
4	D	118	Total	O	0	0
			118	118		
4	E	171	Total	O	0	0
			171	171		
4	F	125	Total	O	0	0
			125	125		

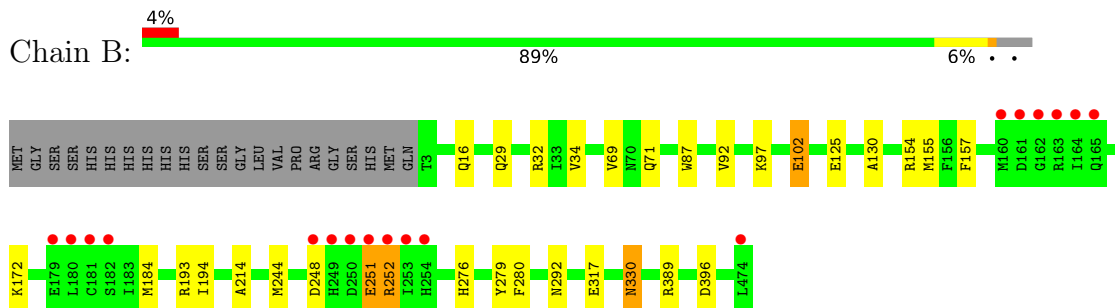
3 Residue-property plots

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.

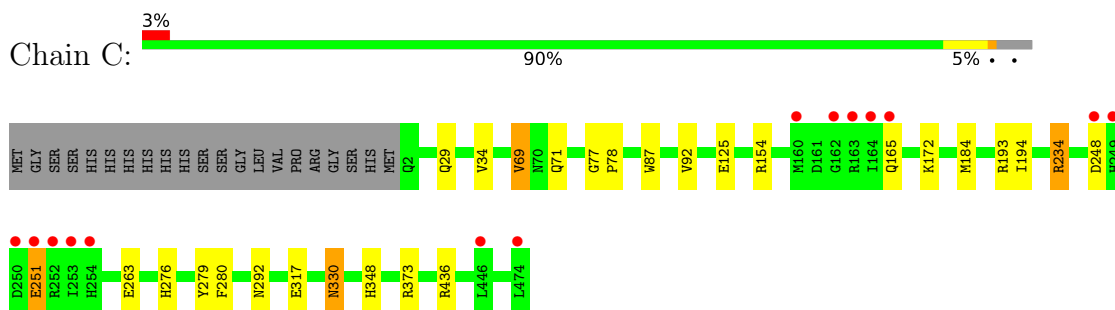
• Molecule 1: ATRAZINE CHLOROHYDROLASE



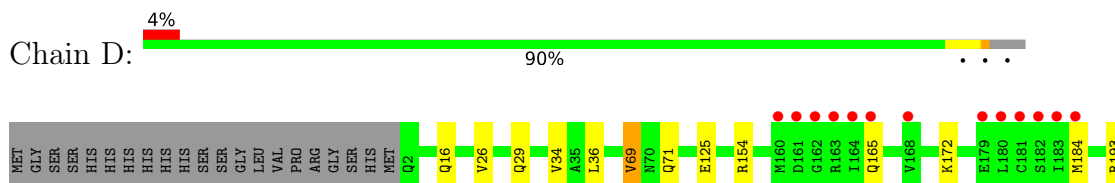
• Molecule 1: ATRAZINE CHLOROHYDROLASE



• Molecule 1: ATRAZINE CHLOROHYDROLASE

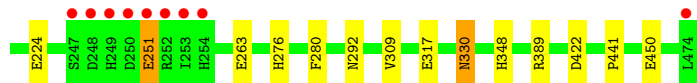
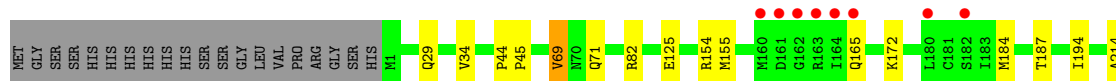
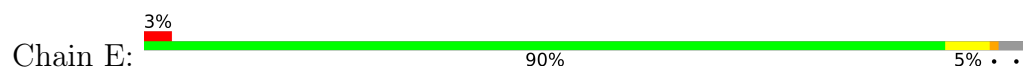


• Molecule 1: ATRAZINE CHLOROHYDROLASE

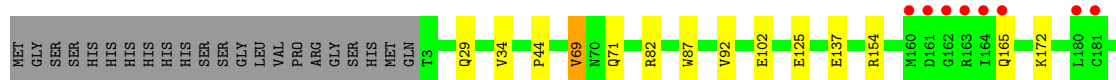
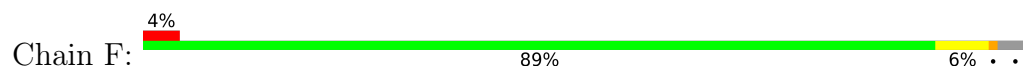




• Molecule 1: ATRAZINE CHLOROHYDROLASE



• Molecule 1: ATRAZINE CHLOROHYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.27Å 146.06Å 196.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.19 – 2.20 117.19 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (117.19-2.20) 99.5 (117.19-2.20)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.166 , 0.196 0.174 , 0.202	Depositor DCC
R_{free} test set	8345 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23156	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.11	2/3781 (0.1%)	1.00	3/5133 (0.1%)
1	B	1.12	1/3784 (0.0%)	0.98	0/5136
1	C	1.18	1/3781 (0.0%)	1.00	1/5133 (0.0%)
1	D	1.10	2/3773 (0.1%)	0.99	2/5122 (0.0%)
1	E	1.18	3/3791 (0.1%)	1.03	2/5145 (0.0%)
1	F	1.17	4/3773 (0.1%)	1.02	2/5122 (0.0%)
All	All	1.15	13/22683 (0.1%)	1.00	10/30791 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	45	PRO	CA-C	6.30	1.55	1.51
1	E	441	PRO	CA-C	6.02	1.55	1.51
1	F	244	MET	C-O	5.85	1.30	1.24
1	E	309	VAL	C-O	-5.75	1.18	1.24
1	D	244	MET	C-O	5.73	1.30	1.24
1	F	44	PRO	C-O	-5.37	1.20	1.24
1	F	312	VAL	C-O	-5.34	1.20	1.24
1	A	45	PRO	C-O	-5.21	1.20	1.25
1	D	399	HIS	CA-CB	-5.15	1.47	1.53
1	B	244	MET	C-O	5.13	1.29	1.24
1	F	44	PRO	CA-C	5.10	1.55	1.52
1	A	311	PRO	CA-C	5.08	1.58	1.53
1	C	436	ARG	CA-C	5.04	1.59	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	VAL	N-CA-C	7.33	117.93	110.82
1	E	69	VAL	N-CA-C	6.75	117.37	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	VAL	N-CA-C	6.49	117.11	110.82
1	A	181	CYS	N-CA-C	6.38	119.13	109.23
1	C	69	VAL	N-CA-C	6.35	116.98	110.82
1	D	165	GLN	N-CA-C	5.83	118.86	111.69
1	A	3	THR	N-CA-C	5.40	118.03	109.50
1	F	385	GLU	CB-CG-CD	5.33	121.66	112.60
1	E	44	PRO	N-CA-C	5.18	115.44	110.47
1	F	69	VAL	N-CA-C	5.09	115.75	110.82

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	3704	0	3637	17	0
1	B	3707	0	3641	20	0
1	C	3704	0	3644	16	0
1	D	3696	0	3632	13	0
1	E	3714	0	3661	13	0
1	F	3696	0	3631	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	7	0	10	0	0
3	B	7	0	10	0	0
3	C	7	0	10	1	0
3	D	7	0	10	1	0
3	E	7	0	10	1	0
3	F	7	0	10	0	0
4	A	161	0	0	0	0
4	B	127	0	0	2	0
4	C	185	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	118	0	0	3	0
4	E	171	0	0	3	0
4	F	125	0	0	2	0
All	All	23156	0	21906	91	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 2.

All (91) 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:A:422[B]:ASP:OD1	1:A:434:ASN:HA	1.71	0.89
1:A:4:LEU:CD1	1:A:49:ARG:HG3	2.11	0.80
1:F:187:THR:HG21	1:F:224:GLU:OE1	1.89	0.72
1:A:4:LEU:HD12	1:A:49:ARG:HG3	1.73	0.68
1:E:187:THR:HG21	1:E:224:GLU:OE1	1.94	0.67
1:E:29:GLN:HB3	1:E:34:VAL:HG21	1.77	0.64
1:D:26:VAL:HG22	1:D:36:LEU:HD22	1.82	0.61
1:F:379:HIS:HD2	4:F:2044:HOH:O	1.83	0.60
1:F:154:ARG:HG3	1:F:194:ILE:HG12	1.83	0.60
1:F:154:ARG:CG	1:F:194:ILE:HG12	2.33	0.58
1:D:26:VAL:HG22	1:D:36:LEU:CD2	2.33	0.58
1:D:154:ARG:CG	1:D:194:ILE:HG12	2.35	0.57
1:A:154:ARG:CG	1:A:194:ILE:HG12	2.34	0.57
1:C:154:ARG:CG	1:C:194:ILE:HG12	2.35	0.56
1:E:154:ARG:CG	1:E:194:ILE:HG12	2.35	0.56
1:B:154:ARG:CG	1:B:194:ILE:HG12	2.36	0.56
1:A:4:LEU:CD1	1:A:49:ARG:CG	2.81	0.55
1:D:154:ARG:HG2	1:D:194:ILE:HG12	1.90	0.54
1:B:29:GLN:HB3	1:B:34:VAL:HG21	1.89	0.53
1:D:29:GLN:HB3	1:D:34:VAL:HG21	1.90	0.53
1:A:29:GLN:HB3	1:A:34:VAL:HG21	1.91	0.53
1:C:154:ARG:HG2	1:C:194:ILE:HG12	1.91	0.52
1:B:154:ARG:HG2	1:B:194:ILE:HG12	1.92	0.51
1:C:29:GLN:HB3	1:C:34:VAL:HG21	1.91	0.51
1:E:154:ARG:HG2	1:E:194:ILE:HG12	1.92	0.51
1:F:69:VAL:HG23	1:F:125:GLU:OE1	2.10	0.51
1:D:399:HIS:HE1	4:D:2104:HOH:O	1.94	0.51
1:B:69:VAL:HG23	1:B:125:GLU:OE1	2.11	0.51
1:F:29:GLN:HB3	1:F:34:VAL:HG21	1.93	0.50
1:C:348:HIS:HD2	4:C:2116:HOH:O	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:GLN:HB3	1:E:330:ASN:ND2	2.27	0.49
1:F:71:GLN:HB3	1:F:330:ASN:ND2	2.26	0.49
1:B:396:ASP:OD2	4:B:2117:HOH:O	2.20	0.49
1:A:154:ARG:HG3	1:A:194:ILE:HG12	1.93	0.49
1:A:69:VAL:HG23	1:A:125:GLU:OE1	2.13	0.48
1:C:69:VAL:HG23	1:C:125:GLU:OE1	2.13	0.48
1:C:263:GLU:HG2	3:C:1475:PEG:H42	1.96	0.47
1:D:69:VAL:HG23	1:D:125:GLU:OE1	2.14	0.47
1:A:71:GLN:HB3	1:A:330:ASN:ND2	2.30	0.47
1:D:283:LYS:HZ3	3:D:1475:PEG:H31	1.78	0.47
1:E:69:VAL:HG23	1:E:125:GLU:OE1	2.14	0.47
1:D:248:ASP:HA	1:D:251:GLU:HG3	1.96	0.47
1:E:263:GLU:HG2	3:E:1475:PEG:H41	1.97	0.47
1:A:422[B]:ASP:CG	1:A:434:ASN:HD22	2.23	0.46
1:B:102[A]:GLU:H	1:B:102[A]:GLU:CD	2.23	0.46
1:A:154:ARG:HG2	1:A:194:ILE:HG12	1.96	0.46
1:A:248:ASP:HA	1:A:251:GLU:HG3	1.97	0.46
1:F:248:ASP:HA	1:F:251:GLU:HG3	1.96	0.46
1:B:248:ASP:HA	1:B:251:GLU:HG3	1.97	0.46
1:E:155:MET:HA	1:E:214:ALA:O	2.16	0.45
1:B:32:ARG:HG3	1:B:389:ARG:NH2	2.31	0.45
1:C:71:GLN:HB3	1:C:330:ASN:ND2	2.32	0.45
1:B:71:GLN:HB3	1:B:330:ASN:ND2	2.32	0.45
1:B:97:LYS:O	1:B:97:LYS:HG3	2.17	0.44
1:F:82:ARG:NE	4:F:2022:HOH:O	2.42	0.44
1:C:248:ASP:HA	1:C:251:GLU:HG3	1.98	0.44
1:A:32:ARG:HG3	1:A:389:ARG:NH2	2.32	0.44
1:D:348:HIS:HD2	4:D:2086:HOH:O	2.01	0.44
1:C:234:ARG:HH11	1:C:234:ARG:HG2	1.82	0.44
1:D:71:GLN:HB3	1:D:330:ASN:ND2	2.33	0.43
1:E:389:ARG:HD3	4:E:2139:HOH:O	2.18	0.43
1:A:4:LEU:HD13	1:A:49:ARG:CG	2.48	0.43
1:A:93:TYR:HB2	1:A:94:PRO:HD3	2.01	0.43
1:C:234:ARG:HG2	1:C:234:ARG:NH1	2.34	0.43
1:C:330:ASN:HD22	1:C:330:ASN:H	1.66	0.43
1:B:130:ALA:CB	1:B:154:ARG:HD3	2.49	0.43
1:B:251:GLU:C	1:B:252:ARG:HD2	2.43	0.43
1:E:154:ARG:HG3	1:E:194:ILE:HG12	2.01	0.43
1:A:155:MET:HA	1:A:214:ALA:O	2.19	0.43
1:B:155:MET:HA	1:B:214:ALA:O	2.19	0.42
1:B:16:GLN:HB2	4:B:2008:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ASP:HB3	1:A:279:TYR:CE2	2.55	0.42
1:D:330:ASN:HD22	1:D:330:ASN:H	1.68	0.42
1:E:330:ASN:H	1:E:330:ASN:HD22	1.67	0.42
1:F:87:TRP:CH2	1:F:92:VAL:HG21	2.55	0.42
1:B:130:ALA:HB3	1:B:154:ARG:HD3	2.02	0.41
1:B:248:ASP:HB3	1:B:279:TYR:CE2	2.55	0.41
1:C:87:TRP:CH2	1:C:92:VAL:HG21	2.55	0.41
1:E:348:HIS:HD2	4:E:2108:HOH:O	2.03	0.41
1:C:87:TRP:CZ2	1:C:92:VAL:HG21	2.55	0.41
1:C:154:ARG:HG3	1:C:194:ILE:HG12	2.01	0.41
1:C:77:GLY:N	1:C:78:PRO:CD	2.83	0.41
1:C:248:ASP:HB3	1:C:279:TYR:CE2	2.55	0.41
1:D:16:GLN:HB2	4:D:2006:HOH:O	2.21	0.41
1:E:82:ARG:NE	4:E:2032:HOH:O	2.29	0.41
1:B:87:TRP:CH2	1:B:92:VAL:HG21	2.56	0.40
1:B:87:TRP:CZ2	1:B:92:VAL:HG21	2.57	0.40
1:B:157:PHE:N	1:B:157:PHE:CD1	2.90	0.40
1:B:330:ASN:HD22	1:B:330:ASN:H	1.69	0.40
1:F:87:TRP:CZ2	1:F:92:VAL:HG21	2.57	0.40
1:F:248:ASP:HB3	1:F:279:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	474/494 (96%)	458 (97%)	14 (3%)	2 (0%)	30 34
1	B	474/494 (96%)	458 (97%)	14 (3%)	2 (0%)	30 34
1	C	474/494 (96%)	457 (96%)	15 (3%)	2 (0%)	30 34
1	D	473/494 (96%)	457 (97%)	14 (3%)	2 (0%)	30 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	475/494 (96%)	458 (96%)	15 (3%)	2 (0%)	30	34
1	F	473/494 (96%)	455 (96%)	15 (3%)	3 (1%)	21	23
All	All	2843/2964 (96%)	2743 (96%)	87 (3%)	13 (0%)	24	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	GLU
1	A	276	HIS
1	B	251	GLU
1	B	276	HIS
1	C	251	GLU
1	C	276	HIS
1	D	251	GLU
1	D	276	HIS
1	E	251	GLU
1	E	276	HIS
1	F	251	GLU
1	F	276	HIS
1	F	327	ASP

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	389/404 (96%)	377 (97%)	12 (3%)	35	48
1	B	389/404 (96%)	378 (97%)	11 (3%)	38	52
1	C	389/404 (96%)	379 (97%)	10 (3%)	40	55
1	D	388/404 (96%)	379 (98%)	9 (2%)	44	59
1	E	390/404 (96%)	380 (97%)	10 (3%)	40	55
1	F	388/404 (96%)	376 (97%)	12 (3%)	35	48
All	All	2333/2424 (96%)	2269 (97%)	64 (3%)	40	53

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	97	LYS
1	A	102	GLU
1	A	137	GLU
1	A	172	LYS
1	A	181	CYS
1	A	184	MET
1	A	193	ARG
1	A	280	PHE
1	A	292	ASN
1	A	317	GLU
1	A	330	ASN
1	B	102[A]	GLU
1	B	102[B]	GLU
1	B	172	LYS
1	B	184	MET
1	B	193	ARG
1	B	252	ARG
1	B	280	PHE
1	B	292	ASN
1	B	317[A]	GLU
1	B	317[B]	GLU
1	B	330	ASN
1	C	165	GLN
1	C	172	LYS
1	C	184	MET
1	C	193	ARG
1	C	234	ARG
1	C	280	PHE
1	C	292	ASN
1	C	317	GLU
1	C	330	ASN
1	C	373	ARG
1	D	172	LYS
1	D	184	MET
1	D	193	ARG
1	D	253	ILE
1	D	280	PHE
1	D	292	ASN
1	D	317[A]	GLU
1	D	317[B]	GLU
1	D	330	ASN

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Mol	Chain	Res	Type
1	E	165	GLN
1	E	172	LYS
1	E	184	MET
1	E	251	GLU
1	E	280	PHE
1	E	292	ASN
1	E	317	GLU
1	E	330	ASN
1	E	422	ASP
1	E	450	GLU
1	F	102	GLU
1	F	137	GLU
1	F	165	GLN
1	F	172	LYS
1	F	184	MET
1	F	193	ARG
1	F	280	PHE
1	F	292	ASN
1	F	317[A]	GLU
1	F	317[B]	GLU
1	F	330	ASN
1	F	444	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	177	GLN
1	A	249	HIS
1	A	302	ASN
1	A	328	ASN
1	A	330	ASN
1	A	348	HIS
1	A	399	HIS
1	A	434	ASN
1	B	7	GLN
1	B	126	ASN
1	B	302	ASN
1	B	328	ASN
1	B	330	ASN
1	B	348	HIS
1	B	399	HIS

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Mol	Chain	Res	Type
1	C	126	ASN
1	C	165	GLN
1	C	302	ASN
1	C	328	ASN
1	C	330	ASN
1	C	348	HIS
1	C	399	HIS
1	D	16	GLN
1	D	200	GLN
1	D	302	ASN
1	D	328	ASN
1	D	330	ASN
1	D	336	ASN
1	D	348	HIS
1	D	399	HIS
1	E	165	GLN
1	E	249	HIS
1	E	292	ASN
1	E	302	ASN
1	E	328	ASN
1	E	330	ASN
1	E	348	HIS
1	E	399	HIS
1	F	70	ASN
1	F	165	GLN
1	F	249	HIS
1	F	276	HIS
1	F	302	ASN
1	F	328	ASN
1	F	330	ASN
1	F	348	HIS
1	F	379	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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	PEG	E	1475	-	6,6,6	0.53	0	5,5,5	0.60	0
3	PEG	A	1475	-	6,6,6	0.33	0	5,5,5	0.57	0
3	PEG	B	1475	-	6,6,6	0.52	0	5,5,5	0.79	0
3	PEG	C	1475	-	6,6,6	0.45	0	5,5,5	0.68	0
3	PEG	D	1475	-	6,6,6	0.28	0	5,5,5	0.79	0
3	PEG	F	1475	-	6,6,6	0.44	0	5,5,5	0.48	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	PEG	E	1475	-	-	3/4/4/4	-
3	PEG	A	1475	-	-	1/4/4/4	-
3	PEG	B	1475	-	-	3/4/4/4	-
3	PEG	C	1475	-	-	1/4/4/4	-
3	PEG	D	1475	-	-	1/4/4/4	-
3	PEG	F	1475	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1475	PEG	O1-C1-C2-O2
3	B	1475	PEG	O1-C1-C2-O2
3	E	1475	PEG	O1-C1-C2-O2
3	B	1475	PEG	O2-C3-C4-O4
3	C	1475	PEG	O1-C1-C2-O2
3	F	1475	PEG	O1-C1-C2-O2
3	F	1475	PEG	C4-C3-O2-C2
3	F	1475	PEG	O2-C3-C4-O4
3	E	1475	PEG	C1-C2-O2-C3
3	A	1475	PEG	C1-C2-O2-C3
3	B	1475	PEG	C4-C3-O2-C2
3	E	1475	PEG	O2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1475	PEG	1	0
3	C	1475	PEG	1	0
3	D	1475	PEG	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	473/494 (95%)	-0.24	19 (4%)	42	39	10, 21, 50, 109	3 (0%)
1	B	472/494 (95%)	-0.28	18 (3%)	44	41	10, 21, 47, 116	4 (0%)
1	C	473/494 (95%)	-0.40	14 (2%)	52	49	9, 19, 40, 110	3 (0%)
1	D	473/494 (95%)	-0.17	22 (4%)	36	33	11, 22, 52, 117	2 (0%)
1	E	474/494 (95%)	-0.37	17 (3%)	46	43	8, 17, 46, 115	3 (0%)
1	F	472/494 (95%)	-0.33	18 (3%)	44	41	9, 19, 45, 107	3 (0%)
All	All	2837/2964 (95%)	-0.30	108 (3%)	44	41	8, 20, 47, 117	18 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	164	ILE	7.5
1	A	164	ILE	6.6
1	B	164	ILE	6.5
1	F	250	ASP	5.5
1	E	164	ILE	5.5
1	D	164	ILE	5.3
1	A	249	HIS	5.2
1	A	160	MET	5.2
1	A	474	LEU	5.1
1	E	163	ARG	5.1
1	A	250	ASP	5.0
1	D	250	ASP	5.0
1	B	250	ASP	4.9
1	D	181	CYS	4.9
1	F	249	HIS	4.9
1	C	164	ILE	4.9
1	B	163	ARG	4.9
1	E	251	GLU	4.8
1	A	252	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	251	GLU	4.6
1	F	252	ARG	4.6
1	D	162	GLY	4.6
1	E	249	HIS	4.5
1	D	249	HIS	4.5
1	E	254	HIS	4.4
1	B	181	CYS	4.4
1	E	250	ASP	4.4
1	B	160	MET	4.4
1	F	254	HIS	4.4
1	F	253	ILE	4.3
1	B	249	HIS	4.2
1	B	254	HIS	4.2
1	C	251	GLU	4.1
1	D	252	ARG	4.0
1	C	250	ASP	4.0
1	C	252	ARG	3.9
1	A	254	HIS	3.9
1	B	253	ILE	3.9
1	D	160	MET	3.9
1	C	163	ARG	3.9
1	F	160	MET	3.8
1	B	251	GLU	3.8
1	E	253	ILE	3.7
1	B	162	GLY	3.7
1	E	161	ASP	3.7
1	B	252	ARG	3.7
1	D	254	HIS	3.7
1	B	474	LEU	3.6
1	D	163	ARG	3.6
1	D	251	GLU	3.6
1	C	474	LEU	3.6
1	A	163	ARG	3.4
1	E	162	GLY	3.4
1	E	252	ARG	3.4
1	F	163	ARG	3.4
1	C	249	HIS	3.4
1	D	180	LEU	3.3
1	C	160	MET	3.3
1	D	253	ILE	3.3
1	A	162	GLY	3.3
1	B	161	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	161	ASP	3.2
1	A	253	ILE	3.2
1	D	165	GLN	3.2
1	C	253	ILE	3.2
1	F	165	GLN	3.1
1	D	474	LEU	3.1
1	F	181	CYS	3.1
1	E	160	MET	3.1
1	F	180	LEU	2.9
1	B	180	LEU	2.9
1	A	251	GLU	2.9
1	A	165	GLN	2.8
1	B	248	ASP	2.8
1	F	162	GLY	2.8
1	C	254	HIS	2.8
1	E	474	LEU	2.7
1	C	165	GLN	2.7
1	D	248	ASP	2.7
1	D	247	SER	2.7
1	A	248	ASP	2.6
1	A	166	GLY	2.6
1	F	161	ASP	2.5
1	A	181	CYS	2.5
1	B	179	GLU	2.5
1	E	248	ASP	2.4
1	A	2	GLN	2.4
1	C	162	GLY	2.4
1	E	165	GLN	2.4
1	F	444	ARG	2.4
1	F	248	ASP	2.3
1	F	474	LEU	2.3
1	E	180	LEU	2.3
1	D	168	VAL	2.3
1	A	161	ASP	2.2
1	C	248	ASP	2.2
1	A	247	SER	2.2
1	E	182	SER	2.2
1	D	183	ILE	2.2
1	B	165	GLN	2.2
1	C	446[A]	LEU	2.1
1	B	182	SER	2.1
1	D	184	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	179	GLU	2.1
1	F	224	GLU	2.1
1	D	182	SER	2.0
1	E	247	SER	2.0
1	A	182	SER	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
3	PEG	C	1475	7/7	0.92	0.10	31,35,42,43	0
3	PEG	D	1475	7/7	0.92	0.11	39,40,43,46	0
3	PEG	A	1475	7/7	0.93	0.10	31,35,37,39	0
3	PEG	B	1475	7/7	0.94	0.09	31,35,36,38	0
3	PEG	E	1475	7/7	0.94	0.09	30,33,39,40	0
3	PEG	F	1475	7/7	0.94	0.08	31,32,35,42	0
2	FE	A	481	1/1	0.95	0.06	29,29,29,29	1
2	FE	B	481	1/1	0.96	0.07	26,26,26,26	1
2	FE	C	481	1/1	0.97	0.04	25,25,25,25	1
2	FE	D	481	1/1	0.97	0.08	27,27,27,27	1
2	FE	F	481	1/1	0.98	0.04	26,26,26,26	1
2	FE	E	481	1/1	0.99	0.03	23,23,23,23	1

6.5 Other polymers [i](#)

There are no such residues in this entry.