Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 06:18 pm BST

PDB ID	:	4V1X
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 (i) 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 (i)) were used in the production of this report:

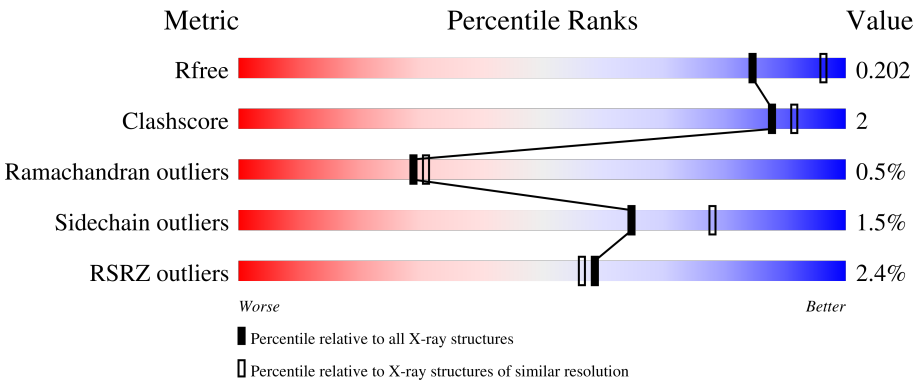
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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% 88% 6% • •
1	B	494	3% 88% 7% • •
1	C	494	2% 88% 7% • •
1	D	494	2% 90% 5% • •
1	E	494	2% 89% 6% • •

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Mol	Chain	Length	Quality of chain
1	F	494	2% 89% 6%

2 Entry composition (i)

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 CHLOROHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	473	3704	2311	682	687	24	0	3	0
1	B	472	3707	2313	683	687	24	0	4	0
1	C	473	3704	2313	682	685	24	0	3	0
1	D	473	3696	2307	680	685	24	0	2	0
1	E	474	3714	2319	685	685	25	0	3	0
1	F	472	3696	2307	680	685	24	0	3	0

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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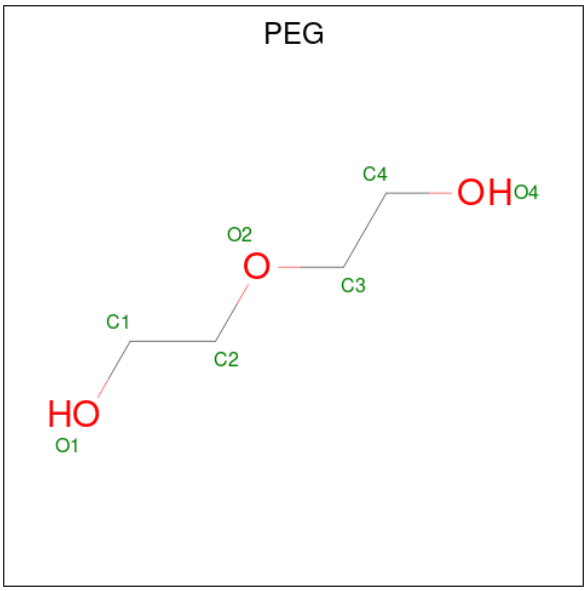
Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP P72156
F	-17	SER	-	expression tag	UNP P72156
F	-16	SER	-	expression tag	UNP P72156
F	-15	HIS	-	expression tag	UNP P72156
F	-14	HIS	-	expression tag	UNP P72156
F	-13	HIS	-	expression tag	UNP P72156
F	-12	HIS	-	expression tag	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 (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is water.

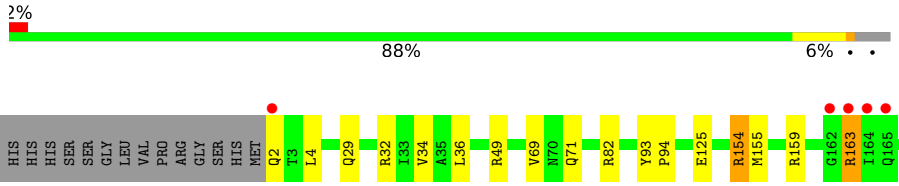
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	161	161	161	0	0
4	B	127	127	127	0	0
4	C	185	185	185	0	0
4	D	118	118	118	0	0
4	E	171	171	171	0	0
4	F	125	125	125	0	0

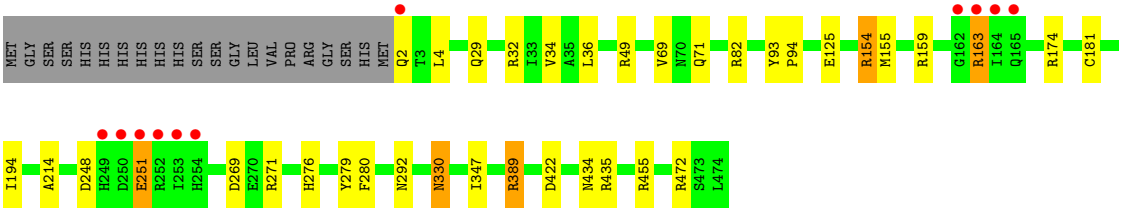
3 Residue-property plots (i)

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

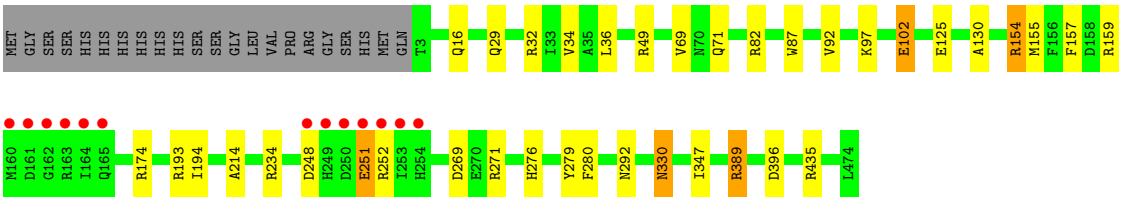
Chain A:





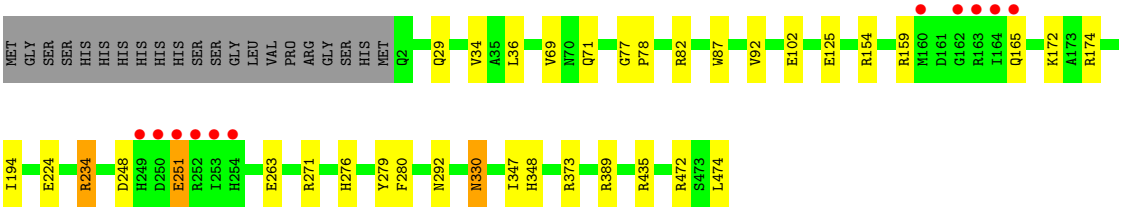
• Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain B:



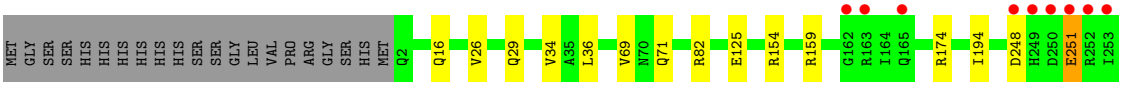
• Molecule 1: ATRAZINE CHLOROHYDROLASE

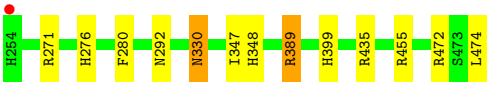
Chain C:



• Molecule 1: ATRAZINE CHLOROHYDROLASE

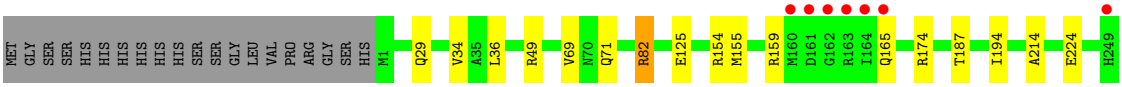
Chain D:

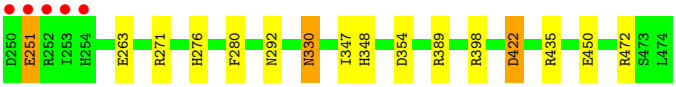




• Molecule 1: ATRAZINE CHLOROHYDROLASE

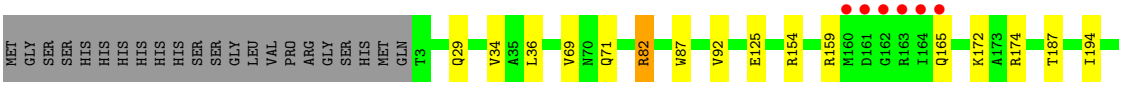
Chain E:

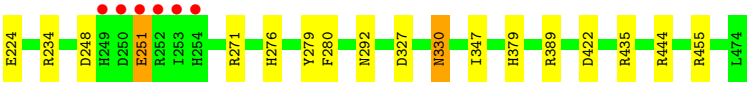




• Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain F:





4 Data and refinement statistics (i)

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 48.74 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (117.19-2.20) 99.5 (48.74-2.20)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.166 , 0.196 0.173 , 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)	0.33 , 30.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.83	0/3781	0.96	20/5133 (0.4%)
1	B	0.83	2/3784 (0.1%)	0.95	19/5136 (0.4%)
1	C	0.87	1/3781 (0.0%)	0.96	18/5133 (0.4%)
1	D	0.82	0/3773	0.95	16/5122 (0.3%)
1	E	0.89	1/3791 (0.0%)	1.01	18/5145 (0.3%)
1	F	0.87	0/3773	0.98	18/5122 (0.4%)
All	All	0.85	4/22683 (0.0%)	0.97	109/30791 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	422	ASP	CB-CG	-5.73	1.39	1.51
1	C	102	GLU	CG-CD	5.69	1.60	1.51
1	B	102[A]	GLU	CD-OE2	-5.05	1.20	1.25
1	B	102[B]	GLU	CD-OE2	-5.05	1.20	1.25

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	271[A]	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	E	271[B]	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	A	271[A]	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	A	271[B]	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	F	422	ASP	CB-CG-OD1	9.30	126.67	118.30
1	E	82	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	F	271[A]	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	F	271[B]	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	C	82	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	E	398	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	E	271[A]	ARG	NE-CZ-NH1	8.89	124.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	271[B]	ARG	NE-CZ-NH1	8.89	124.74	120.30
1	A	82	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	C	82	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	E	398	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	D	82	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	F	82	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	174	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	D	271[A]	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	D	271[B]	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	C	435	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	C	271[A]	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	C	271[B]	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	B	82	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	F	174	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	F	234	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	271[A]	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	271[B]	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	D	174	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	E	49	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	F	82	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	B	82	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	F	271[A]	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	F	271[B]	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	E	82	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	435	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	271[A]	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	271[B]	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	82	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	E	49	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	174	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	D	82	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	271[A]	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	D	271[B]	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	E	174	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	C	174	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	F	422	ASP	CB-CG-OD2	-6.52	112.44	118.30
1	C	474	LEU	CB-CG-CD2	6.50	122.06	111.00
1	F	174	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	C	102	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	E	435	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	174	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	B	435	ARG	NE-CZ-NH1	6.14	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	174	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	D	455	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	D	474	LEU	CB-CG-CD2	6.01	121.22	111.00
1	B	159	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	159	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	E	159	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	36	LEU	CA-CB-CG	5.86	128.77	115.30
1	E	472	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	F	389	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	234	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	389	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	435	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	389	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	F	435	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	174	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	389	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	389	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	163	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	F	36	LEU	CA-CB-CG	5.62	128.22	115.30
1	C	435	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	E	347	ILE	CG1-CB-CG2	-5.54	99.21	111.40
1	F	347	ILE	CG1-CB-CG2	-5.52	99.26	111.40
1	B	269	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	193	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	C	472	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	347	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	C	271[A]	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	C	271[B]	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	455	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	E	354	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	159	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	347	ILE	CG1-CB-CG2	-5.34	99.65	111.40
1	C	373	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	347	ILE	CG1-CB-CG2	-5.29	99.76	111.40
1	D	347	ILE	CG1-CB-CG2	-5.29	99.76	111.40
1	C	36	LEU	CA-CB-CG	5.28	127.44	115.30
1	F	159	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	E	36	LEU	CB-CA-C	-5.26	100.21	110.20
1	A	163	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	154	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	D	435	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	F	455	ARG	NE-CZ-NH1	5.20	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	154	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	154	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	36	LEU	CA-CB-CG	5.17	127.19	115.30
1	F	36	LEU	CB-CA-C	-5.14	100.43	110.20
1	B	271[A]	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	271[B]	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	269	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	174	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	D	472	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	E	36	LEU	CA-CB-CG	5.05	126.91	115.30
1	D	435	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	472	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	49	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	159	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	19	0
1	C	3704	0	3644	16	0
1	D	3696	0	3632	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	0	10	0	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
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	89	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 (89) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:248:ASP:HB3	1:A:279:TYR:CE2	2.55	0.42
1:A:422[B]:ASP:CG	1:A:434:ASN:HD22	2.23	0.42
1:B:102[A]:GLU:H	1:B:102[A]:GLU:CD	2.23	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 (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	474/494 (96%)	458 (97%)	14 (3%)	2 (0%)	34 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	474/494 (96%)	458 (97%)	14 (3%)	2 (0%)	34	37
1	C	474/494 (96%)	457 (96%)	15 (3%)	2 (0%)	34	37
1	D	473/494 (96%)	457 (97%)	14 (3%)	2 (0%)	34	37
1	E	475/494 (96%)	458 (96%)	15 (3%)	2 (0%)	34	37
1	F	473/494 (96%)	455 (96%)	15 (3%)	3 (1%)	25	26
All	All	2843/2964 (96%)	2743 (96%)	87 (3%)	13 (0%)	29	31

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 (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	389/404 (96%)	383 (98%)	6 (2%)	65	78
1	B	389/404 (96%)	385 (99%)	4 (1%)	76	86
1	C	389/404 (96%)	382 (98%)	7 (2%)	59	72
1	D	388/404 (96%)	384 (99%)	4 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	390/404 (96%)	383 (98%)	7 (2%)	59	72
1	F	388/404 (96%)	382 (98%)	6 (2%)	65	78
All	All	2333/2424 (96%)	2299 (98%)	34 (2%)	65	78

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	163	ARG
1	A	181	CYS
1	A	280	PHE
1	A	292	ASN
1	A	330	ASN
1	B	252	ARG
1	B	280	PHE
1	B	292	ASN
1	B	330	ASN
1	C	165	GLN
1	C	172	LYS
1	C	224	GLU
1	C	234	ARG
1	C	280	PHE
1	C	292	ASN
1	C	330	ASN
1	D	280	PHE
1	D	292	ASN
1	D	330	ASN
1	D	389	ARG
1	E	165	GLN
1	E	251	GLU
1	E	280	PHE
1	E	292	ASN
1	E	330	ASN
1	E	422	ASP
1	E	450	GLU
1	F	165	GLN
1	F	172	LYS
1	F	280	PHE
1	F	292	ASN
1	F	330	ASN
1	F	444	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	70	ASN
1	A	200	GLN
1	A	330	ASN
1	A	348	HIS
1	A	399	HIS
1	A	434	ASN
1	B	70	ASN
1	B	200	GLN
1	B	302	ASN
1	B	330	ASN
1	B	348	HIS
1	B	379	HIS
1	C	7	GLN
1	C	70	ASN
1	C	200	GLN
1	C	330	ASN
1	C	348	HIS
1	C	379	HIS
1	C	399	HIS
1	C	434	ASN
1	D	16	GLN
1	D	70	ASN
1	D	200	GLN
1	D	330	ASN
1	D	348	HIS
1	D	399	HIS
1	E	7	GLN
1	E	70	ASN
1	E	200	GLN
1	E	302	ASN
1	E	330	ASN
1	E	348	HIS
1	E	399	HIS
1	F	70	ASN
1	F	330	ASN
1	F	348	HIS
1	F	379	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	1475	-	6,6,6	0.32	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	E	1475	-	6,6,6	0.52	0	5,5,5	0.60	0
3	PEG	D	1475	-	6,6,6	0.27	0	5,5,5	0.79	0
3	PEG	F	1475	-	6,6,6	0.43	0	5,5,5	0.48	0
3	PEG	C	1475	-	6,6,6	0.44	0	5,5,5	0.68	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	A	1475	-	-	1/4/4/4	-
3	PEG	B	1475	-	-	3/4/4/4	-
3	PEG	E	1475	-	-	3/4/4/4	-
3	PEG	D	1475	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	F	1475	-	-	3/4/4/4	-
3	PEG	C	1475	-	-	1/4/4/4	-

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	B	1475	PEG	C4-C3-O2-C2
3	A	1475	PEG	C1-C2-O2-C3
3	E	1475	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1475	PEG	1	0
3	C	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.39	11 (2%)	60	58	12, 21, 50, 109	0
1	B	472/494 (95%)	-0.40	13 (2%)	53	51	12, 21, 47, 116	0
1	C	473/494 (95%)	-0.39	11 (2%)	60	58	12, 19, 40, 110	0
1	D	473/494 (95%)	-0.37	10 (2%)	63	61	12, 22, 52, 117	0
1	E	474/494 (95%)	-0.49	12 (2%)	57	55	9, 17, 46, 115	0
1	F	472/494 (95%)	-0.52	12 (2%)	57	55	10, 19, 45, 107	0
All	All	2837/2964 (95%)	-0.43	69 (2%)	59	56	9, 20, 47, 117	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	ARG	10.0
1	E	163	ARG	9.2
1	C	163	ARG	6.5
1	D	163	ARG	6.4
1	F	163	ARG	6.1
1	A	252	ARG	5.8
1	E	164	ILE	5.5
1	A	163	ARG	5.3
1	B	252	ARG	5.3
1	D	162	GLY	5.2
1	F	250	ASP	5.2
1	C	250	ASP	5.1
1	D	251	GLU	5.0
1	E	162	GLY	5.0
1	D	249	HIS	4.9
1	B	162	GLY	4.8
1	F	164	ILE	4.7
1	F	252	ARG	4.6
1	C	252	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	251	GLU	4.5
1	D	250	ASP	4.4
1	E	254	HIS	4.3
1	F	254	HIS	4.3
1	E	250	ASP	4.3
1	F	162	GLY	4.3
1	C	251	GLU	4.2
1	C	164	ILE	4.1
1	D	165	GLN	4.0
1	B	254	HIS	4.0
1	B	164	ILE	3.9
1	B	250	ASP	3.9
1	A	254	HIS	3.8
1	A	165	GLN	3.7
1	C	254	HIS	3.7
1	A	162	GLY	3.6
1	C	162	GLY	3.6
1	D	252	ARG	3.6
1	E	161	ASP	3.5
1	E	251	GLU	3.3
1	F	161	ASP	3.3
1	B	161	ASP	3.3
1	B	251	GLU	3.2
1	E	249	HIS	3.2
1	A	164	ILE	3.2
1	B	165	GLN	3.2
1	F	253	ILE	3.1
1	A	249	HIS	3.1
1	B	249	HIS	3.1
1	D	253	ILE	3.0
1	E	252	ARG	3.0
1	F	249	HIS	3.0
1	E	253	ILE	3.0
1	C	249	HIS	2.9
1	D	248	ASP	2.9
1	F	160	MET	2.8
1	C	253	ILE	2.6
1	A	250	ASP	2.6
1	C	165	GLN	2.6
1	A	253	ILE	2.5
1	B	160	MET	2.5
1	F	165	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	165	GLN	2.4
1	D	254	HIS	2.3
1	C	160	MET	2.3
1	E	160	MET	2.3
1	B	253	ILE	2.3
1	A	251	GLU	2.3
1	B	248	ASP	2.1
1	A	2	GLN	2.1

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 monosaccharides 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(Å^2)	Q<0.9
3	PEG	E	1475	7/7	0.92	0.10	30,33,39,40	0
3	PEG	C	1475	7/7	0.93	0.11	31,35,42,43	0
3	PEG	D	1475	7/7	0.93	0.13	39,40,43,46	0
3	PEG	B	1475	7/7	0.93	0.10	31,35,36,38	0
3	PEG	A	1475	7/7	0.94	0.13	31,35,37,39	0
3	PEG	F	1475	7/7	0.94	0.10	31,32,35,42	0
2	FE	A	481	1/1	0.95	0.12	29,29,29,29	1
2	FE	D	481	1/1	0.97	0.07	27,27,27,27	1
2	FE	C	481	1/1	0.98	0.11	25,25,25,25	1
2	FE	E	481	1/1	0.98	0.10	23,23,23,23	1
2	FE	F	481	1/1	0.98	0.08	26,26,26,26	1
2	FE	B	481	1/1	0.99	0.11	26,26,26,26	1

6.5 Other polymers (i)

There are no such residues in this entry.