



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2023 – 10:08 PM EDT

PDB ID : 3U0G
Title : Crystal structure of branched-chain amino acid aminotransferase from burkholderia pseudomallei
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2011-09-28
Resolution : 1.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

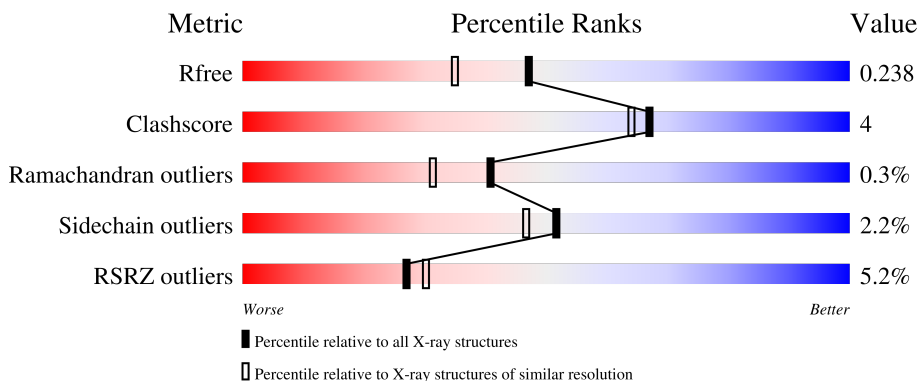
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	328	 4% 85% 7% 8%
1	B	328	 2% 79% 9% 10%
1	C	328	 3% 84% 6% 9%
1	D	328	 5% 83% 8% 9%
1	E	328	 9% 79% 10% 10%

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Mol	Chain	Length	Quality of chain
1	F	328	

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
4	GOL	C	309	-	-	X	-
4	GOL	E	309	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14643 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 Putative branched-chain amino acid aminotransferase IlvE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	Total 2346	C 1484	N 413	O 442	S 7	0	1	0
1	B	295	Total 2296	C 1450	N 404	O 435	S 7	0	0	0
1	C	299	Total 2318	C 1464	N 407	O 440	S 7	0	1	0
1	D	299	Total 2312	C 1458	N 407	O 440	S 7	0	1	0
1	E	296	Total 2308	C 1460	N 403	O 438	S 7	0	1	0
1	F	305	Total 2337	C 1476	N 410	O 444	S 7	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q63WU8
A	-19	ALA	-	expression tag	UNP Q63WU8
A	-18	HIS	-	expression tag	UNP Q63WU8
A	-17	HIS	-	expression tag	UNP Q63WU8
A	-16	HIS	-	expression tag	UNP Q63WU8
A	-15	HIS	-	expression tag	UNP Q63WU8
A	-14	HIS	-	expression tag	UNP Q63WU8
A	-13	HIS	-	expression tag	UNP Q63WU8
A	-12	MET	-	expression tag	UNP Q63WU8
A	-11	GLY	-	expression tag	UNP Q63WU8
A	-10	THR	-	expression tag	UNP Q63WU8
A	-9	LEU	-	expression tag	UNP Q63WU8
A	-8	GLU	-	expression tag	UNP Q63WU8
A	-7	ALA	-	expression tag	UNP Q63WU8
A	-6	GLN	-	expression tag	UNP Q63WU8
A	-5	THR	-	expression tag	UNP Q63WU8
A	-4	GLN	-	expression tag	UNP Q63WU8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q63WU8
A	-2	PRO	-	expression tag	UNP Q63WU8
A	-1	GLY	-	expression tag	UNP Q63WU8
A	0	SER	-	expression tag	UNP Q63WU8
B	-20	MET	-	expression tag	UNP Q63WU8
B	-19	ALA	-	expression tag	UNP Q63WU8
B	-18	HIS	-	expression tag	UNP Q63WU8
B	-17	HIS	-	expression tag	UNP Q63WU8
B	-16	HIS	-	expression tag	UNP Q63WU8
B	-15	HIS	-	expression tag	UNP Q63WU8
B	-14	HIS	-	expression tag	UNP Q63WU8
B	-13	HIS	-	expression tag	UNP Q63WU8
B	-12	MET	-	expression tag	UNP Q63WU8
B	-11	GLY	-	expression tag	UNP Q63WU8
B	-10	THR	-	expression tag	UNP Q63WU8
B	-9	LEU	-	expression tag	UNP Q63WU8
B	-8	GLU	-	expression tag	UNP Q63WU8
B	-7	ALA	-	expression tag	UNP Q63WU8
B	-6	GLN	-	expression tag	UNP Q63WU8
B	-5	THR	-	expression tag	UNP Q63WU8
B	-4	GLN	-	expression tag	UNP Q63WU8
B	-3	GLY	-	expression tag	UNP Q63WU8
B	-2	PRO	-	expression tag	UNP Q63WU8
B	-1	GLY	-	expression tag	UNP Q63WU8
B	0	SER	-	expression tag	UNP Q63WU8
C	-20	MET	-	expression tag	UNP Q63WU8
C	-19	ALA	-	expression tag	UNP Q63WU8
C	-18	HIS	-	expression tag	UNP Q63WU8
C	-17	HIS	-	expression tag	UNP Q63WU8
C	-16	HIS	-	expression tag	UNP Q63WU8
C	-15	HIS	-	expression tag	UNP Q63WU8
C	-14	HIS	-	expression tag	UNP Q63WU8
C	-13	HIS	-	expression tag	UNP Q63WU8
C	-12	MET	-	expression tag	UNP Q63WU8
C	-11	GLY	-	expression tag	UNP Q63WU8
C	-10	THR	-	expression tag	UNP Q63WU8
C	-9	LEU	-	expression tag	UNP Q63WU8
C	-8	GLU	-	expression tag	UNP Q63WU8
C	-7	ALA	-	expression tag	UNP Q63WU8
C	-6	GLN	-	expression tag	UNP Q63WU8
C	-5	THR	-	expression tag	UNP Q63WU8
C	-4	GLN	-	expression tag	UNP Q63WU8

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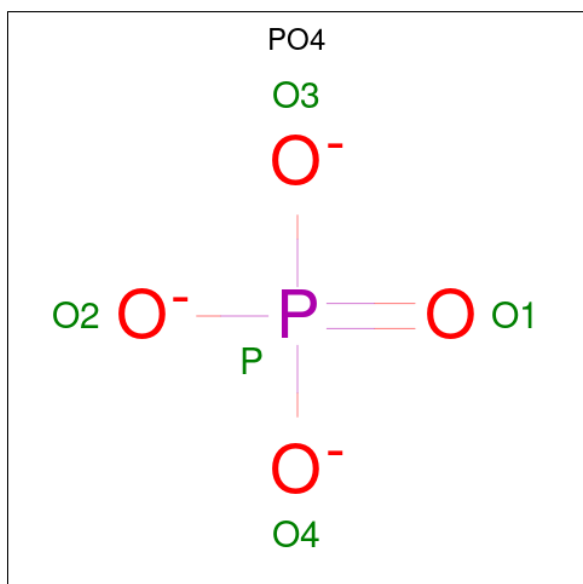
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q63WU8
C	-2	PRO	-	expression tag	UNP Q63WU8
C	-1	GLY	-	expression tag	UNP Q63WU8
C	0	SER	-	expression tag	UNP Q63WU8
D	-20	MET	-	expression tag	UNP Q63WU8
D	-19	ALA	-	expression tag	UNP Q63WU8
D	-18	HIS	-	expression tag	UNP Q63WU8
D	-17	HIS	-	expression tag	UNP Q63WU8
D	-16	HIS	-	expression tag	UNP Q63WU8
D	-15	HIS	-	expression tag	UNP Q63WU8
D	-14	HIS	-	expression tag	UNP Q63WU8
D	-13	HIS	-	expression tag	UNP Q63WU8
D	-12	MET	-	expression tag	UNP Q63WU8
D	-11	GLY	-	expression tag	UNP Q63WU8
D	-10	THR	-	expression tag	UNP Q63WU8
D	-9	LEU	-	expression tag	UNP Q63WU8
D	-8	GLU	-	expression tag	UNP Q63WU8
D	-7	ALA	-	expression tag	UNP Q63WU8
D	-6	GLN	-	expression tag	UNP Q63WU8
D	-5	THR	-	expression tag	UNP Q63WU8
D	-4	GLN	-	expression tag	UNP Q63WU8
D	-3	GLY	-	expression tag	UNP Q63WU8
D	-2	PRO	-	expression tag	UNP Q63WU8
D	-1	GLY	-	expression tag	UNP Q63WU8
D	0	SER	-	expression tag	UNP Q63WU8
E	-20	MET	-	expression tag	UNP Q63WU8
E	-19	ALA	-	expression tag	UNP Q63WU8
E	-18	HIS	-	expression tag	UNP Q63WU8
E	-17	HIS	-	expression tag	UNP Q63WU8
E	-16	HIS	-	expression tag	UNP Q63WU8
E	-15	HIS	-	expression tag	UNP Q63WU8
E	-14	HIS	-	expression tag	UNP Q63WU8
E	-13	HIS	-	expression tag	UNP Q63WU8
E	-12	MET	-	expression tag	UNP Q63WU8
E	-11	GLY	-	expression tag	UNP Q63WU8
E	-10	THR	-	expression tag	UNP Q63WU8
E	-9	LEU	-	expression tag	UNP Q63WU8
E	-8	GLU	-	expression tag	UNP Q63WU8
E	-7	ALA	-	expression tag	UNP Q63WU8
E	-6	GLN	-	expression tag	UNP Q63WU8
E	-5	THR	-	expression tag	UNP Q63WU8
E	-4	GLN	-	expression tag	UNP Q63WU8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP Q63WU8
E	-2	PRO	-	expression tag	UNP Q63WU8
E	-1	GLY	-	expression tag	UNP Q63WU8
E	0	SER	-	expression tag	UNP Q63WU8
F	-20	MET	-	expression tag	UNP Q63WU8
F	-19	ALA	-	expression tag	UNP Q63WU8
F	-18	HIS	-	expression tag	UNP Q63WU8
F	-17	HIS	-	expression tag	UNP Q63WU8
F	-16	HIS	-	expression tag	UNP Q63WU8
F	-15	HIS	-	expression tag	UNP Q63WU8
F	-14	HIS	-	expression tag	UNP Q63WU8
F	-13	HIS	-	expression tag	UNP Q63WU8
F	-12	MET	-	expression tag	UNP Q63WU8
F	-11	GLY	-	expression tag	UNP Q63WU8
F	-10	THR	-	expression tag	UNP Q63WU8
F	-9	LEU	-	expression tag	UNP Q63WU8
F	-8	GLU	-	expression tag	UNP Q63WU8
F	-7	ALA	-	expression tag	UNP Q63WU8
F	-6	GLN	-	expression tag	UNP Q63WU8
F	-5	THR	-	expression tag	UNP Q63WU8
F	-4	GLN	-	expression tag	UNP Q63WU8
F	-3	GLY	-	expression tag	UNP Q63WU8
F	-2	PRO	-	expression tag	UNP Q63WU8
F	-1	GLY	-	expression tag	UNP Q63WU8
F	0	SER	-	expression tag	UNP Q63WU8

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0


- Molecule 5 is water.

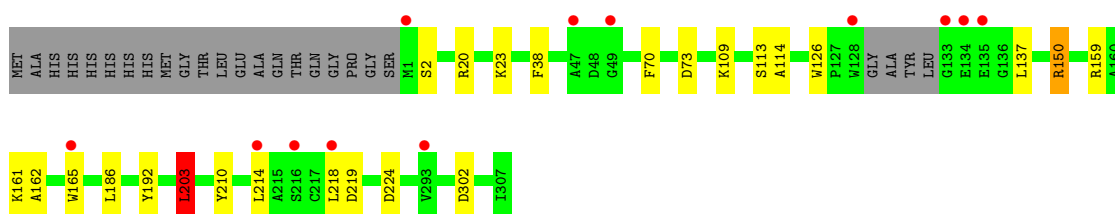
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	125	Total O 125 125	0	0
5	B	133	Total O 133 133	0	0
5	C	132	Total O 132 132	0	0
5	D	97	Total O 97 97	0	0
5	E	100	Total O 100 100	0	0
5	F	85	Total O 85 85	0	0

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.

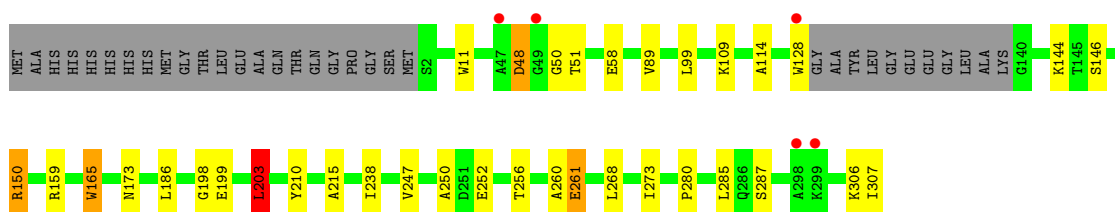
- Molecule 1: Putative branched-chain amino acid aminotransferase IlvE

Chain A: 




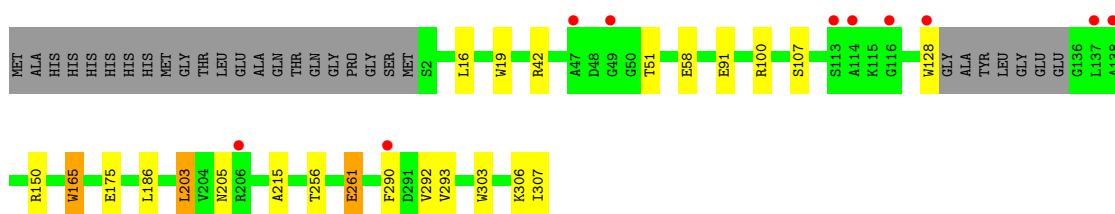
- Molecule 1: Putative branched-chain amino acid aminotransferase IlvE

Chain B: 




- Molecule 1: Putative branched-chain amino acid aminotransferase IlvE

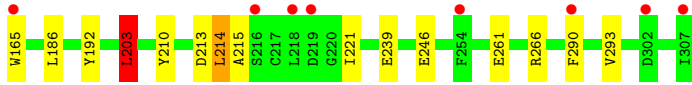
Chain C: 



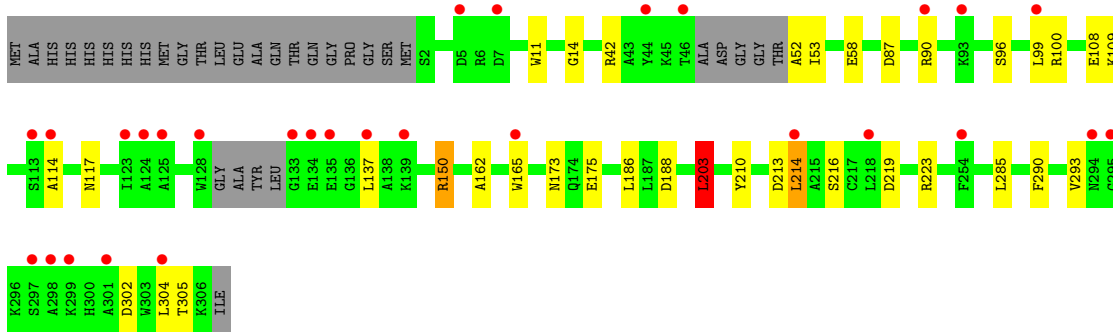
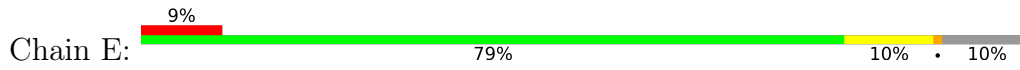
- Molecule 1: Putative branched-chain amino acid aminotransferase IlvE

Chain D: 

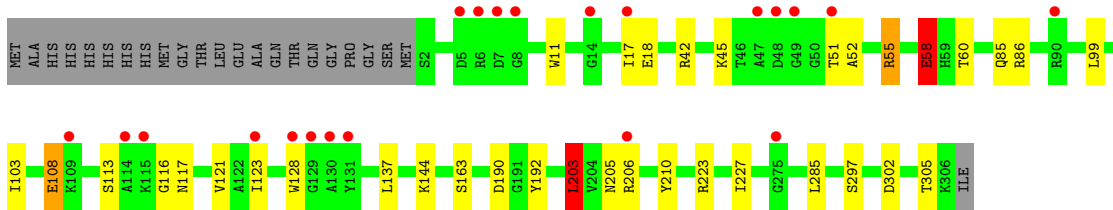
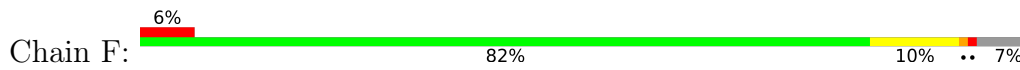




- Molecule 1: Putative branched-chain amino acid aminotransferase IlvE



- Molecule 1: Putative branched-chain amino acid aminotransferase IlvE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	106.97Å 139.27Å 290.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.90) 99.8 (20.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.192 , 0.230 0.198 , 0.238	Depositor DCC
R_{free} test set	8508 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14643	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: CL, GOL, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.86	1/2393 (0.0%)	0.91	3/3243 (0.1%)
1	B	0.88	4/2340 (0.2%)	0.93	4/3168 (0.1%)
1	C	0.83	4/2363 (0.2%)	0.90	5/3202 (0.2%)
1	D	0.82	1/2357 (0.0%)	0.87	1/3194 (0.0%)
1	E	0.79	0/2354	0.89	6/3191 (0.2%)
1	F	0.82	4/2384 (0.2%)	0.88	5/3235 (0.2%)
All	All	0.83	14/14191 (0.1%)	0.90	24/19233 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	163	SER	CB-OG	6.85	1.51	1.42
1	B	165	TRP	CE2-CZ2	-6.64	1.28	1.39
1	C	165	TRP	CE2-CZ2	-6.30	1.29	1.39
1	C	165	TRP	CE3-CZ3	-6.05	1.28	1.38
1	B	165	TRP	CE3-CZ3	-5.92	1.28	1.38
1	A	126	TRP	CD2-CE2	5.82	1.48	1.41
1	B	11	TRP	CD2-CE2	5.71	1.48	1.41
1	D	126	TRP	CD2-CE2	5.66	1.48	1.41
1	F	11	TRP	CD2-CE2	5.61	1.48	1.41
1	C	128	TRP	CD2-CE2	5.48	1.48	1.41
1	B	128	TRP	CD2-CE2	5.42	1.47	1.41
1	C	19	TRP	CD2-CE2	5.14	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	58	GLU	CG-CD	5.03	1.59	1.51
1	F	128	TRP	CD2-CE2	5.01	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	LEU	CA-CB-CG	8.98	135.97	115.30
1	C	203	LEU	CA-CB-CG	8.88	135.72	115.30
1	A	203	LEU	CA-CB-CG	8.51	134.88	115.30
1	E	188	ASP	CB-CG-OD1	8.17	125.66	118.30
1	E	203	LEU	CA-CB-CG	8.01	133.73	115.30
1	C	42	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	150	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	C	42	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	E	58	GLU	OE1-CD-OE2	-6.94	114.97	123.30
1	F	42	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	D	203	LEU	CA-CB-CG	6.49	130.23	115.30
1	B	150	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	E	203	LEU	CB-CG-CD2	6.08	121.34	111.00
1	F	42	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	C	58	GLU	OE1-CD-OE2	-5.94	116.17	123.30
1	A	150	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	100	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	F	203	LEU	CA-CB-CG	5.75	128.53	115.30
1	F	190	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	58	GLU	CG-CD-OE2	5.42	129.13	118.30
1	E	100	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	E	150	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	F	55	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	150	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	161	LYS	Peptide

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	2346	0	2289	23	0
1	B	2296	0	2264	24	0
1	C	2318	0	2262	9	0
1	D	2312	0	2244	17	0
1	E	2308	0	2238	24	0
1	F	2337	0	2262	17	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	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
4	C	6	0	8	4	0
4	E	6	0	8	4	0
4	F	6	0	8	0	0
5	A	125	0	0	6	0
5	B	133	0	0	1	0
5	C	132	0	0	0	0
5	D	97	0	0	2	0
5	E	100	0	0	4	0
5	F	85	0	0	1	0
All	All	14643	0	13583	106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (106) 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:B:51:THR:HG22	1:B:307:ILE:HD12	1.58	0.85
1:A:38:PHE:HD1	5:A:561:HOH:O	1.60	0.83
1:E:109:LYS:HB2	1:E:114:ALA:HB1	1.65	0.78
1:F:55:ARG:NE	1:F:58:GLU:OE2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ALA:HB3	1:D:165[B]:TRP:CD1	2.19	0.78
1:E:216:SER:HB2	5:E:617:HOH:O	1.84	0.77
1:D:214:LEU:CB	5:D:589:HOH:O	2.32	0.76
1:E:52:ALA:HA	1:E:305:THR:O	1.88	0.73
1:A:73:ASP:HB2	5:A:598:HOH:O	1.88	0.71
1:A:214:LEU:HD23	4:E:309:GOL:H32	1.73	0.71
1:B:51:THR:HG22	1:B:307:ILE:CD1	2.22	0.69
1:F:17:ILE:HD12	1:F:18:GLU:H	1.58	0.69
1:B:51:THR:CG2	1:B:307:ILE:HD12	2.24	0.68
1:C:16:LEU:HD13	1:C:91:GLU:HG3	1.75	0.66
1:D:150:ARG:HD3	1:D:186:LEU:HD22	1.78	0.65
1:F:108:GLU:HG3	1:F:117:ASN:HA	1.78	0.64
1:E:150:ARG:HD3	1:E:186:LEU:HD22	1.80	0.64
1:A:224:ASP:OD2	5:A:380:HOH:O	2.16	0.61
1:A:150:ARG:HD3	1:A:186:LEU:HD22	1.82	0.60
1:A:214:LEU:HD23	4:E:309:GOL:C3	2.32	0.59
1:B:89:VAL:HG11	1:B:307:ILE:CD1	2.33	0.58
1:E:162:ALA:HB3	1:E:165[B]:TRP:CD1	2.39	0.57
1:D:203:LEU:HD22	1:D:210:TYR:HB2	1.86	0.57
1:D:27:LEU:HD22	1:D:110:LEU:HD22	1.86	0.57
1:A:38:PHE:CD1	5:A:561:HOH:O	2.45	0.57
1:B:51:THR:CG2	1:B:307:ILE:CD1	2.83	0.57
1:B:89:VAL:HG11	1:B:307:ILE:HD13	1.87	0.56
1:C:175:GLU:OE2	1:F:144:LYS:NZ	2.36	0.56
1:B:252:GLU:OE1	1:B:280:PRO:HD2	2.05	0.56
1:B:210:TYR:CE2	1:B:238:ILE:HD12	2.41	0.56
1:F:85:GLN:HG3	1:F:123:ILE:HD13	1.88	0.56
1:E:11:TRP:CZ2	1:E:14:GLY:HA2	2.41	0.55
4:C:309:GOL:O1	1:E:214:LEU:HD22	2.05	0.55
1:D:214:LEU:CB	5:F:552:HOH:O	2.54	0.54
1:A:161:LYS:HG2	5:A:592:HOH:O	2.07	0.54
1:F:205:ASN:OD1	1:F:206:ARG:HG3	2.08	0.54
4:C:309:GOL:H11	1:E:214:LEU:HD23	1.91	0.53
1:E:87:ASP:OD1	1:E:90:ARG:NH1	2.39	0.52
1:C:150:ARG:HD3	1:C:186:LEU:HD22	1.90	0.52
1:E:213:ASP:HB2	5:E:315:HOH:O	2.09	0.52
1:F:203:LEU:HD22	1:F:210:TYR:HB2	1.91	0.52
1:C:16:LEU:CD1	1:C:91:GLU:HG3	2.39	0.51
1:F:86:ARG:HD2	1:F:305:THR:HG21	1.93	0.50
1:D:215:ALA:HB1	1:F:192:TYR:OH	2.11	0.50
1:F:108:GLU:CG	1:F:117:ASN:HA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:VAL:HG11	1:C:303:TRP:HE3	1.77	0.49
1:E:108:GLU:HG2	1:E:117:ASN:HA	1.94	0.49
1:F:45:LYS:HA	1:F:51:THR:HG22	1.94	0.49
1:A:218:LEU:HD13	5:A:348:HOH:O	2.12	0.49
1:A:150:ARG:NH2	1:A:165[A]:TRP:CH2	2.80	0.49
1:E:150:ARG:NH2	1:E:165[A]:TRP:CH2	2.81	0.49
1:A:113:SER:HB2	1:B:173:ASN:OD1	2.12	0.48
1:B:273:ILE:HD13	1:B:273:ILE:N	2.28	0.48
1:E:52:ALA:HB1	1:E:304:LEU:HB3	1.96	0.48
1:A:159:ARG:NH1	1:A:214:LEU:O	2.44	0.48
1:E:42:ARG:HD3	5:E:349:HOH:O	2.13	0.48
1:B:48:ASP:HB3	1:B:50:GLY:H	1.80	0.47
1:B:198:GLY:O	1:B:199:GLU:HG3	2.15	0.47
1:A:203:LEU:HD22	1:A:210:TYR:HB2	1.97	0.47
1:B:89:VAL:CG1	1:B:307:ILE:HD13	2.45	0.46
1:F:103:ILE:HG12	1:F:121:VAL:HG22	1.96	0.46
1:D:51:THR:HG21	1:D:95:GLU:HB3	1.96	0.46
1:B:48:ASP:CB	1:B:50:GLY:H	2.29	0.46
1:F:85:GLN:CG	1:F:123:ILE:HD13	2.46	0.46
1:E:214:LEU:HD13	1:E:223:ARG:NH1	2.30	0.45
1:A:165[B]:TRP:HA	1:A:165[B]:TRP:CE3	2.50	0.45
1:A:214:LEU:HD11	1:A:219:ASP:HA	1.98	0.45
1:B:144:LYS:NZ	1:E:175:GLU:OE2	2.36	0.45
1:B:109:LYS:HB2	1:B:114:ALA:HB1	1.98	0.45
4:C:309:GOL:O1	1:E:214:LEU:CD2	2.64	0.45
1:B:146:SER:CB	5:B:580:HOH:O	2.64	0.45
1:D:51:THR:HG21	1:D:95:GLU:CB	2.47	0.45
1:A:109:LYS:HB2	1:A:114:ALA:HB1	1.98	0.45
1:C:290:PHE:HA	1:C:293:VAL:HG22	1.99	0.45
1:E:52:ALA:N	5:E:313:HOH:O	2.50	0.45
1:C:256:THR:HA	1:C:261:GLU:O	2.18	0.44
1:A:165[B]:TRP:HA	1:A:165[B]:TRP:HE3	1.81	0.44
1:B:203:LEU:HG	1:B:250:ALA:HB2	2.00	0.44
1:E:173:ASN:OD1	1:F:113:SER:HB2	2.17	0.44
1:F:52:ALA:HA	1:F:305:THR:O	2.17	0.44
1:D:109:LYS:HB2	1:D:114:ALA:HB1	2.00	0.44
1:D:213:ASP:HA	1:D:239:GLU:HB3	1.98	0.44
1:B:150:ARG:HD3	1:B:186:LEU:HD22	2.00	0.43
1:C:306:LYS:O	1:C:307:ILE:CB	2.67	0.43
1:A:165[B]:TRP:CE3	1:A:165[B]:TRP:CA	3.01	0.43
1:E:53:ILE:HD13	1:E:99:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:LEU:HD22	1:E:210:TYR:HB2	2.00	0.43
1:A:20:ARG:O	1:A:23:LYS:HE3	2.18	0.43
1:A:192:TYR:OH	1:C:215:ALA:HB1	2.18	0.43
1:D:290:PHE:HA	1:D:293:VAL:HG22	2.01	0.43
1:B:247:VAL:HG11	1:B:268:LEU:HD22	2.01	0.42
1:A:214:LEU:HD23	4:E:309:GOL:O3	2.20	0.42
1:B:260:ALA:O	1:B:261:GLU:HB2	2.19	0.42
1:F:60:THR:HG22	1:F:60:THR:O	2.20	0.42
1:E:214:LEU:HD11	1:E:219:ASP:HA	2.01	0.42
1:E:290:PHE:HA	1:E:293:VAL:HG22	2.01	0.42
4:C:309:GOL:H11	1:E:214:LEU:CD2	2.49	0.41
1:D:68:LYS:NZ	5:D:354:HOH:O	2.52	0.41
1:B:215:ALA:HB1	1:D:192:TYR:OH	2.19	0.41
1:B:256:THR:HA	1:B:261:GLU:O	2.21	0.41
1:F:223:ARG:O	1:F:227:ILE:HG13	2.21	0.41
1:A:70:PHE:CE2	1:A:162:ALA:HB2	2.55	0.41
1:A:214:LEU:CD2	4:E:309:GOL:O3	2.68	0.41
1:B:159:ARG:HE	1:D:246:GLU:HG3	1.86	0.40
1:D:261:GLU:OE2	1:D:290:PHE:HE1	2.05	0.40
1:D:139:LYS:O	1:D:266:ARG:HD3	2.22	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	300/328 (92%)	293 (98%)	7 (2%)	0	100 100
1	B	291/328 (89%)	283 (97%)	6 (2%)	2 (1%)	22 12
1	C	296/328 (90%)	283 (96%)	12 (4%)	1 (0%)	41 31
1	D	296/328 (90%)	288 (97%)	7 (2%)	1 (0%)	41 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	291/328 (89%)	279 (96%)	11 (4%)	1 (0%)	41 31
1	F	303/328 (92%)	291 (96%)	11 (4%)	1 (0%)	41 31
All	All	1777/1968 (90%)	1717 (97%)	54 (3%)	6 (0%)	41 31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	214	LEU
1	E	214	LEU
1	B	48	ASP
1	B	261	GLU
1	C	261	GLU
1	F	116	GLY

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	238/264 (90%)	234 (98%)	4 (2%)	60 57
1	B	238/264 (90%)	232 (98%)	6 (2%)	47 41
1	C	237/264 (90%)	232 (98%)	5 (2%)	53 48
1	D	235/264 (89%)	232 (99%)	3 (1%)	69 68
1	E	236/264 (89%)	231 (98%)	5 (2%)	53 48
1	F	235/264 (89%)	227 (97%)	8 (3%)	37 28
All	All	1419/1584 (90%)	1388 (98%)	31 (2%)	52 47

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	137	LEU
1	A	203	LEU
1	A	302	ASP

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Mol	Chain	Res	Type
1	B	99	LEU
1	B	165	TRP
1	B	203	LEU
1	B	285	LEU
1	B	287	SER
1	B	306	LYS
1	C	51	THR
1	C	107	SER
1	C	165	TRP
1	C	203	LEU
1	C	205	ASN
1	D	137	LEU
1	D	203	LEU
1	D	221	ILE
1	E	96	SER
1	E	137	LEU
1	E	203	LEU
1	E	285	LEU
1	E	302	ASP
1	F	58	GLU
1	F	99	LEU
1	F	108	GLU
1	F	137	LEU
1	F	203	LEU
1	F	285	LEU
1	F	297	SER
1	F	302	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	205	ASN

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 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	PO4	F	308	-	4,4,4	0.81	0	6,6,6	1.22	1 (16%)
2	PO4	B	308	-	4,4,4	0.56	0	6,6,6	0.98	0
4	GOL	E	309	-	5,5,5	0.40	0	5,5,5	0.57	0
4	GOL	C	309	-	5,5,5	0.38	0	5,5,5	1.10	0
4	GOL	F	309	-	5,5,5	1.07	0	5,5,5	1.14	0
2	PO4	A	308	-	4,4,4	1.08	0	6,6,6	1.43	1 (16%)
2	PO4	C	308	-	4,4,4	1.17	0	6,6,6	1.08	0
2	PO4	E	308	-	4,4,4	1.12	0	6,6,6	0.83	0
2	PO4	D	308	-	4,4,4	0.74	0	6,6,6	1.07	1 (16%)

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
4	GOL	F	309	-	-	4/4/4/4	-
4	GOL	E	309	-	-	4/4/4/4	-
4	GOL	C	309	-	-	4/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	308	PO4	O3-P-O2	2.39	115.63	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	308	PO4	O3-P-O1	-2.21	102.83	110.89
2	A	308	PO4	O4-P-O3	2.13	114.81	107.97

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	309	GOL	O1-C1-C2-C3
4	C	309	GOL	C1-C2-C3-O3
4	C	309	GOL	O2-C2-C3-O3
4	E	309	GOL	O1-C1-C2-C3
4	E	309	GOL	C1-C2-C3-O3
4	F	309	GOL	O1-C1-C2-C3
4	F	309	GOL	C1-C2-C3-O3
4	E	309	GOL	O1-C1-C2-O2
4	F	309	GOL	O2-C2-C3-O3
4	C	309	GOL	O1-C1-C2-O2
4	E	309	GOL	O2-C2-C3-O3
4	F	309	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	309	GOL	4	0
4	C	309	GOL	4	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	303/328 (92%)	-0.07	12 (3%) 38 41	16, 32, 54, 81	0
1	B	295/328 (89%)	-0.10	5 (1%) 70 72	16, 32, 54, 70	0
1	C	299/328 (91%)	-0.02	10 (3%) 46 49	17, 33, 60, 70	0
1	D	299/328 (91%)	0.17	16 (5%) 25 29	17, 38, 61, 68	0
1	E	296/328 (90%)	0.33	29 (9%) 7 8	17, 41, 79, 113	0
1	F	305/328 (92%)	0.33	21 (6%) 16 19	18, 47, 75, 90	0
All	All	1797/1968 (91%)	0.11	93 (5%) 27 30	16, 36, 67, 113	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	7	ASP	6.0
1	D	165[A]	TRP	5.9
1	D	218	LEU	5.9
1	E	133	GLY	5.9
1	C	137	LEU	5.7
1	E	114	ALA	5.6
1	E	165[A]	TRP	5.4
1	E	128	TRP	5.2
1	D	114	ALA	5.2
1	A	133	GLY	5.1
1	A	165[A]	TRP	4.9
1	D	138	ALA	4.9
1	F	5	ASP	4.6
1	E	134	GLU	4.6
1	F	130	ALA	4.5
1	F	131	TYR	4.5
1	D	137	LEU	4.2
1	A	1	MET	4.1
1	F	129	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	298	ALA	4.0
1	A	47	ALA	4.0
1	F	47	ALA	4.0
1	E	295	GLY	3.9
1	C	47	ALA	3.8
1	E	113	SER	3.8
1	E	7	ASP	3.7
1	E	124	ALA	3.5
1	F	114	ALA	3.5
1	E	99	LEU	3.3
1	F	49	GLY	3.3
1	B	47	ALA	3.3
1	A	128	TRP	3.2
1	E	299	LYS	3.2
1	B	298	ALA	3.1
1	E	297	SER	3.1
1	C	113	SER	3.0
1	E	125	ALA	3.0
1	C	138	ALA	2.9
1	B	299	LYS	2.9
1	E	123	ILE	2.9
1	F	6	ARG	2.9
1	C	114	ALA	2.9
1	C	49	GLY	2.8
1	E	46	THR	2.8
1	A	214	LEU	2.8
1	F	109	LYS	2.8
1	E	218	LEU	2.7
1	F	206	ARG	2.7
1	F	90	ARG	2.7
1	E	294	ASN	2.7
1	D	116	GLY	2.6
1	E	135	GLU	2.6
1	E	301	ALA	2.6
1	B	128	TRP	2.6
1	C	290	PHE	2.5
1	A	218	LEU	2.5
1	A	49	GLY	2.5
1	D	2	SER	2.5
1	D	290	PHE	2.5
1	F	115	LYS	2.4
1	E	90	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	216	SER	2.4
1	E	214	LEU	2.4
1	E	44	TYR	2.4
1	F	14	GLY	2.4
1	F	123	ILE	2.4
1	F	17	ILE	2.4
1	F	275	GLY	2.4
1	D	113	SER	2.4
1	C	128	TRP	2.3
1	D	115	LYS	2.3
1	E	5	ASP	2.3
1	E	254	PHE	2.2
1	E	304	LEU	2.2
1	E	139	LYS	2.2
1	D	307	ILE	2.2
1	A	134	GLU	2.2
1	F	48	ASP	2.2
1	D	128	TRP	2.2
1	D	302	ASP	2.2
1	F	51	THR	2.2
1	F	128	TRP	2.1
1	F	8	GLY	2.1
1	C	206	ARG	2.1
1	E	93	LYS	2.1
1	E	137	LEU	2.1
1	D	219	ASP	2.1
1	A	135	GLU	2.1
1	C	116	GLY	2.1
1	D	254	PHE	2.0
1	A	216	SER	2.0
1	A	293	VAL	2.0
1	B	49	GLY	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 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
4	GOL	F	309	6/6	0.67	0.18	45,48,49,50	0
3	CL	D	309	1/1	0.83	0.14	58,58,58,58	0
4	GOL	C	309	6/6	0.85	0.14	44,48,49,51	0
4	GOL	E	309	6/6	0.88	0.14	43,50,51,55	0
3	CL	A	309	1/1	0.90	0.09	46,46,46,46	0
3	CL	E	310	1/1	0.92	0.07	61,61,61,61	0
2	PO4	D	308	5/5	0.93	0.20	45,54,59,60	0
2	PO4	A	308	5/5	0.94	0.17	47,47,50,54	0
3	CL	C	310	1/1	0.96	0.06	48,48,48,48	0
3	CL	B	309	1/1	0.96	0.07	43,43,43,43	0
2	PO4	F	308	5/5	0.97	0.09	38,39,42,51	0
2	PO4	E	308	5/5	0.97	0.14	43,45,50,50	0
3	CL	F	310	1/1	0.97	0.12	44,44,44,44	0
2	PO4	B	308	5/5	0.98	0.10	35,38,42,44	0
2	PO4	C	308	5/5	0.98	0.10	37,37,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.