



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:06 AM UTC

PDB ID : 8QNN / pdb_00008qnn
Title : Structure of the toxin-antitoxin NatRT complex from *Pseudomonas aeruginosa*. NatTE29D mutant
Authors : Dias Teixeira, R.; Hiller, S.; Jenal, U.
Deposited on : 2023-09-27
Resolution : 2.39 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

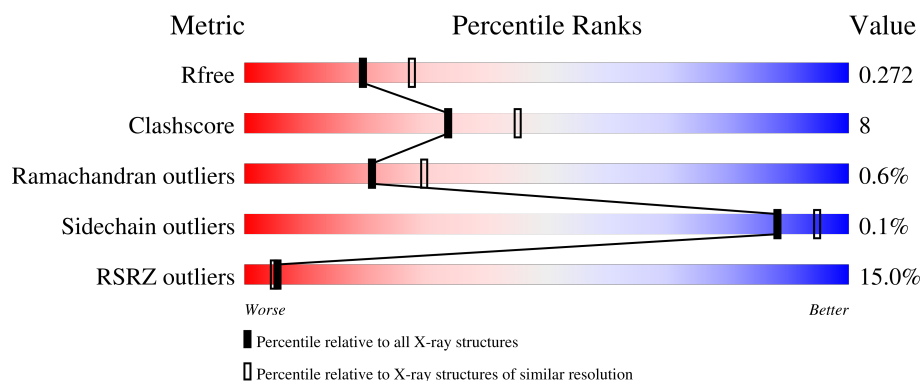
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	129	6% 86% 13%
1	B	129	29% 78% 12% 10%
1	D	129	8% 82% 17%
1	E	129	24% 61% 26% 12%
2	C	264	4% 81% 13% 5%

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Mol	Chain	Length	Quality of chain
2	F	264	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7812 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 Antitoxin Xre/MbcA/ParS-like toxin-binding domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	93	0	0
			989	629	182	176	2			
1	B	116	Total	C	N	O	S	20	0	0
			896	568	167	159	2			
1	D	128	Total	C	N	O	S	0	0	0
			989	629	182	176	2			
1	E	113	Total	C	N	O	S	27	0	0
			876	555	163	156	2			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9I4U5
A	-5	ALA	-	expression tag	UNP Q9I4U5
A	-4	ASP	-	expression tag	UNP Q9I4U5
A	-3	LEU	-	expression tag	UNP Q9I4U5
A	-2	ASN	-	expression tag	UNP Q9I4U5
A	-1	TRP	-	expression tag	UNP Q9I4U5
A	0	ILE	-	expression tag	UNP Q9I4U5
A	1	SER	-	expression tag	UNP Q9I4U5
A	2	SER	-	expression tag	UNP Q9I4U5
A	3	ALA	-	expression tag	UNP Q9I4U5
A	4	LEU	-	expression tag	UNP Q9I4U5
A	5	ILE	-	expression tag	UNP Q9I4U5
A	6	LYS	-	expression tag	UNP Q9I4U5
A	7	GLU	-	expression tag	UNP Q9I4U5
A	8	ARG	-	expression tag	UNP Q9I4U5
A	9	PRO	-	expression tag	UNP Q9I4U5
A	10	SER	-	expression tag	UNP Q9I4U5
A	11	ALA	-	expression tag	UNP Q9I4U5
A	12	ASP	-	expression tag	UNP Q9I4U5
A	13	ALA	-	expression tag	UNP Q9I4U5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	VAL	-	expression tag	UNP Q9I4U5
A	15	LEU	-	expression tag	UNP Q9I4U5
A	16	ALA	-	expression tag	UNP Q9I4U5
A	17	LYS	-	expression tag	UNP Q9I4U5
A	18	ALA	-	expression tag	UNP Q9I4U5
A	19	VAL	-	expression tag	UNP Q9I4U5
A	20	LEU	-	expression tag	UNP Q9I4U5
A	21	ALA	-	expression tag	UNP Q9I4U5
A	22	ALA	-	expression tag	UNP Q9I4U5
A	23	ARG	-	expression tag	UNP Q9I4U5
A	24	GLU	-	expression tag	UNP Q9I4U5
A	25	GLN	-	expression tag	UNP Q9I4U5
A	26	LEU	-	expression tag	UNP Q9I4U5
A	27	GLY	-	expression tag	UNP Q9I4U5
A	28	LEU	-	expression tag	UNP Q9I4U5
B	-6	MET	-	initiating methionine	UNP Q9I4U5
B	-5	ALA	-	expression tag	UNP Q9I4U5
B	-4	ASP	-	expression tag	UNP Q9I4U5
B	-3	LEU	-	expression tag	UNP Q9I4U5
B	-2	ASN	-	expression tag	UNP Q9I4U5
B	-1	TRP	-	expression tag	UNP Q9I4U5
B	0	ILE	-	expression tag	UNP Q9I4U5
B	1	SER	-	expression tag	UNP Q9I4U5
B	2	SER	-	expression tag	UNP Q9I4U5
B	3	ALA	-	expression tag	UNP Q9I4U5
B	4	LEU	-	expression tag	UNP Q9I4U5
B	5	ILE	-	expression tag	UNP Q9I4U5
B	6	LYS	-	expression tag	UNP Q9I4U5
B	7	GLU	-	expression tag	UNP Q9I4U5
B	8	ARG	-	expression tag	UNP Q9I4U5
B	9	PRO	-	expression tag	UNP Q9I4U5
B	10	SER	-	expression tag	UNP Q9I4U5
B	11	ALA	-	expression tag	UNP Q9I4U5
B	12	ASP	-	expression tag	UNP Q9I4U5
B	13	ALA	-	expression tag	UNP Q9I4U5
B	14	VAL	-	expression tag	UNP Q9I4U5
B	15	LEU	-	expression tag	UNP Q9I4U5
B	16	ALA	-	expression tag	UNP Q9I4U5
B	17	LYS	-	expression tag	UNP Q9I4U5
B	18	ALA	-	expression tag	UNP Q9I4U5
B	19	VAL	-	expression tag	UNP Q9I4U5
B	20	LEU	-	expression tag	UNP Q9I4U5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ALA	-	expression tag	UNP Q9I4U5
B	22	ALA	-	expression tag	UNP Q9I4U5
B	23	ARG	-	expression tag	UNP Q9I4U5
B	24	GLU	-	expression tag	UNP Q9I4U5
B	25	GLN	-	expression tag	UNP Q9I4U5
B	26	LEU	-	expression tag	UNP Q9I4U5
B	27	GLY	-	expression tag	UNP Q9I4U5
B	28	LEU	-	expression tag	UNP Q9I4U5
D	-6	MET	-	initiating methionine	UNP Q9I4U5
D	-5	ALA	-	expression tag	UNP Q9I4U5
D	-4	ASP	-	expression tag	UNP Q9I4U5
D	-3	LEU	-	expression tag	UNP Q9I4U5
D	-2	ASN	-	expression tag	UNP Q9I4U5
D	-1	TRP	-	expression tag	UNP Q9I4U5
D	0	ILE	-	expression tag	UNP Q9I4U5
D	1	SER	-	expression tag	UNP Q9I4U5
D	2	SER	-	expression tag	UNP Q9I4U5
D	3	ALA	-	expression tag	UNP Q9I4U5
D	4	LEU	-	expression tag	UNP Q9I4U5
D	5	ILE	-	expression tag	UNP Q9I4U5
D	6	LYS	-	expression tag	UNP Q9I4U5
D	7	GLU	-	expression tag	UNP Q9I4U5
D	8	ARG	-	expression tag	UNP Q9I4U5
D	9	PRO	-	expression tag	UNP Q9I4U5
D	10	SER	-	expression tag	UNP Q9I4U5
D	11	ALA	-	expression tag	UNP Q9I4U5
D	12	ASP	-	expression tag	UNP Q9I4U5
D	13	ALA	-	expression tag	UNP Q9I4U5
D	14	VAL	-	expression tag	UNP Q9I4U5
D	15	LEU	-	expression tag	UNP Q9I4U5
D	16	ALA	-	expression tag	UNP Q9I4U5
D	17	LYS	-	expression tag	UNP Q9I4U5
D	18	ALA	-	expression tag	UNP Q9I4U5
D	19	VAL	-	expression tag	UNP Q9I4U5
D	20	LEU	-	expression tag	UNP Q9I4U5
D	21	ALA	-	expression tag	UNP Q9I4U5
D	22	ALA	-	expression tag	UNP Q9I4U5
D	23	ARG	-	expression tag	UNP Q9I4U5
D	24	GLU	-	expression tag	UNP Q9I4U5
D	25	GLN	-	expression tag	UNP Q9I4U5
D	26	LEU	-	expression tag	UNP Q9I4U5
D	27	GLY	-	expression tag	UNP Q9I4U5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	28	LEU	-	expression tag	UNP Q9I4U5
E	-6	MET	-	initiating methionine	UNP Q9I4U5
E	-5	ALA	-	expression tag	UNP Q9I4U5
E	-4	ASP	-	expression tag	UNP Q9I4U5
E	-3	LEU	-	expression tag	UNP Q9I4U5
E	-2	ASN	-	expression tag	UNP Q9I4U5
E	-1	TRP	-	expression tag	UNP Q9I4U5
E	0	ILE	-	expression tag	UNP Q9I4U5
E	1	SER	-	expression tag	UNP Q9I4U5
E	2	SER	-	expression tag	UNP Q9I4U5
E	3	ALA	-	expression tag	UNP Q9I4U5
E	4	LEU	-	expression tag	UNP Q9I4U5
E	5	ILE	-	expression tag	UNP Q9I4U5
E	6	LYS	-	expression tag	UNP Q9I4U5
E	7	GLU	-	expression tag	UNP Q9I4U5
E	8	ARG	-	expression tag	UNP Q9I4U5
E	9	PRO	-	expression tag	UNP Q9I4U5
E	10	SER	-	expression tag	UNP Q9I4U5
E	11	ALA	-	expression tag	UNP Q9I4U5
E	12	ASP	-	expression tag	UNP Q9I4U5
E	13	ALA	-	expression tag	UNP Q9I4U5
E	14	VAL	-	expression tag	UNP Q9I4U5
E	15	LEU	-	expression tag	UNP Q9I4U5
E	16	ALA	-	expression tag	UNP Q9I4U5
E	17	LYS	-	expression tag	UNP Q9I4U5
E	18	ALA	-	expression tag	UNP Q9I4U5
E	19	VAL	-	expression tag	UNP Q9I4U5
E	20	LEU	-	expression tag	UNP Q9I4U5
E	21	ALA	-	expression tag	UNP Q9I4U5
E	22	ALA	-	expression tag	UNP Q9I4U5
E	23	ARG	-	expression tag	UNP Q9I4U5
E	24	GLU	-	expression tag	UNP Q9I4U5
E	25	GLN	-	expression tag	UNP Q9I4U5
E	26	LEU	-	expression tag	UNP Q9I4U5
E	27	GLY	-	expression tag	UNP Q9I4U5
E	28	LEU	-	expression tag	UNP Q9I4U5

- Molecule 2 is a protein called RES domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	250	Total	C	N	O	S	0	0	0
			1990	1274	353	355	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	250	Total	C	N	O	S	6	0	0
			1990	1274	353	355	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	MET	-	initiating methionine	UNP Q9I4U4
C	-11	GLY	-	expression tag	UNP Q9I4U4
C	-10	SER	-	expression tag	UNP Q9I4U4
C	-9	SER	-	expression tag	UNP Q9I4U4
C	-8	HIS	-	expression tag	UNP Q9I4U4
C	-7	HIS	-	expression tag	UNP Q9I4U4
C	-6	HIS	-	expression tag	UNP Q9I4U4
C	-5	HIS	-	expression tag	UNP Q9I4U4
C	-4	HIS	-	expression tag	UNP Q9I4U4
C	-3	HIS	-	expression tag	UNP Q9I4U4
C	-2	SER	-	expression tag	UNP Q9I4U4
C	-1	GLN	-	expression tag	UNP Q9I4U4
C	0	ASP	-	expression tag	UNP Q9I4U4
C	1	PRO	-	expression tag	UNP Q9I4U4
C	29	ASP	GLU	engineered mutation	UNP Q9I4U4
F	-12	MET	-	initiating methionine	UNP Q9I4U4
F	-11	GLY	-	expression tag	UNP Q9I4U4
F	-10	SER	-	expression tag	UNP Q9I4U4
F	-9	SER	-	expression tag	UNP Q9I4U4
F	-8	HIS	-	expression tag	UNP Q9I4U4
F	-7	HIS	-	expression tag	UNP Q9I4U4
F	-6	HIS	-	expression tag	UNP Q9I4U4
F	-5	HIS	-	expression tag	UNP Q9I4U4
F	-4	HIS	-	expression tag	UNP Q9I4U4
F	-3	HIS	-	expression tag	UNP Q9I4U4
F	-2	SER	-	expression tag	UNP Q9I4U4
F	-1	GLN	-	expression tag	UNP Q9I4U4
F	0	ASP	-	expression tag	UNP Q9I4U4
F	1	PRO	-	expression tag	UNP Q9I4U4
F	29	ASP	GLU	engineered mutation	UNP Q9I4U4

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

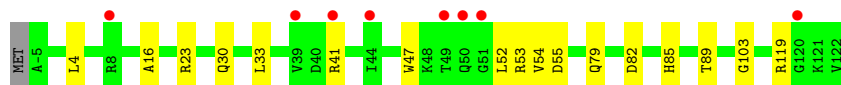
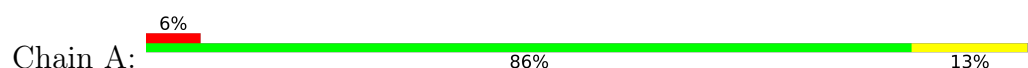
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	5	Total	O	0	0
			5	5		
4	C	27	Total	O	0	0
			27	27		
4	D	11	Total	O	0	0
			11	11		
4	E	1	Total	O	0	0
			1	1		
4	F	13	Total	O	0	0
			13	13		

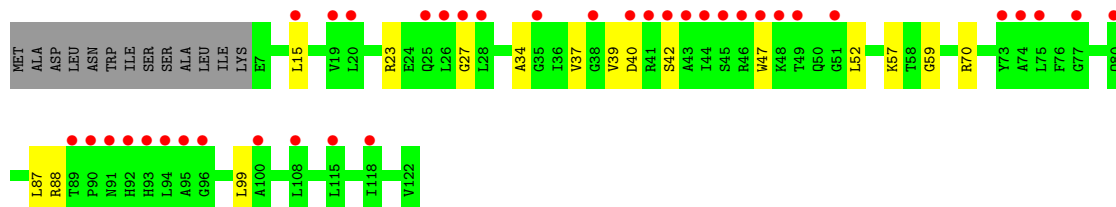
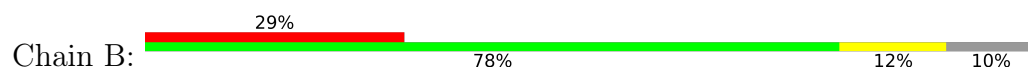
3 Residue-property plots

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.

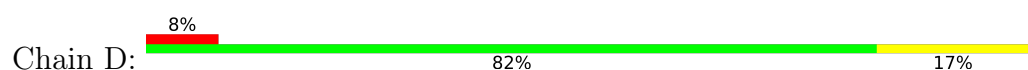
- Molecule 1: Antitoxin Xre/MbcA/ParS-like toxin-binding domain-containing protein



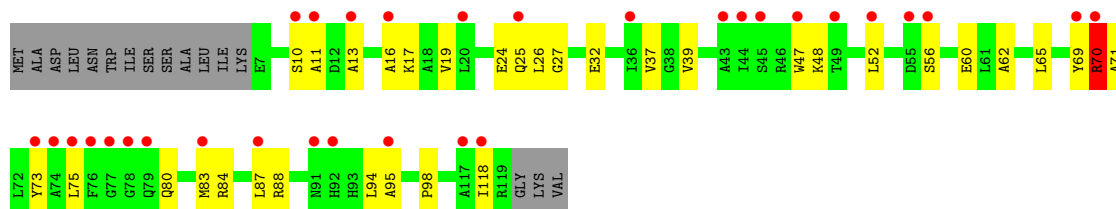
- Molecule 1: Antitoxin Xre/MbcA/ParS-like toxin-binding domain-containing protein



- Molecule 1: Antitoxin Xre/MbcA/ParS-like toxin-binding domain-containing protein

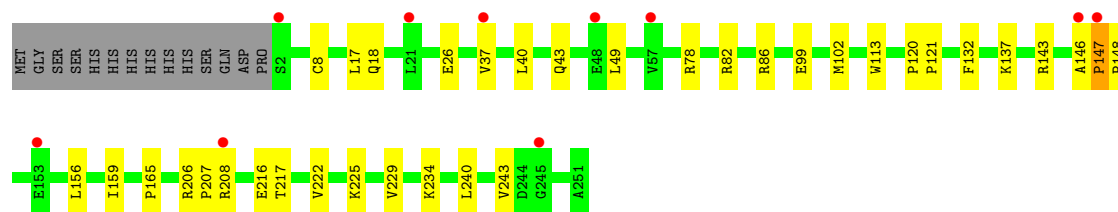


- Molecule 1: Antitoxin Xre/MbcA/ParS-like toxin-binding domain-containing protein



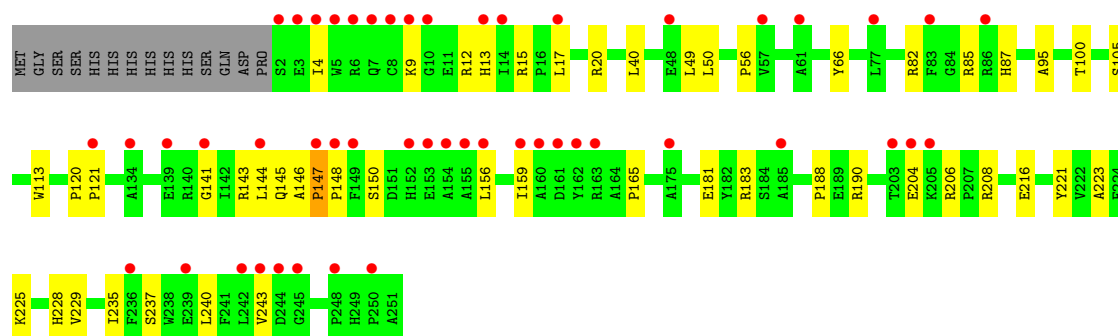
- Molecule 2: RES domain-containing protein

Chain C: 



• Molecule 2: RES domain-containing protein

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.42Å 107.71Å 93.53Å 90.00° 104.06° 90.00°	Depositor
Resolution (Å)	53.85 – 2.39 53.85 – 2.39	Depositor EDS
% Data completeness (in resolution range)	92.2 (53.85-2.39) 92.2 (53.85-2.39)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.234 , 0.270 0.236 , 0.272	Depositor DCC
R_{free} test set	1972 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7812	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.24	0/1004	0.56	3/1358 (0.2%)
1	B	0.15	0/909	0.41	0/1228
1	D	0.08	0/1004	0.26	0/1358
1	E	0.25	0/889	0.40	0/1202
2	C	0.19	0/2051	0.34	0/2791
2	F	0.18	0/2051	0.40	0/2791
All	All	0.19	0/7908	0.40	3/10728 (0.0%)

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	B	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LEU	CA-CB-CG	7.48	142.48	116.30
1	A	4	LEU	CA-C-N	-6.37	110.51	121.97
1	A	4	LEU	C-N-CA	-6.37	110.51	121.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	ARG	Sidechain
1	E	70	ARG	Sidechain

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	989	0	1030	11	0
1	B	896	0	930	10	0
1	D	989	0	1030	15	0
1	E	876	0	905	25	0
2	C	1990	0	1965	30	0
2	F	1990	0	1965	43	0
3	C	10	0	0	1	0
3	F	10	0	0	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	27	0	0	0	0
4	D	11	0	0	0	0
4	E	1	0	0	0	0
4	F	13	0	0	0	0
All	All	7812	0	7825	117	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 8.

All (117) 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)
2:F:9:LYS:HE2	2:F:12:ARG:HD2	1.37	1.02
2:F:9:LYS:HE2	2:F:12:ARG:CD	2.02	0.89
2:C:206:ARG:HH22	2:C:208:ARG:HH11	1.29	0.81
2:F:9:LYS:CE	2:F:12:ARG:HD2	2.13	0.79
2:F:145:GLN:HE22	2:F:181:GLU:HB2	1.49	0.78
2:C:147:PRO:HB2	2:C:148:PRO:CD	2.17	0.75
2:F:159:ILE:HD13	2:F:243:VAL:HG11	1.66	0.75
2:F:145:GLN:NE2	2:F:181:GLU:HB2	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:PRO:HB2	2:F:148:PRO:CD	2.17	0.75
1:B:52:LEU:HD21	1:B:59:GLY:HA2	1.70	0.72
1:E:16:ALA:HB1	1:E:47:TRP:HB3	1.71	0.72
2:F:144:LEU:HD23	2:F:156:LEU:HD13	1.71	0.72
1:A:53:ARG:HH21	1:A:55:ASP:HB3	1.54	0.72
1:E:25:GLN:OE1	1:E:80:GLN:NE2	2.26	0.68
2:F:9:LYS:HB2	2:F:13:HIS:CD2	2.30	0.67
2:C:208:ARG:HH21	2:F:206:ARG:HH21	1.44	0.66
1:E:13:ALA:O	1:E:17:LYS:HB2	1.95	0.65
2:F:156:LEU:HA	2:F:165:PRO:HG3	1.80	0.64
2:F:183:ARG:HD3	2:F:190:ARG:HG2	1.79	0.63
1:D:19:VAL:HG11	1:D:62:ALA:HB1	1.81	0.62
1:E:80:GLN:OE1	1:E:84:ARG:NH2	2.33	0.62
1:E:95:ALA:HB3	2:F:56:PRO:HG2	1.82	0.61
2:F:15:ARG:O	2:F:141:GLY:N	2.32	0.60
2:C:225:LYS:HD2	2:F:40:LEU:HG	1.84	0.60
2:C:40:LEU:HG	2:F:225:LYS:HD2	1.83	0.59
2:C:156:LEU:HA	2:C:165:PRO:HG3	1.83	0.59
2:F:147:PRO:HB2	2:F:148:PRO:HD3	1.85	0.58
2:C:99:GLU:H	2:C:99:GLU:CD	2.12	0.58
1:E:70:ARG:O	1:E:73:TYR:N	2.37	0.57
2:C:147:PRO:HB2	2:C:148:PRO:HD3	1.86	0.56
2:C:206:ARG:HH22	2:C:208:ARG:NH1	2.02	0.56
1:D:54:VAL:HG11	2:F:49:LEU:HD22	1.87	0.56
1:A:79:GLN:NE2	1:A:82:ASP:OD2	2.39	0.56
2:F:82:ARG:NH1	2:F:156:LEU:O	2.39	0.56
1:A:16:ALA:HB2	1:A:52:LEU:H	1.71	0.55
2:C:216:GLU:HB2	2:F:40:LEU:HD13	1.88	0.55
2:F:223:ALA:HB2	2:F:235:ILE:HD13	1.89	0.55
1:B:37:VAL:HG23	1:B:39:VAL:HG12	1.89	0.54
1:D:119:ARG:NH2	3:F:301:PO4:O2	2.35	0.54
1:E:24:GLU:C	1:E:26:LEU:H	2.16	0.54
1:D:2:SER:HA	1:D:5:ILE:HG22	1.90	0.54
2:C:82:ARG:NH1	2:C:156:LEU:O	2.41	0.54
2:C:40:LEU:HD13	2:F:216:GLU:HB2	1.88	0.54
2:C:17:LEU:HD11	2:C:143:ARG:HG3	1.90	0.53
2:C:159:ILE:HD12	2:C:243:VAL:HG21	1.90	0.53
1:A:54:VAL:HG11	2:C:49:LEU:HD22	1.89	0.53
2:F:221:TYR:HA	2:F:237:SER:HA	1.89	0.53
2:F:9:LYS:HE2	2:F:12:ARG:NE	2.23	0.53
1:E:26:LEU:HA	1:E:84:ARG:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLY:O	1:B:88:ARG:NH2	2.40	0.53
1:E:16:ALA:HB2	1:E:52:LEU:HB3	1.91	0.52
1:D:31:LEU:HG	1:D:41:ARG:HD2	1.93	0.51
1:E:17:LYS:HD3	1:E:17:LYS:C	2.36	0.51
2:C:8:CYS:HB3	2:C:148:PRO:HG2	1.93	0.50
1:E:19:VAL:HG21	1:E:62:ALA:HB1	1.92	0.50
2:F:206:ARG:HB2	2:F:206:ARG:NH1	2.27	0.50
1:B:39:VAL:HG22	1:B:40:ASP:O	2.11	0.50
2:C:37:VAL:HG11	2:C:43:GLN:HB2	1.93	0.49
1:E:26:LEU:HD13	1:E:87:LEU:HD11	1.94	0.49
2:C:113:TRP:CE2	2:C:120:PRO:HD2	2.48	0.49
1:A:119:ARG:NH2	3:C:301:PO4:O2	2.42	0.49
1:B:47:TRP:CZ2	1:B:52:LEU:HD12	2.47	0.49
2:C:18:GLN:HG3	2:C:137:LYS:HB2	1.94	0.49
1:E:16:ALA:HB2	1:E:52:LEU:CB	2.43	0.49
1:E:71:ALA:O	1:E:75:LEU:HB2	2.13	0.48
2:F:188:PRO:HB3	2:F:240:LEU:HD22	1.95	0.48
2:C:208:ARG:NH2	2:F:206:ARG:HH21	2.09	0.48
2:F:113:TRP:CE2	2:F:120:PRO:HD2	2.49	0.47
1:D:122:VAL:HG23	2:F:105:SER:HB3	1.96	0.47
2:F:95:ALA:HB1	2:F:100:THR:HB	1.97	0.47
2:C:132:PHE:CD1	2:C:207:PRO:HB3	2.50	0.47
1:D:20:LEU:HD13	1:D:48:LYS:HE3	1.96	0.47
1:D:32:GLU:OE2	1:D:88:ARG:NH1	2.48	0.47
1:E:37:VAL:HG23	1:E:39:VAL:HG22	1.96	0.47
2:C:206:ARG:HH11	2:C:206:ARG:HG2	1.79	0.47
2:F:4:ILE:H	2:F:4:ILE:HD12	1.79	0.47
1:B:34:ALA:HB1	1:B:39:VAL:O	2.15	0.47
1:A:85:HIS:O	1:A:89:THR:OG1	2.32	0.46
1:D:79:GLN:NE2	1:D:82:ASP:OD2	2.48	0.46
1:A:30:GLN:OE1	1:A:41:ARG:NH2	2.48	0.46
2:C:102:MET:HE1	2:C:234:LYS:HD2	1.98	0.46
2:F:17:LEU:HD11	2:F:143:ARG:HG2	1.97	0.46
1:E:27:GLY:O	1:E:88:ARG:NH2	2.48	0.46
1:E:24:GLU:OE1	1:E:25:GLN:NE2	2.44	0.45
1:E:56:SER:O	1:E:60:GLU:HG3	2.17	0.45
1:E:69:TYR:CE1	1:E:83:MET:HE1	2.51	0.45
1:D:16:ALA:HB1	1:D:47:TRP:HB3	1.98	0.44
1:B:87:LEU:HD21	1:B:99:LEU:HD13	1.98	0.44
2:C:208:ARG:HH22	2:F:208:ARG:HD2	1.83	0.44
2:F:228:HIS:CD2	2:F:229:VAL:HG13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:THR:HG23	2:C:222:VAL:HG22	1.99	0.43
1:E:19:VAL:HG13	1:E:65:LEU:HD23	2.00	0.43
2:F:145:GLN:O	2:F:150:SER:HB3	2.18	0.43
1:B:37:VAL:HG23	1:B:39:VAL:CG1	2.48	0.43
2:F:85:ARG:HD2	2:F:87:HIS:HE1	1.83	0.43
1:A:103:GLY:O	1:B:57:LYS:NZ	2.52	0.42
1:E:48:LYS:HB3	1:E:48:LYS:HE3	1.88	0.42
2:F:183:ARG:HH11	2:F:190:ARG:HG2	1.83	0.42
2:C:78:ARG:HA	2:C:86:ARG:HD3	2.02	0.42
2:C:120:PRO:HA	2:C:121:PRO:HD3	1.89	0.42
2:F:120:PRO:HA	2:F:121:PRO:HD3	1.90	0.42
1:A:23:ARG:HD3	1:A:33:LEU:HD22	2.01	0.42
1:E:10:SER:OG	1:E:11:ALA:N	2.53	0.42
1:A:119:ARG:HG2	2:C:26:GLU:HG3	2.02	0.42
1:D:15:LEU:O	1:D:19:VAL:HG13	2.20	0.41
1:E:94:LEU:HD12	1:E:98:PRO:HG3	2.02	0.41
2:C:229:VAL:HG12	2:F:66:TYR:HB3	2.01	0.41
1:A:16:ALA:HB1	1:A:47:TRP:HB3	2.01	0.41
1:E:32:GLU:OE2	1:E:88:ARG:NH1	2.54	0.41
1:D:12:ASP:OD1	1:D:54:VAL:HG23	2.21	0.41
1:D:67:ARG:HG3	2:F:50:LEU:HD22	2.02	0.41
1:B:15:LEU:HG	1:B:52:LEU:HD22	2.02	0.41
1:D:85:HIS:CG	2:F:121:PRO:HD3	2.56	0.41
1:E:75:LEU:HD11	1:E:118:ILE:CG2	2.51	0.41
2:C:240:LEU:HD21	1:D:-2:ASN:HA	2.03	0.41
2:F:20:ARG:NH2	2:F:204:GLU:OE1	2.53	0.41
2:F:206:ARG:HB2	2:F:206:ARG:HH11	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
1	B	114/129 (88%)	109 (96%)	3 (3%)	2 (2%)	6	8
1	D	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
1	E	111/129 (86%)	106 (96%)	5 (4%)	0	100	100
2	C	248/264 (94%)	240 (97%)	6 (2%)	2 (1%)	16	23
2	F	248/264 (94%)	240 (97%)	6 (2%)	2 (1%)	16	23
All	All	973/1044 (93%)	939 (96%)	28 (3%)	6 (1%)	21	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	SER
2	C	147	PRO
2	F	147	PRO
1	B	23	ARG
2	F	146	ALA
2	C	146	ALA

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	101/102 (99%)	101 (100%)	0	100	100
1	B	91/102 (89%)	91 (100%)	0	100	100
1	D	101/102 (99%)	101 (100%)	0	100	100
1	E	89/102 (87%)	88 (99%)	1 (1%)	65	81
2	C	209/222 (94%)	209 (100%)	0	100	100
2	F	209/222 (94%)	209 (100%)	0	100	100
All	All	800/852 (94%)	799 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
2	C	7	GLN
2	C	228	HIS
2	C	249	HIS
1	D	93	HIS
2	F	145	GLN
2	F	249	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	PO4	F	302	-	4,4,4	0.97	0	6,6,6	0.45	0
3	PO4	C	301	-	4,4,4	0.95	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	C	302	-	4,4,4	0.97	0	6,6,6	0.47	0
3	PO4	F	301	-	4,4,4	0.97	0	6,6,6	0.46	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	PO4	1	0
3	F	301	PO4	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	116/129 (89%)	0.79	8 (6%) 23 21	28, 40, 72, 83	0
1	B	113/129 (87%)	1.59	37 (32%) 1 1	44, 68, 92, 97	0
1	D	128/129 (99%)	0.70	10 (7%) 19 17	29, 44, 66, 71	0
1	E	110/129 (85%)	1.60	31 (28%) 1 1	43, 65, 86, 92	0
2	C	250/264 (94%)	0.60	10 (4%) 42 42	26, 40, 56, 68	0
2	F	249/264 (94%)	1.26	49 (19%) 3 2	33, 52, 81, 92	0
All	All	966/1044 (92%)	1.03	145 (15%) 5 5	26, 48, 80, 97	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	16	ALA	8.3
2	F	250	PRO	6.0
2	C	147	PRO	5.1
1	A	51	GLY	4.9
1	E	69	TYR	4.8
2	F	10	GLY	4.6
1	B	43	ALA	4.4
1	B	92	HIS	4.4
1	A	49	THR	4.3
1	A	120	GLY	4.3
1	D	120	GLY	4.3
2	F	2	SER	3.9
2	F	162	TYR	3.9
1	E	77	GLY	3.8
2	F	155	ALA	3.7
2	F	149	PHE	3.6
2	F	148	PRO	3.6
1	E	11	ALA	3.6
1	E	44	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	26	LEU	3.5
2	F	8	CYS	3.4
2	F	161	ASP	3.4
2	F	244	ASP	3.4
2	C	37	VAL	3.4
2	F	17	LEU	3.4
2	F	159	ILE	3.4
2	F	147	PRO	3.4
1	D	122	VAL	3.3
2	F	154	ALA	3.2
1	B	89	THR	3.2
2	F	160	ALA	3.1
1	E	20	LEU	3.1
1	E	73	TYR	3.1
2	F	242	LEU	3.1
2	F	243	VAL	3.1
1	A	50	GLN	3.1
2	C	146	ALA	3.0
1	B	90	PRO	3.0
2	F	4	ILE	3.0
2	F	153	GLU	3.0
2	F	245	GLY	3.0
1	B	47	TRP	3.0
2	F	239	GLU	3.0
1	B	100	ALA	2.9
2	F	185	ALA	2.9
1	B	28	LEU	2.9
2	F	77	LEU	2.8
2	F	14	ILE	2.8
1	B	96	GLY	2.8
1	E	70	ARG	2.8
1	E	76	PHE	2.8
2	F	9	LYS	2.8
1	B	44	ILE	2.8
1	E	75	LEU	2.8
1	E	49	THR	2.8
1	B	91	ASN	2.8
1	E	91	ASN	2.8
2	C	153	GLU	2.8
1	E	52	LEU	2.8
1	B	20	LEU	2.7
1	B	118	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	42	SER	2.7
1	B	94	LEU	2.7
1	B	35	GLY	2.7
1	E	10	SER	2.7
1	E	74	ALA	2.7
1	B	25	GLN	2.7
1	E	55	ASP	2.7
2	C	21	LEU	2.7
2	F	5	TRP	2.7
2	F	156	LEU	2.7
1	B	42	SER	2.6
2	F	134	ALA	2.6
1	A	8	ARG	2.6
2	C	208	ARG	2.6
2	F	236	PHE	2.6
1	E	118	ILE	2.6
2	F	141	GLY	2.6
1	E	92	HIS	2.5
1	D	-2	ASN	2.5
1	B	80	GLN	2.5
1	D	104	GLN	2.5
1	B	73	TYR	2.5
1	E	83	MET	2.5
2	F	61	ALA	2.5
1	B	77	GLY	2.5
1	E	78	GLY	2.5
1	B	93	HIS	2.4
2	F	3	GLU	2.4
1	B	48	LYS	2.4
1	A	44	ILE	2.3
2	F	248	PRO	2.3
1	E	95	ALA	2.3
1	E	45	SER	2.3
1	E	56	SER	2.3
1	D	5	ILE	2.3
2	F	48	GLU	2.3
2	F	57	VAL	2.3
2	F	204	GLU	2.3
1	A	41	ARG	2.3
2	F	152	HIS	2.3
2	F	7	GLN	2.3
1	D	44	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	57	VAL	2.3
1	B	108	LEU	2.3
1	B	95	ALA	2.3
1	D	-1	TRP	2.3
1	E	13	ALA	2.3
1	B	45	SER	2.3
2	F	13	HIS	2.3
1	B	27	GLY	2.2
1	B	46	ARG	2.2
2	F	175	ALA	2.2
1	E	36	ILE	2.2
1	B	115	LEU	2.2
2	F	6	ARG	2.2
1	B	38	GLY	2.2
2	C	245	GLY	2.2
1	E	117	ALA	2.2
1	B	40	ASP	2.2
1	B	41	ARG	2.2
2	F	205	LYS	2.2
1	D	49	THR	2.2
1	A	39	VAL	2.2
2	F	83	PHE	2.2
1	B	75	LEU	2.1
2	F	121	PRO	2.1
1	E	25	GLN	2.1
1	B	49	THR	2.1
1	D	46	ARG	2.1
2	F	163	ARG	2.1
1	E	87	LEU	2.1
2	F	139	GLU	2.1
1	E	79	GLN	2.1
1	B	51	GLY	2.1
1	E	43	ALA	2.1
2	F	144	LEU	2.1
1	E	47	TRP	2.1
2	C	2	SER	2.1
1	B	74	ALA	2.1
1	B	19	VAL	2.1
1	B	15	LEU	2.0
2	C	48	GLU	2.0
2	F	203	THR	2.0
2	F	86	ARG	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	PO4	F	302	5/5	0.94	0.08	43,46,48,58	0
3	PO4	C	302	5/5	0.98	0.07	28,30,33,34	0
3	PO4	F	301	5/5	0.98	0.06	25,35,41,46	0
3	PO4	C	301	5/5	0.98	0.05	33,34,38,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.