Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 04:43 AM EDT

PDB ID	:	4MZR
Title	:	Crystal structure of a polypeptide p53 mutant bound to DNA
Authors	:	Emamzadah, S.T.; Tropia, L.; Vincenti, I.; Falquet, B.; Halazonetis, T.D.
Deposited on	:	2013-09-30
Resolution	:	2.90 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 (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 (1)) were used in the production of this report:

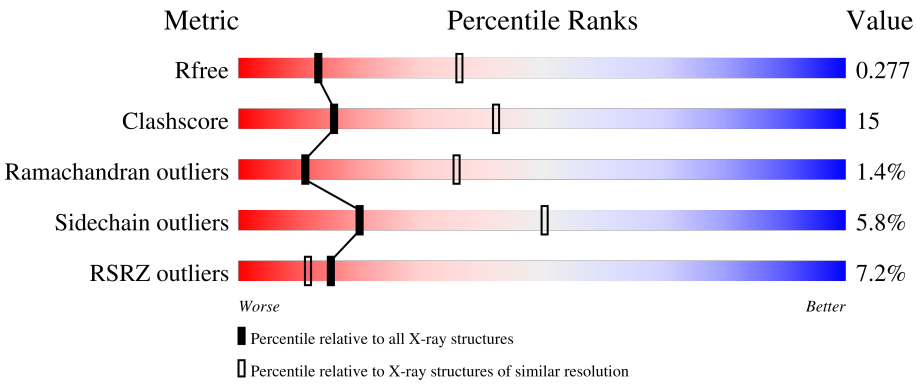
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	237	3% 77% 21%
1	B	237	17% 44% 49% 6%
1	C	237	3% 68% 28%
1	D	237	7% 73% 24%
2	K	26	46% 54%

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Mol	Chain	Length	Quality of chain
3	L	26	62% 38%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8593 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	1865	1160	339	353	13	0	0	0
1	B	234	1865	1160	339	353	13	0	0	0
1	C	234	1865	1160	339	353	13	0	0	0
1	D	234	1865	1160	339	353	13	0	0	0

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	MET	-	initiating methionine	UNP P04637
A	121	PHE	SER	engineered mutation	UNP P04637
A	122	GLY	VAL	engineered mutation	UNP P04637
A	135	VAL	CYS	engineered mutation	UNP P04637
A	141	VAL	CYS	engineered mutation	UNP P04637
A	146	TYR	TRP	engineered mutation	UNP P04637
A	182	SER	CYS	engineered mutation	UNP P04637
A	203	ALA	VAL	engineered mutation	UNP P04637
A	209	PRO	ARG	engineered mutation	UNP P04637
A	229	TYR	CYS	engineered mutation	UNP P04637
A	233	TYR	HIS	engineered mutation	UNP P04637
A	234	PHE	TYR	engineered mutation	UNP P04637
A	235	LYS	ASN	engineered mutation	UNP P04637
A	236	PHE	TYR	engineered mutation	UNP P04637
A	253	VAL	THR	engineered mutation	UNP P04637
A	268	ASP	ASN	engineered mutation	UNP P04637
A	?	-	LYS	deletion	UNP P04637
A	?	-	GLY	deletion	UNP P04637
A	?	-	GLU	deletion	UNP P04637
A	?	-	PRO	deletion	UNP P04637
A	?	-	HIS	deletion	UNP P04637

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P04637
A	?	-	GLU	deletion	UNP P04637
A	?	-	LEU	deletion	UNP P04637
A	?	-	PRO	deletion	UNP P04637
A	?	-	PRO	deletion	UNP P04637
A	?	-	GLY	deletion	UNP P04637
A	?	-	SER	deletion	UNP P04637
A	?	-	THR	deletion	UNP P04637
A	?	-	LYS	deletion	UNP P04637
A	?	-	ARG	deletion	UNP P04637
A	?	-	ALA	deletion	UNP P04637
A	?	-	LEU	deletion	UNP P04637
A	?	-	PRO	deletion	UNP P04637
A	?	-	ASN	deletion	UNP P04637
A	?	-	ASN	deletion	UNP P04637
A	?	-	SER	deletion	UNP P04637
A	?	-	SER	deletion	UNP P04637
A	?	-	SER	deletion	UNP P04637
A	?	-	PRO	deletion	UNP P04637
A	?	-	GLN	deletion	UNP P04637
A	?	-	PRO	deletion	UNP P04637
A	?	-	LYS	deletion	UNP P04637
A	?	-	LYS	deletion	UNP P04637
A	322	THR	PRO	conflict	UNP P04637
A	323	MET	LEU	variant	UNP P04637
A	340	GLN	MET	conflict	UNP P04637
A	344	ARG	LEU	variant	UNP P04637
A	356	THR	GLY	conflict	UNP P04637
A	357	GLU	LYS	conflict	UNP P04637
B	93	MET	-	initiating methionine	UNP P04637
B	121	PHE	SER	engineered mutation	UNP P04637
B	122	GLY	VAL	engineered mutation	UNP P04637
B	135	VAL	CYS	engineered mutation	UNP P04637
B	141	VAL	CYS	engineered mutation	UNP P04637
B	146	TYR	TRP	engineered mutation	UNP P04637
B	182	SER	CYS	engineered mutation	UNP P04637
B	203	ALA	VAL	engineered mutation	UNP P04637
B	209	PRO	ARG	engineered mutation	UNP P04637
B	229	TYR	CYS	engineered mutation	UNP P04637
B	233	TYR	HIS	engineered mutation	UNP P04637
B	234	PHE	TYR	engineered mutation	UNP P04637
B	235	LYS	ASN	engineered mutation	UNP P04637

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Chain	Residue	Modelled	Actual	Comment	Reference
B	236	PHE	TYR	engineered mutation	UNP P04637
B	253	VAL	THR	engineered mutation	UNP P04637
B	268	ASP	ASN	engineered mutation	UNP P04637
B	?	-	GLY	deletion	UNP P04637
B	?	-	GLU	deletion	UNP P04637
B	?	-	PRO	deletion	UNP P04637
B	?	-	HIS	deletion	UNP P04637
B	?	-	HIS	deletion	UNP P04637
B	?	-	GLU	deletion	UNP P04637
B	?	-	LEU	deletion	UNP P04637
B	?	-	PRO	deletion	UNP P04637
B	?	-	PRO	deletion	UNP P04637
B	?	-	GLY	deletion	UNP P04637
B	?	-	SER	deletion	UNP P04637
B	?	-	THR	deletion	UNP P04637
B	?	-	LYS	deletion	UNP P04637
B	?	-	ARG	deletion	UNP P04637
B	?	-	ALA	deletion	UNP P04637
B	?	-	LEU	deletion	UNP P04637
B	?	-	PRO	deletion	UNP P04637
B	?	-	ASN	deletion	UNP P04637
B	?	-	ASN	deletion	UNP P04637
B	?	-	SER	deletion	UNP P04637
B	?	-	SER	deletion	UNP P04637
B	?	-	SER	deletion	UNP P04637
B	?	-	PRO	deletion	UNP P04637
B	?	-	GLN	deletion	UNP P04637
B	?	-	PRO	deletion	UNP P04637
B	?	-	LYS	deletion	UNP P04637
B	?	-	LYS	deletion	UNP P04637
B	?	-	LYS	deletion	UNP P04637
B	?	-	PRO	deletion	UNP P04637
B	323	MET	LEU	variant	UNP P04637
B	340	GLN	MET	conflict	UNP P04637
B	344	ARG	LEU	variant	UNP P04637
B	356	THR	GLY	conflict	UNP P04637
B	357	GLU	LYS	conflict	UNP P04637
C	93	MET	-	initiating methionine	UNP P04637
C	121	PHE	SER	engineered mutation	UNP P04637
C	122	GLY	VAL	engineered mutation	UNP P04637
C	135	VAL	CYS	engineered mutation	UNP P04637
C	141	VAL	CYS	engineered mutation	UNP P04637

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Chain	Residue	Modelled	Actual	Comment	Reference
C	146	TYR	TRP	engineered mutation	UNP P04637
C	182	SER	CYS	engineered mutation	UNP P04637
C	203	ALA	VAL	engineered mutation	UNP P04637
C	209	PRO	ARG	engineered mutation	UNP P04637
C	229	TYR	CYS	engineered mutation	UNP P04637
C	233	TYR	HIS	engineered mutation	UNP P04637
C	234	PHE	TYR	engineered mutation	UNP P04637
C	235	LYS	ASN	engineered mutation	UNP P04637
C	236	PHE	TYR	engineered mutation	UNP P04637
C	253	VAL	THR	conflict	UNP P04637
C	268	ASP	ASN	conflict	UNP P04637
C	?	-	GLY	deletion	UNP P04637
C	?	-	GLU	deletion	UNP P04637
C	?	-	PRO	deletion	UNP P04637
C	?	-	HIS	deletion	UNP P04637
C	?	-	HIS	deletion	UNP P04637
C	?	-	GLU	deletion	UNP P04637
C	?	-	LEU	deletion	UNP P04637
C	?	-	PRO	deletion	UNP P04637
C	?	-	PRO	deletion	UNP P04637
C	?	-	GLY	deletion	UNP P04637
C	?	-	SER	deletion	UNP P04637
C	?	-	THR	deletion	UNP P04637
C	?	-	LYS	deletion	UNP P04637
C	?	-	ARG	deletion	UNP P04637
C	?	-	ALA	deletion	UNP P04637
C	?	-	LEU	deletion	UNP P04637
C	?	-	PRO	deletion	UNP P04637
C	?	-	ASN	deletion	UNP P04637
C	?	-	ASN	deletion	UNP P04637
C	?	-	SER	deletion	UNP P04637
C	?	-	SER	deletion	UNP P04637
C	?	-	SER	deletion	UNP P04637
C	?	-	PRO	deletion	UNP P04637
C	?	-	GLN	deletion	UNP P04637
C	?	-	PRO	deletion	UNP P04637
C	?	-	LYS	deletion	UNP P04637
C	?	-	LYS	deletion	UNP P04637
C	?	-	LYS	deletion	UNP P04637
C	?	-	PRO	deletion	UNP P04637
C	323	MET	LEU	variant	UNP P04637
C	340	GLN	MET	conflict	UNP P04637

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Chain	Residue	Modelled	Actual	Comment	Reference
C	344	ARG	LEU	variant	UNP P04637
C	356	THR	GLY	conflict	UNP P04637
C	357	GLU	LYS	conflict	UNP P04637
D	93	MET	-	initiating methionine	UNP P04637
D	121	PHE	SER	engineered mutation	UNP P04637
D	122	GLY	VAL	engineered mutation	UNP P04637
D	135	VAL	CYS	engineered mutation	UNP P04637
D	141	VAL	CYS	engineered mutation	UNP P04637
D	146	TYR	TRP	engineered mutation	UNP P04637
D	182	SER	CYS	engineered mutation	UNP P04637
D	203	ALA	VAL	engineered mutation	UNP P04637
D	209	PRO	ARG	engineered mutation	UNP P04637
D	229	TYR	CYS	engineered mutation	UNP P04637
D	233	TYR	HIS	engineered mutation	UNP P04637
D	234	PHE	TYR	engineered mutation	UNP P04637
D	235	LYS	ASN	engineered mutation	UNP P04637
D	236	PHE	TYR	engineered mutation	UNP P04637
D	253	VAL	THR	engineered mutation	UNP P04637
D	268	ASP	ASN	engineered mutation	UNP P04637
D	?	-	GLY	deletion	UNP P04637
D	?	-	GLU	deletion	UNP P04637
D	?	-	PRO	deletion	UNP P04637
D	?	-	HIS	deletion	UNP P04637
D	?	-	HIS	deletion	UNP P04637
D	?	-	GLU	deletion	UNP P04637
D	?	-	LEU	deletion	UNP P04637
D	?	-	PRO	deletion	UNP P04637
D	?	-	PRO	deletion	UNP P04637
D	?	-	GLY	deletion	UNP P04637
D	?	-	SER	deletion	UNP P04637
D	?	-	THR	deletion	UNP P04637
D	?	-	LYS	deletion	UNP P04637
D	?	-	ARG	deletion	UNP P04637
D	?	-	ALA	deletion	UNP P04637
D	?	-	LEU	deletion	UNP P04637
D	?	-	PRO	deletion	UNP P04637
D	?	-	ASN	deletion	UNP P04637
D	?	-	ASN	deletion	UNP P04637
D	?	-	SER	deletion	UNP P04637
D	?	-	SER	deletion	UNP P04637
D	?	-	SER	deletion	UNP P04637
D	?	-	PRO	deletion	UNP P04637

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLN	deletion	UNP P04637
D	?	-	PRO	deletion	UNP P04637
D	?	-	LYS	deletion	UNP P04637
D	?	-	LYS	deletion	UNP P04637
D	?	-	LYS	deletion	UNP P04637
D	?	-	PRO	deletion	UNP P04637
D	323	MET	LEU	variant	UNP P04637
D	340	GLN	MET	conflict	UNP P04637
D	344	ARG	LEU	variant	UNP P04637
D	356	THR	GLY	conflict	UNP P04637
D	357	GLU	LYS	conflict	UNP P04637

- Molecule 2 is a DNA chain called consensus DNA sense strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	K	26	525	252	90	158	25	0	0	0

- Molecule 3 is a DNA chain called consensus DNA anti-sense strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	L	26	535	254	106	150	25	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	15	15	15	0	0

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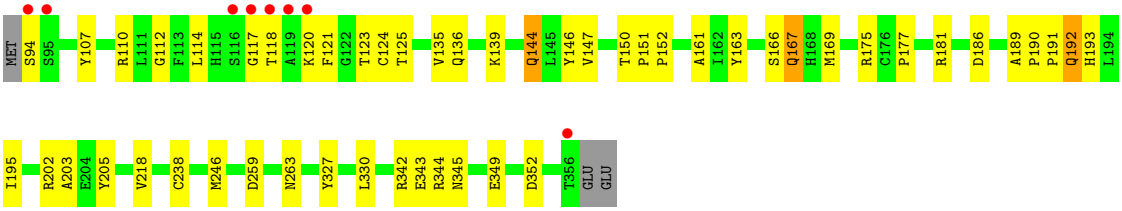
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	1	1	1	0	0
			Total	O		
5	C	31	31	31	0	0
			Total	O		
5	D	21	21	21	0	0
			Total	O		
5	L	1	1	1	0	0

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.

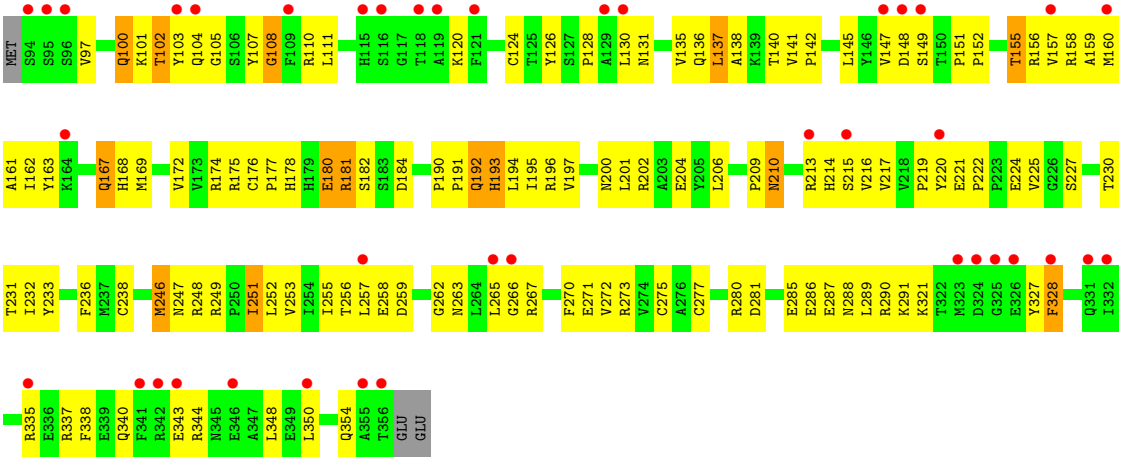
- Molecule 1: Cellular tumor antigen p53

Chain A:



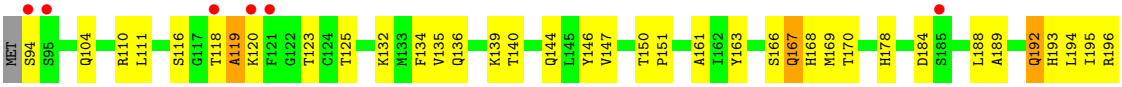
- Molecule 1: Cellular tumor antigen p53

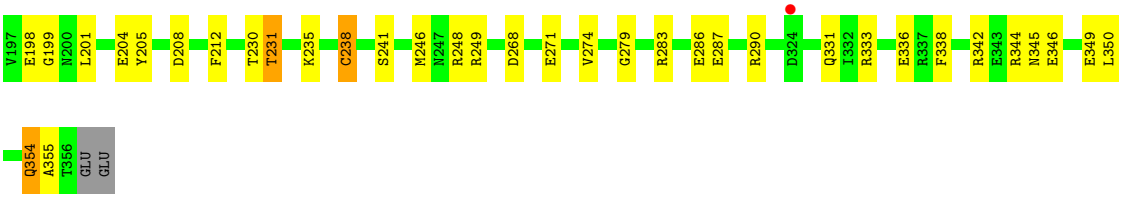
Chain B:



- Molecule 1: Cellular tumor antigen p53

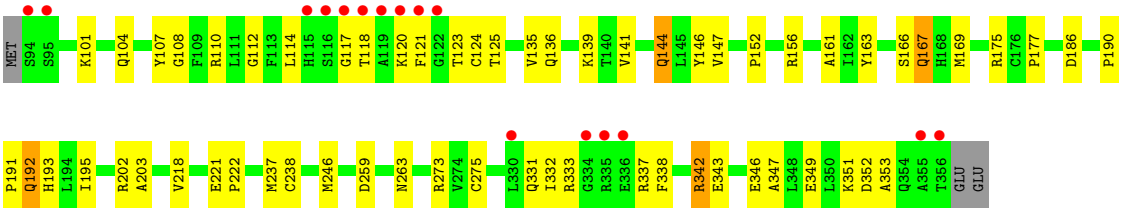
Chain C:





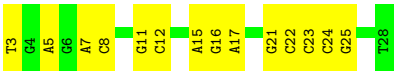
• Molecule 1: Cellular tumor antigen p53

Chain D:



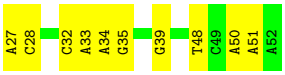
• Molecule 2: consensus DNA sense strand

Chain K:



• Molecule 3: consensus DNA anti-sense strand

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.30Å 169.76Å 55.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 2.90 52.69 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (80.00-2.90) 92.0 (52.69-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.281 0.233 , 0.277	Depositor DCC
R_{free} test set	1618 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8593	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.72% 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: ZN

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	0.35	0/1906	0.54	0/2574
1	B	0.34	0/1906	0.48	0/2574
1	C	0.40	0/1906	0.58	0/2574
1	D	0.35	0/1906	0.54	0/2574
2	K	0.40	0/586	0.76	0/902
3	L	0.36	0/602	0.73	0/928
All	All	0.36	0/8812	0.57	0/12126

There are no bond length outliers.

There are no bond angle outliers.

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	1865	0	1820	40	0
1	B	1865	0	1821	110	0
1	C	1865	0	1820	45	0
1	D	1865	0	1820	45	0
2	K	525	0	296	11	0
3	L	535	0	292	14	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	15	0	0	0	0
5	B	1	0	0	0	0
5	C	31	0	0	0	0
5	D	21	0	0	1	0
5	L	1	0	0	0	0
All	All	8593	0	7869	241	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 15.

All (241) 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:D:192:GLN:H	1:D:192:GLN:HE21	1.08	0.99
1:B:327:TYR:HB3	1:D:331:GLN:HB3	1.43	0.99
3:L:27:DA:H4'	3:L:28:DC:H5'	1.44	0.98
3:L:33:DA:H2"	3:L:34:DA:H5"	1.47	0.97
1:A:192:GLN:H	1:A:192:GLN:HE21	1.08	0.94
1:D:166:SER:HA	1:D:169:MET:HG3	1.55	0.89
1:A:94:SER:HB3	1:C:199:GLY:H	1.39	0.87
1:A:166:SER:HA	1:A:169:MET:HG3	1.55	0.86
1:D:117:GLY:HA2	1:D:121:PHE:HB2	1.59	0.83
1:B:258:GLU:HB2	1:B:262:GLY:HA2	1.58	0.83
1:A:117:GLY:HA2	1:A:121:PHE:HB2	1.59	0.82
2:K:3:DT:H3	3:L:50:DA:H61	1.26	0.82
1:D:167:GLN:H	1:D:167:GLN:HE21	1.27	0.81
1:B:256:THR:HG22	1:B:267:ARG:HD3	1.64	0.79
1:A:192:GLN:HE21	1:A:192:GLN:N	1.80	0.79
1:D:192:GLN:HE21	1:D:192:GLN:N	1.80	0.78
2:K:5:DA:H61	3:L:48:DT:H3	1.30	0.77
1:A:192:GLN:H	1:A:192:GLN:NE2	1.83	0.77
1:D:114:LEU:H	1:D:144:GLN:HE22	1.33	0.77
1:A:167:GLN:H	1:A:167:GLN:HE21	1.30	0.77
1:C:166:SER:HA	1:C:169:MET:HG3	1.67	0.77
1:B:103:TYR:HB3	1:B:267:ARG:HB3	1.68	0.76
1:D:156:ARG:HD3	5:D:508:HOH:O	1.87	0.75
1:A:114:LEU:H	1:A:144:GLN:HE22	1.32	0.74
1:D:192:GLN:H	1:D:192:GLN:NE2	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ILE:HG22	1:B:252:LEU:H	1.52	0.72
1:B:126:TYR:OH	1:B:131:ASN:HA	1.91	0.70
1:B:287:GLU:HG2	1:B:291:LYS:HE3	1.71	0.70
1:D:167:GLN:H	1:D:167:GLN:NE2	1.91	0.68
1:B:192:GLN:H	1:B:192:GLN:NE2	1.91	0.68
2:K:23:DC:H2"	2:K:24:DC:H5'	1.76	0.68
2:K:21:DG:H2"	2:K:22:DC:H5'	1.76	0.67
1:B:156:ARG:NH1	1:B:219:PRO:HG3	2.10	0.67
1:D:332:ILE:HB	1:D:338:PHE:HD1	1.59	0.67
1:A:167:GLN:H	1:A:167:GLN:NE2	1.93	0.66
1:B:108:GLY:O	1:B:147:VAL:HA	1.95	0.66
1:B:175:ARG:HG2	1:B:238:CYS:HB2	1.77	0.66
1:B:191:PRO:HG2	1:B:192:GLN:NE2	2.13	0.63
1:B:101:LYS:O	1:B:267:ARG:HG2	1.99	0.63
1:C:345:ASN:O	1:C:349:GLU:HG3	1.98	0.63
1:D:167:GLN:HE21	1:D:167:GLN:N	1.97	0.62
1:C:119:ALA:O	1:C:279:GLY:HA3	1.99	0.62
1:C:241:SER:HA	1:C:248:ARG:H	1.65	0.62
1:A:94:SER:HB3	1:C:199:GLY:N	2.13	0.62
1:B:145:LEU:HB2	1:B:230:THR:HB	1.82	0.62
1:A:344:ARG:HH21	1:C:344:ARG:HH11	1.48	0.61
1:D:123:THR:HG21	1:D:139:LYS:HG3	1.82	0.61
1:A:123:THR:HG21	1:A:139:LYS:HG3	1.82	0.61
1:A:167:GLN:HE21	1:A:167:GLN:N	1.98	0.61
1:C:167:GLN:H	1:C:167:GLN:HE21	1.49	0.61
2:K:7:DA:H2"	2:K:8:DC:O5'	2.00	0.61
1:B:135:VAL:HG21	1:B:141:VAL:HG22	1.84	0.60
2:K:11:DG:H2"	2:K:12:DC:H5'	1.83	0.60
1:D:259:ASP:OD2	1:D:263:ASN:HB2	2.02	0.59
1:B:135:VAL:HG21	1:B:141:VAL:CG2	2.32	0.59
1:A:107:TYR:OH	1:A:152:PRO:HD3	2.03	0.59
1:B:161:ALA:HB2	1:B:195:ILE:HD11	1.84	0.59
1:C:120:LYS:HG3	3:L:39:DG:H2'	1.86	0.58
1:B:168:HIS:CD2	1:B:249:ARG:HH11	2.22	0.57
1:B:184:ASP:CB	1:B:196:ARG:HH22	2.17	0.57
1:B:162:ILE:HG22	1:B:213:ARG:NH1	2.20	0.56
1:B:172:VAL:HG11	1:B:174:ARG:HH11	1.70	0.56
1:B:224:GLU:HB3	1:B:227:SER:HB2	1.86	0.56
1:B:163:TYR:OH	1:B:246:MET:HA	2.05	0.56
1:B:288:ASN:HA	1:B:291:LYS:HD2	1.88	0.56
1:B:344:ARG:HE	1:B:348:LEU:HG	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LEU:O	1:B:354:GLN:HG2	2.06	0.56
1:C:178:HIS:HA	1:D:177:PRO:HG2	1.87	0.56
1:B:190:PRO:O	1:B:193:HIS:HB2	2.04	0.56
1:A:203:ALA:HA	1:A:218:VAL:HG12	1.88	0.55
1:D:342:ARG:O	1:D:346:GLU:HG2	2.07	0.55
1:D:107:TYR:HB3	1:D:147:VAL:CG2	2.36	0.55
3:L:33:DA:C2'	3:L:34:DA:H5"	2.29	0.55
1:B:111:LEU:HD11	1:B:255:ILE:HG13	1.89	0.55
1:B:348:LEU:HB2	1:D:337:ARG:HH21	1.72	0.55
1:C:118:THR:HG21	1:C:283:ARG:HG3	1.90	0.55
1:B:136:GLN:HA	1:B:275:CYS:O	2.07	0.54
1:C:167:GLN:H	1:C:167:GLN:NE2	2.04	0.54
1:C:342:ARG:O	1:C:346:GLU:HG3	2.08	0.54
1:A:107:TYR:HB3	1:A:147:VAL:CG2	2.38	0.54
3:L:34:DA:H2"	3:L:35:DG:C8	2.43	0.54
1:A:163:TYR:OH	1:A:246:MET:HA	2.07	0.54
1:A:259:ASP:OD2	1:A:263:ASN:HB2	2.07	0.54
1:D:117:GLY:HA2	1:D:121:PHE:CB	2.35	0.53
1:C:163:TYR:OH	1:C:246:MET:HA	2.09	0.53
1:D:203:ALA:HA	1:D:218:VAL:HG12	1.91	0.53
2:K:5:DA:N6	3:L:48:DT:H3	2.03	0.53
1:B:236:PHE:CE2	1:B:272:VAL:HG11	2.44	0.53
1:C:194:LEU:CD1	1:C:238:CYS:HB2	2.39	0.53
1:C:350:LEU:O	1:C:354:GLN:HG3	2.08	0.53
1:D:163:TYR:OH	1:D:246:MET:HA	2.08	0.53
1:D:347:ALA:O	1:D:351:LYS:HG3	2.09	0.52
1:B:273:ARG:HH22	3:L:34:DA:H5'	1.74	0.52
1:B:145:LEU:HD11	1:B:232:ILE:HG22	1.91	0.52
1:B:277:CYS:HB3	1:B:280:ARG:HB3	1.91	0.52
1:A:327:TYR:CZ	1:C:333:ARG:HD3	2.45	0.52
3:L:34:DA:H2"	3:L:35:DG:H8	1.74	0.52
1:B:120:LYS:HB2	2:K:15:DA:OP2	2.09	0.51
1:B:107:TYR:CD1	1:B:149:SER:HB2	2.45	0.51
1:B:175:ARG:HB2	1:B:180:GLU:OE2	2.09	0.51
1:D:107:TYR:OH	1:D:152:PRO:HD3	2.10	0.51
1:D:124:CYS:HB3	1:D:135:VAL:HG23	1.93	0.51
1:B:103:TYR:HB3	1:B:267:ARG:CB	2.39	0.51
1:B:97:VAL:HG11	1:B:169:MET:SD	2.51	0.51
1:D:107:TYR:HB3	1:D:147:VAL:HG23	1.91	0.51
1:B:161:ALA:HB2	1:B:253:VAL:HG22	1.92	0.50
1:B:335:ARG:O	1:B:338:PHE:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLU:O	1:B:291:LYS:HG3	2.12	0.50
1:C:189:ALA:HB2	1:C:205:TYR:CZ	2.47	0.50
1:B:224:GLU:HG3	1:B:225:VAL:N	2.27	0.50
1:B:286:GLU:O	1:B:290:ARG:HG3	2.12	0.50
1:B:327:TYR:HA	1:D:332:ILE:O	2.12	0.50
1:B:175:ARG:HD3	1:B:191:PRO:O	2.11	0.50
1:B:151:PRO:HD2	1:B:220:TYR:CE2	2.46	0.49
1:A:107:TYR:HB3	1:A:147:VAL:HG23	1.94	0.49
1:B:209:PRO:HG2	1:B:210:ASN:H	1.76	0.49
1:B:337:ARG:HA	1:B:340:GLN:HG2	1.92	0.49
1:C:198:GLU:OE2	1:C:235:LYS:HG3	2.13	0.49
1:C:192:GLN:H	1:C:192:GLN:NE2	2.10	0.49
1:B:124:CYS:SG	1:B:135:VAL:HB	2.53	0.48
1:A:330:LEU:HD13	1:C:338:PHE:HE1	1.78	0.48
1:A:124:CYS:HB3	1:A:135:VAL:HG23	1.96	0.48
1:B:152:PRO:HG2	1:B:155:THR:OG1	2.14	0.48
1:B:128:PRO:O	1:B:350:LEU:HD11	2.14	0.48
1:B:107:TYR:CE2	1:B:151:PRO:HG3	2.49	0.47
1:D:332:ILE:HG21	1:D:338:PHE:HA	1.94	0.47
3:L:50:DA:H2"	3:L:51:DA:C8	2.49	0.47
1:C:135:VAL:HG22	1:C:136:GLN:N	2.29	0.47
1:A:117:GLY:HA2	1:A:121:PHE:CB	2.35	0.47
1:A:349:GLU:O	1:A:352:ASP:HB2	2.14	0.47
1:C:123:THR:HG23	1:C:139:LYS:HB3	1.95	0.47
1:A:135:VAL:HG22	1:A:136:GLN:N	2.30	0.47
1:B:184:ASP:HB2	1:B:196:ARG:HH22	1.80	0.47
1:C:135:VAL:O	1:C:274:VAL:HA	2.14	0.47
3:L:32:DC:H2"	3:L:33:DA:C8	2.50	0.47
2:K:24:DC:H2"	2:K:25:DG:C8	2.50	0.47
1:A:175:ARG:HD3	1:A:191:PRO:O	2.14	0.46
1:C:246:MET:O	1:C:249:ARG:HB2	2.15	0.46
3:L:27:DA:H1'	3:L:28:DC:C6	2.50	0.46
1:B:174:ARG:NH2	1:B:192:GLN:HG3	2.30	0.46
1:B:155:THR:HG23	1:B:258:GLU:O	2.16	0.46
1:B:281:ASP:O	1:B:285:GLU:HG3	2.14	0.46
1:D:333:ARG:HB3	1:D:337:ARG:HH11	1.80	0.46
1:B:145:LEU:HD12	1:B:145:LEU:N	2.30	0.46
1:B:151:PRO:HB3	1:B:152:PRO:HD2	1.96	0.46
1:C:116:SER:HB2	1:C:125:THR:OG1	2.15	0.46
1:D:349:GLU:HA	1:D:352:ASP:OD2	2.15	0.46
1:D:114:LEU:H	1:D:144:GLN:NE2	2.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ARG:HD3	1:D:191:PRO:O	2.16	0.45
1:B:192:GLN:HG2	1:B:214:HIS:HE1	1.81	0.45
1:B:247:ASN:C	1:B:249:ARG:H	2.19	0.45
1:D:190:PRO:HB2	1:D:193:HIS:HD2	1.81	0.45
1:B:200:ASN:C	1:B:201:LEU:HD22	2.37	0.45
1:A:345:ASN:O	1:A:349:GLU:HG2	2.16	0.45
1:B:273:ARG:NH2	3:L:34:DA:H5'	2.32	0.45
1:B:103:TYR:CE1	1:B:105:GLY:HA2	2.52	0.45
1:B:162:ILE:HD12	1:B:162:ILE:O	2.17	0.45
1:B:190:PRO:HB2	1:B:193:HIS:HD2	1.82	0.45
1:C:193:HIS:CE1	1:C:205:TYR:HB3	2.52	0.45
1:B:172:VAL:HG11	1:B:174:ARG:NH1	2.32	0.45
1:B:197:VAL:CG1	1:B:232:ILE:HD11	2.47	0.45
1:D:161:ALA:HB2	1:D:195:ILE:HD11	1.98	0.45
1:B:101:LYS:HD2	1:B:102:THR:H	1.82	0.44
1:B:152:PRO:HG2	1:B:155:THR:HG1	1.82	0.44
1:C:283:ARG:O	1:C:287:GLU:HB2	2.17	0.44
1:B:142:PRO:HB3	1:B:233:TYR:CE2	2.53	0.44
1:B:197:VAL:HA	1:B:233:TYR:O	2.18	0.44
1:B:202:ARG:HE	1:B:219:PRO:HG2	1.82	0.44
1:C:144:GLN:HE21	1:C:146:TYR:HE1	1.65	0.44
1:A:167:GLN:HA	1:C:140:THR:HB	1.99	0.44
1:C:168:HIS:CD2	1:C:249:ARG:HH11	2.36	0.44
1:B:130:LEU:HD21	1:B:289:LEU:HD22	1.98	0.44
1:B:191:PRO:HG2	1:B:192:GLN:HE22	1.82	0.44
1:C:111:LEU:HG	1:C:268:ASP:HB3	1.98	0.44
1:B:197:VAL:HG13	1:B:232:ILE:HD11	2.00	0.44
1:B:252:LEU:HD12	1:B:271:GLU:HA	2.00	0.44
1:C:94:SER:HA	1:C:170:THR:HG21	1.99	0.43
1:B:246:MET:O	1:B:249:ARG:HB2	2.18	0.43
1:A:177:PRO:HB2	1:B:177:PRO:HB2	2.01	0.43
1:B:135:VAL:HG22	1:B:136:GLN:O	2.17	0.43
1:D:135:VAL:HG21	1:D:141:VAL:HG22	2.00	0.43
1:B:257:LEU:HB3	1:B:266:GLY:HA3	2.00	0.43
1:B:192:GLN:HG2	1:B:214:HIS:CE1	2.54	0.43
1:B:236:PHE:CD1	1:B:236:PHE:N	2.86	0.43
1:C:184:ASP:HB2	1:C:196:ARG:HH12	1.82	0.43
1:A:190:PRO:HB2	1:A:193:HIS:HD2	1.83	0.43
1:D:135:VAL:HG22	1:D:136:GLN:N	2.34	0.43
1:B:209:PRO:HG2	1:B:210:ASN:OD1	2.19	0.42
1:B:194:LEU:CD1	1:B:238:CYS:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:SER:HA	1:D:101:LYS:HD3	2.00	0.42
1:B:251:ILE:N	1:B:251:ILE:HD12	2.34	0.42
1:B:128:PRO:HG2	1:B:343:GLU:OE2	2.19	0.42
1:C:286:GLU:O	1:C:290:ARG:HB2	2.18	0.42
1:A:112:GLY:HA3	1:A:146:TYR:HE1	1.84	0.42
1:B:157:VAL:HG22	1:B:257:LEU:CD1	2.49	0.42
1:B:137:LEU:O	1:B:138:ALA:HB3	2.19	0.42
1:B:140:THR:HB	1:D:167:GLN:HA	2.02	0.42
1:B:177:PRO:HB3	1:B:181:ARG:HH12	1.84	0.42
2:K:16:DG:H2"	2:K:17:DA:O5'	2.20	0.42
1:A:330:LEU:HD13	1:C:338:PHE:CE1	2.55	0.42
1:C:208:ASP:O	1:C:212:PHE:HA	2.19	0.42
1:B:156:ARG:HB3	1:B:217:VAL:HG12	2.01	0.42
1:B:100:GLN:HA	1:B:267:ARG:HD2	2.00	0.42
1:B:158:ARG:NH2	1:B:217:VAL:HG21	2.34	0.42
1:B:101:LYS:O	1:B:103:TYR:N	2.53	0.42
1:D:104:GLN:HB3	1:D:108:GLY:HA2	2.02	0.42
1:A:150:THR:HA	1:A:151:PRO:HD3	1.78	0.42
1:B:167:GLN:CD	1:B:167:GLN:H	2.21	0.42
1:C:150:THR:HA	1:C:151:PRO:HD3	1.77	0.42
1:B:107:TYR:CD2	1:B:151:PRO:HG3	2.55	0.41
1:B:328:PHE:HB2	1:D:338:PHE:CE1	2.55	0.41
1:C:354:GLN:HG3	1:C:354:GLN:H	1.52	0.41
1:B:204:GLU:O	1:B:216:VAL:HA	2.20	0.41
1:A:118:THR:C	1:A:120:LYS:H	2.23	0.41
1:B:159:ALA:HB3	1:B:216:VAL:HG13	2.02	0.41
1:B:175:ARG:HA	1:B:238:CYS:SG	2.60	0.41
1:C:125:THR:O	1:C:125:THR:HG23	2.20	0.41
1:A:114:LEU:H	1:A:144:GLN:NE2	2.07	0.41
1:C:132:LYS:HD2	1:C:271:GLU:OE2	2.20	0.41
1:A:189:ALA:HA	1:A:190:PRO:HD3	1.93	0.41
1:B:157:VAL:HG22	1:B:257:LEU:HD13	2.03	0.41
1:B:156:ARG:O	1:B:257:LEU:HD12	2.20	0.41
1:B:160:MET:CE	1:B:215:SER:HB3	2.51	0.41
1:B:221:GLU:HA	1:B:222:PRO:HD3	1.96	0.41
1:C:230:THR:HG22	1:C:231:THR:N	2.35	0.41
1:D:112:GLY:HA3	1:D:146:TYR:HE1	1.85	0.41
1:D:118:THR:C	1:D:120:LYS:H	2.24	0.41
1:D:136:GLN:HA	1:D:275:CYS:O	2.20	0.41
1:A:181:ARG:O	1:A:181:ARG:HG3	2.21	0.41
1:B:131:ASN:ND2	1:B:270:PHE:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:HD22	1:B:201:LEU:N	2.37	0.41
1:D:175:ARG:NH2	1:D:237:MET:HB3	2.36	0.40
1:D:273:ARG:HH11	1:D:273:ARG:HG3	1.87	0.40
1:A:161:ALA:HB2	1:A:195:ILE:HD11	2.02	0.40
1:C:132:LYS:HE2	1:C:134:PHE:CZ	2.57	0.40
1:A:189:ALA:HB2	1:A:205:TYR:CZ	2.57	0.40
1:B:120:LYS:HD3	2:K:15:DA:OP2	2.21	0.40
1:A:167:GLN:HB3	1:C:123:THR:HG21	2.04	0.40
1:B:176:CYS:SG	1:B:178:HIS:HB3	2.61	0.40
1:C:161:ALA:HB2	1:C:195:ILE:HD11	2.03	0.40
1:D:221:GLU:HA	1:D:222:PRO:HD3	1.86	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	232/237 (98%)	219 (94%)	13 (6%)	0	100 100
1	B	232/237 (98%)	184 (79%)	38 (16%)	10 (4%)	2 10
1	C	232/237 (98%)	210 (90%)	20 (9%)	2 (1%)	17 48
1	D	232/237 (98%)	212 (91%)	19 (8%)	1 (0%)	34 66
All	All	928/948 (98%)	825 (89%)	90 (10%)	13 (1%)	11 36

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	ASP
1	C	355	ALA
1	B	102	THR
1	B	182	SER

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Mol	Chain	Res	Type
1	B	263	ASN
1	C	119	ALA
1	B	155	THR
1	B	206	LEU
1	B	265	LEU
1	D	353	ALA
1	B	100	GLN
1	B	248	ARG
1	B	108	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	207/210 (99%)	197 (95%)	10 (5%)	25	58
1	B	207/210 (99%)	192 (93%)	15 (7%)	14	39
1	C	207/210 (99%)	194 (94%)	13 (6%)	18	46
1	D	207/210 (99%)	197 (95%)	10 (5%)	25	58
All	All	828/840 (99%)	780 (94%)	48 (6%)	20	50

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	125	THR
1	A	144	GLN
1	A	167	GLN
1	A	186	ASP
1	A	192	GLN
1	A	202	ARG
1	A	238	CYS
1	A	342	ARG
1	A	343	GLU
1	B	104	GLN
1	B	110	ARG

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Mol	Chain	Res	Type
1	B	137	LEU
1	B	167	GLN
1	B	180	GLU
1	B	181	ARG
1	B	192	GLN
1	B	193	HIS
1	B	210	ASN
1	B	231	THR
1	B	246	MET
1	B	251	ILE
1	B	259	ASP
1	B	321	LYS
1	B	328	PHE
1	C	104	GLN
1	C	110	ARG
1	C	147	VAL
1	C	167	GLN
1	C	188	LEU
1	C	192	GLN
1	C	201	LEU
1	C	204	GLU
1	C	231	THR
1	C	238	CYS
1	C	331	GLN
1	C	336	GLU
1	C	354	GLN
1	D	110	ARG
1	D	125	THR
1	D	144	GLN
1	D	167	GLN
1	D	186	ASP
1	D	192	GLN
1	D	202	ARG
1	D	238	CYS
1	D	342	ARG
1	D	343	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	115	HIS

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Mol	Chain	Res	Type
1	A	144	GLN
1	A	167	GLN
1	A	192	GLN
1	B	104	GLN
1	B	131	ASN
1	B	144	GLN
1	B	167	GLN
1	B	168	HIS
1	B	192	GLN
1	B	193	HIS
1	B	214	HIS
1	B	263	ASN
1	B	340	GLN
1	C	104	GLN
1	C	144	GLN
1	C	167	GLN
1	C	168	HIS
1	C	192	GLN
1	C	239	ASN
1	C	331	GLN
1	C	340	GLN
1	D	104	GLN
1	D	115	HIS
1	D	144	GLN
1	D	167	GLN
1	D	192	GLN

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	234/237 (98%)	0.06	8 (3%) 45 40	27, 49, 95, 95	0
1	B	234/237 (98%)	0.96	40 (17%) 1 1	63, 95, 95, 95	0
1	C	234/237 (98%)	0.03	7 (2%) 50 45	20, 39, 90, 95	0
1	D	234/237 (98%)	0.28	16 (6%) 17 13	30, 48, 95, 95	0
2	K	26/26 (100%)	-0.10	0 100 100	36, 59, 87, 93	0
3	L	26/26 (100%)	-0.24	0 100 100	44, 64, 86, 90	0
All	All	988/1000 (98%)	0.31	71 (7%) 15 11	20, 55, 95, 95	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	SER	5.7
1	B	95	SER	5.7
1	C	95	SER	5.2
1	B	94	SER	5.0
1	C	94	SER	4.9
1	D	116	SER	4.6
1	B	323	MET	4.6
1	D	121	PHE	4.4
1	D	119	ALA	4.4
1	D	120	LYS	4.3
1	B	119	ALA	4.2
1	A	356	THR	4.2
1	D	115	HIS	4.2
1	B	121	PHE	4.0
1	B	331	GLN	3.9
1	B	115	HIS	3.8
1	C	185	SER	3.8
1	B	355	ALA	3.8
1	D	94	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	350	LEU	3.7
1	B	324	ASP	3.6
1	B	341	PHE	3.5
1	B	116	SER	3.4
1	B	265	LEU	3.4
1	D	95	SER	3.4
1	B	356	THR	3.3
1	B	103	TYR	3.3
1	D	334	GLY	3.2
1	C	120	LYS	3.2
1	B	343	GLU	3.2
1	B	346	GLU	3.2
1	A	116	SER	3.2
1	A	118	THR	3.1
1	B	104	GLN	3.0
1	A	117	GLY	3.0
1	B	118	THR	3.0
1	B	109	PHE	2.9
1	D	122	GLY	2.9
1	D	355	ALA	2.8
1	D	117	GLY	2.8
1	B	342	ARG	2.8
1	B	266	GLY	2.7
1	B	149	SER	2.7
1	B	96	SER	2.7
1	A	119	ALA	2.6
1	B	326	GLU	2.6
1	A	95	SER	2.6
1	B	213	ARG	2.5
1	B	257	LEU	2.5
1	C	118	THR	2.5
1	B	332	ILE	2.4
1	B	325	GLY	2.3
1	B	335	ARG	2.3
1	B	220	TYR	2.3
1	D	330	LEU	2.3
1	D	335	ARG	2.3
1	B	328	PHE	2.2
1	C	121	PHE	2.2
1	A	120	LYS	2.2
1	B	130	LEU	2.1
1	D	356	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	164	LYS	2.1
1	B	215	SER	2.1
1	D	118	THR	2.1
1	B	157	VAL	2.1
1	B	147	VAL	2.1
1	D	336	GLU	2.1
1	B	160	MET	2.1
1	C	324	ASP	2.0
1	B	129	ALA	2.0
1	B	148	ASP	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	ZN	B	401	1/1	0.90	0.23	82,82,82,82	0
4	ZN	A	401	1/1	0.99	0.21	49,49,49,49	0
4	ZN	C	401	1/1	0.99	0.19	35,35,35,35	0
4	ZN	D	401	1/1	0.99	0.22	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.