



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 12:15 PM BST

PDB ID : 6XLQ
Title : Crystal Structure of the Human BTN3A1 Ectodomain in Complex with the CTX-2026 Fab
Authors : Payne, K.K.; Mine, J.A.; Biswas, S.; Chaurio, R.A.; Perales-Puchalt, A.; Anadon, C.M.; Costich, T.L.; Harro, C.M.; Walrath, J.; Ming, Q.; Tcyganov, E.; Buras, A.L.; Rigolizzo, K.E.; Mandal, G.; Lajoie, J.; Ophir, M.; Tchou, J.; Marchion, D.; Luca, V.C.; Bobrowicz, P.; McLaughlin, B.; Eskiocak, U.; Schmidt, M.; Cubillos-Ruiz, J.R.; Rodriguez, P.C.; Gabrilovich, D.I.; Conejo-Garcia, J.R.
Deposited on : 2020-06-29
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

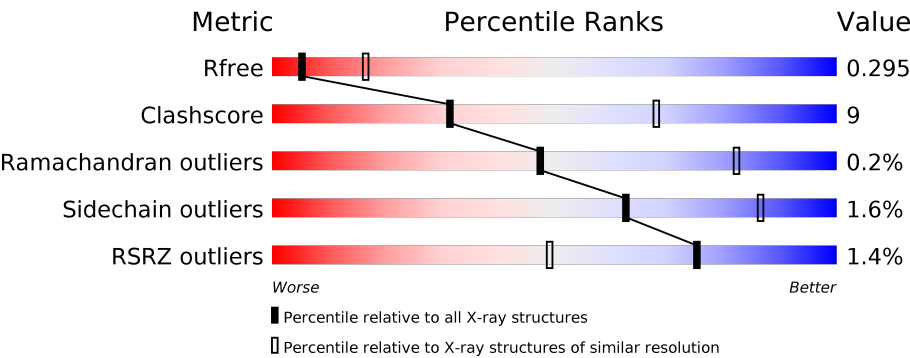
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	226	<div><div>%</div><div><div></div><div>73%</div><div>19%</div><div>• 7%</div></div></div>
1	D	226	<div><div>2%</div><div><div></div><div>75%</div><div>17%</div><div>7%</div></div></div>
1	G	226	<div><div></div><div><div></div><div>73%</div><div>19%</div><div>• 7%</div></div></div>
1	J	226	<div><div>%</div><div><div></div><div>73%</div><div>19%</div><div>• 7%</div></div></div>
2	B	223	<div><div>2%</div><div><div></div><div>73%</div><div>23%</div><div>• •</div></div></div>

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Mol	Chain	Length	Quality of chain
2	E	223	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>70%</div><div>26%</div><div>••</div></div></div>
2	H	223	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>74%</div><div>22%</div><div>••</div></div></div>
2	K	223	<div><div><div></div><div></div><div></div></div><div><div></div><div>75%</div><div>21%</div><div>••</div></div></div>
3	C	212	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>83%</div><div>15%</div><div>•</div></div></div>
3	F	212	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>84%</div><div>16%</div><div></div></div></div>
3	I	212	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>86%</div><div>14%</div><div></div></div></div>
3	L	212	<div><div><div></div><div></div><div></div></div><div><div></div><div>83%</div><div>17%</div><div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19387 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 Butyrophilin subfamily 3 member A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1588	1003	270	307	8			
1	D	210	Total	C	N	O	S	0	0	0
			1588	1003	270	307	8			
1	G	210	Total	C	N	O	S	0	0	0
			1588	1003	270	307	8			
1	J	210	Total	C	N	O	S	0	0	0
			1588	1003	270	307	8			

- Molecule 2 is a protein called CTX-2026 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1641	1038	277	316	10			
2	E	216	Total	C	N	O	S	0	0	0
			1641	1038	277	316	10			
2	H	216	Total	C	N	O	S	0	0	0
			1641	1038	277	316	10			
2	K	216	Total	C	N	O	S	0	0	0
			1641	1038	277	316	10			

- Molecule 3 is a protein called CTX-2026 Light Chain.

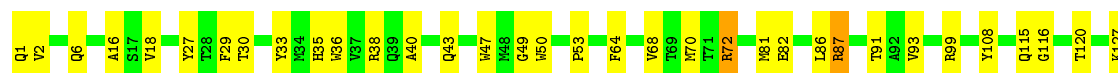
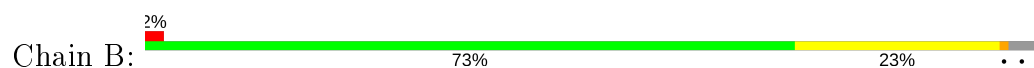
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	212	Total	C	N	O	S	0	0	0
			1611	1009	270	327	5			
3	F	212	Total	C	N	O	S	0	0	0
			1611	1009	270	327	5			
3	I	212	Total	C	N	O	S	0	0	0
			1611	1009	270	327	5			
3	L	212	Total	C	N	O	S	0	0	0
			1611	1009	270	327	5			

- Molecule 4 is water.

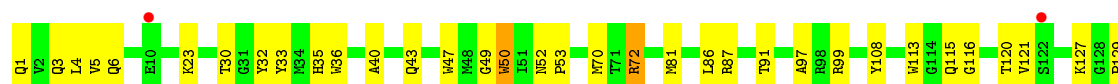
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	1	Total 1	O 1	0	0
4	C	2	Total 2	O 2	0	0
4	D	1	Total 1	O 1	0	0
4	F	1	Total 1	O 1	0	0
4	G	5	Total 5	O 5	0	0
4	H	1	Total 1	O 1	0	0
4	J	6	Total 6	O 6	0	0
4	K	3	Total 3	O 3	0	0
4	L	5	Total 5	O 5	0	0



- Molecule 2: CTX-2026 Heavy Chain



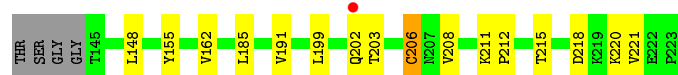
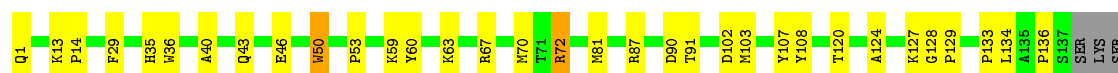
- Molecule 2: CTX-2026 Heavy Chain



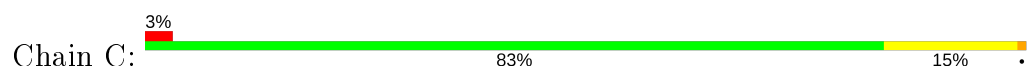
- Molecule 2: CTX-2026 Heavy Chain

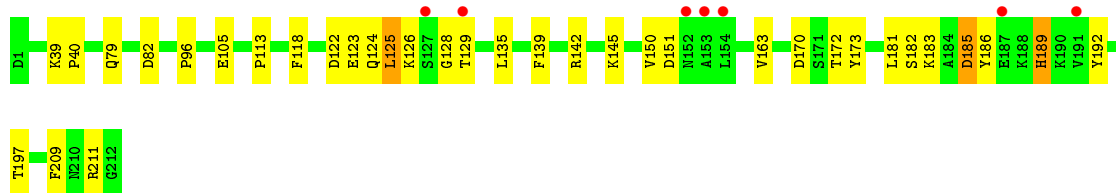


- Molecule 2: CTX-2026 Heavy Chain

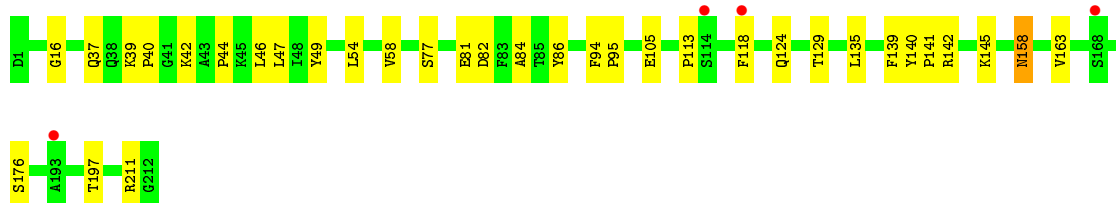
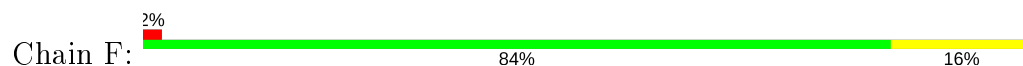


- Molecule 3: CTX-2026 Light Chain

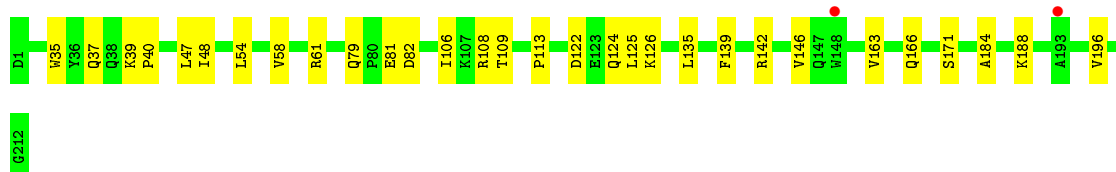
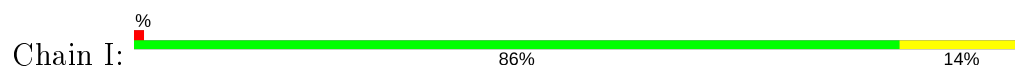




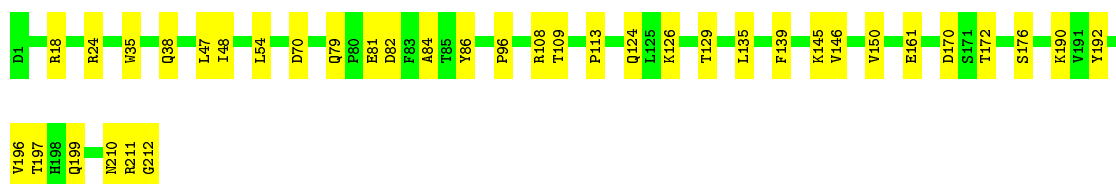
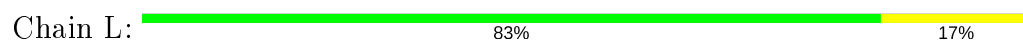
- Molecule 3: CTX-2026 Light Chain



- Molecule 3: CTX-2026 Light Chain



- Molecule 3: CTX-2026 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.31Å 159.85Å 188.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.17 – 3.00 38.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.17-3.00) 98.6 (38.17-3.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.246 , 0.296 0.248 , 0.295	Depositor DCC
R_{free} test set	3332 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19387	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5208e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: PCA

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	0.29	0/1620	0.54	0/2197
1	D	0.28	0/1620	0.52	0/2197
1	G	0.30	0/1620	0.55	0/2197
1	J	0.31	0/1620	0.56	0/2197
2	B	0.50	0/1676	0.60	0/2283
2	E	0.31	0/1676	0.58	1/2283 (0.0%)
2	H	0.31	0/1676	0.60	2/2283 (0.1%)
2	K	0.32	0/1676	0.56	0/2283
3	C	0.38	0/1647	0.56	1/2238 (0.0%)
3	F	0.27	0/1647	0.52	0/2238
3	I	0.29	0/1647	0.53	0/2238
3	L	0.29	0/1647	0.56	0/2238
All	All	0.33	0/19772	0.56	4/26872 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	203	THR	CA-CB-CG2	7.29	122.61	112.40
2	E	50	TRP	CA-CB-CG	6.44	125.93	113.70
3	C	125	LEU	CA-CB-CG	-5.39	102.91	115.30
2	H	220	LYS	CD-CE-NZ	-5.37	99.35	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1588	0	1566	28	0
1	D	1588	0	1566	24	0
1	G	1588	0	1566	36	1
1	J	1588	0	1566	32	0
2	B	1641	0	1600	42	0
2	E	1641	0	1600	46	0
2	H	1641	0	1600	34	0
2	K	1641	0	1600	32	0
3	C	1611	0	1567	38	0
3	F	1611	0	1567	24	0
3	I	1611	0	1567	20	0
3	L	1611	0	1567	22	1
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	5	0	0	0	0
4	H	1	0	0	0	0
4	J	6	0	0	0	0
4	K	3	0	0	0	0
4	L	5	0	0	0	0
All	All	19387	0	18932	346	1

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 9.

The worst 5 of 346 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:G:37:LYS:HE2	2:H:103:MET:SD	1.88	1.14
2:H:198:SER:OG	2:H:202:GLN:HG3	1.56	1.06
2:B:219:LYS:NZ	3:C:123:GLU:OE2	2.01	0.94
2:E:35:HIS:CE1	2:E:50:TRP:CD1	2.56	0.94
3:C:151:ASP:CG	3:C:189:HIS:HB3	1.89	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:SER:OG	3:L:190:LYS:NZ[3_555]	2.19	0.01

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	206/226 (91%)	204 (99%)	1 (0%)	1 (0%)	29	68
1	D	206/226 (91%)	202 (98%)	3 (2%)	1 (0%)	29	68
1	G	206/226 (91%)	204 (99%)	1 (0%)	1 (0%)	29	68
1	J	206/226 (91%)	204 (99%)	1 (0%)	1 (0%)	29	68
2	B	212/223 (95%)	205 (97%)	7 (3%)	0	100	100
2	E	212/223 (95%)	207 (98%)	5 (2%)	0	100	100
2	H	212/223 (95%)	208 (98%)	4 (2%)	0	100	100
2	K	212/223 (95%)	207 (98%)	5 (2%)	0	100	100
3	C	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
3	F	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
3	I	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
3	L	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
All	All	2512/2644 (95%)	2452 (98%)	56 (2%)	4 (0%)	47	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	22	PRO
1	G	22	PRO
1	J	22	PRO
1	A	22	PRO

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	171/181 (94%)	167 (98%)	4 (2%)	50	80
1	D	171/181 (94%)	170 (99%)	1 (1%)	86	95
1	G	171/181 (94%)	169 (99%)	2 (1%)	71	90
1	J	171/181 (94%)	165 (96%)	6 (4%)	36	71
2	B	181/186 (97%)	176 (97%)	5 (3%)	43	77
2	E	181/186 (97%)	178 (98%)	3 (2%)	60	85
2	H	181/186 (97%)	177 (98%)	4 (2%)	52	81
2	K	181/186 (97%)	177 (98%)	4 (2%)	52	81
3	C	183/183 (100%)	180 (98%)	3 (2%)	62	86
3	F	183/183 (100%)	182 (100%)	1 (0%)	88	96
3	I	183/183 (100%)	183 (100%)	0	100	100
3	L	183/183 (100%)	182 (100%)	1 (0%)	88	96
All	All	2140/2200 (97%)	2106 (98%)	34 (2%)	62	86

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	206	CYS
2	H	50	TRP
2	K	102	ASP
1	G	41	SER
2	B	72	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
2	PCA	H	1	2	7,8,9	1.82	1 (14%)	9,10,12	2.19	5 (55%)
2	PCA	B	1	2	7,8,9	1.82	1 (14%)	9,10,12	2.22	5 (55%)
2	PCA	K	1	2	7,8,9	1.83	1 (14%)	9,10,12	2.23	5 (55%)
2	PCA	E	1	2	7,8,9	1.80	1 (14%)	9,10,12	2.21	5 (55%)

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
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1
2	PCA	K	1	2	-	0/0/11/13	0/1/1/1
2	PCA	E	1	2	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	PCA	CD-N	4.74	1.47	1.34
2	H	1	PCA	CD-N	4.69	1.47	1.34
2	B	1	PCA	CD-N	4.69	1.47	1.34
2	E	1	PCA	CD-N	4.63	1.46	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	PCA	CB-CA-C	-3.17	108.34	112.70
2	K	1	PCA	OE-CD-CG	-3.13	121.30	126.76
2	H	1	PCA	OE-CD-CG	-3.08	121.39	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	PCA	OE-CD-CG	-3.07	121.41	126.76
2	B	1	PCA	OE-CD-CG	-3.06	121.42	126.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	210/226 (92%)	-0.08	2 (0%) 82 59	49, 79, 113, 127	0
1	D	210/226 (92%)	0.01	4 (1%) 66 37	51, 75, 114, 133	0
1	G	210/226 (92%)	-0.19	0 100 100	35, 59, 106, 129	0
1	J	210/226 (92%)	-0.18	3 (1%) 75 49	46, 64, 109, 135	0
2	B	215/223 (96%)	-0.20	4 (1%) 66 37	40, 61, 123, 146	0
2	E	215/223 (96%)	0.28	6 (2%) 53 25	61, 98, 148, 173	0
2	H	215/223 (96%)	0.04	2 (0%) 84 63	38, 71, 134, 156	0
2	K	215/223 (96%)	-0.26	1 (0%) 91 75	41, 59, 95, 132	0
3	C	212/212 (100%)	-0.05	7 (3%) 46 20	43, 77, 137, 150	0
3	F	212/212 (100%)	0.11	4 (1%) 66 37	46, 105, 132, 149	0
3	I	212/212 (100%)	-0.07	2 (0%) 84 63	33, 76, 108, 124	0
3	L	212/212 (100%)	-0.29	0 100 100	41, 63, 85, 96	0
All	All	2548/2644 (96%)	-0.07	35 (1%) 75 49	33, 72, 127, 173	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	195	PRO	3.3
1	J	164	PRO	3.3
2	B	202	GLN	3.3
2	E	194	VAL	3.3
3	C	191	VAL	3.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	PCA	E	1	8/9	0.81	0.41	89,95,100,103	0
2	PCA	K	1	8/9	0.86	0.22	66,80,86,89	0
2	PCA	H	1	8/9	0.86	0.31	57,75,89,95	0
2	PCA	B	1	8/9	0.89	0.23	73,76,81,82	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.