WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 05:43 PM EDT

PDB ID	:	3EDT
Title	:	Crystal structure of the mutated S328N hKLC2 TPR domain
Authors	:	Zhu, H.; Shen, Y.; MacKenzie, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on	:	2008-09-03
Resolution	:	2.70 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 following versions of software and data (see references ⓘ) were used in the production of this report:

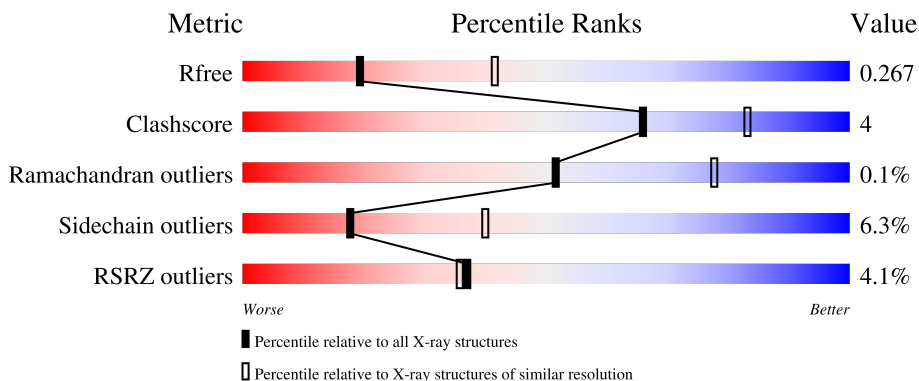|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.70 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		6.3%
RSRZ outliers		4.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	B	283	5% / 81% / 8% · 9%
1	D	283	3% / 76% / 14% 10%
1	F	283	4% / 81% / 9% · 9%
1	H	283	4% / 75% / 14% · 10%

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
2	UNX	D	1	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8095 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 Kinesin light chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	258	Total 2030	C 1261	N 374	O 387	S 8	0	0	0
1	D	255	Total 2013	C 1252	N 370	O 383	S 8	0	0	0
1	F	258	Total 2029	C 1261	N 374	O 386	S 8	0	0	0
1	H	254	Total 2005	C 1247	N 369	O 381	S 8	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	198	MET	-	expression tag	UNP Q9H0B6
B	199	GLY	-	expression tag	UNP Q9H0B6
B	200	SER	-	expression tag	UNP Q9H0B6
B	201	SER	-	expression tag	UNP Q9H0B6
B	202	HIS	-	expression tag	UNP Q9H0B6
B	203	HIS	-	expression tag	UNP Q9H0B6
B	204	HIS	-	expression tag	UNP Q9H0B6
B	205	HIS	-	expression tag	UNP Q9H0B6
B	206	HIS	-	expression tag	UNP Q9H0B6
B	207	HIS	-	expression tag	UNP Q9H0B6
B	208	SER	-	expression tag	UNP Q9H0B6
B	209	SER	-	expression tag	UNP Q9H0B6
B	210	GLY	-	expression tag	UNP Q9H0B6
B	211	LEU	-	expression tag	UNP Q9H0B6
B	212	VAL	-	expression tag	UNP Q9H0B6
B	213	PRO	-	expression tag	UNP Q9H0B6
B	214	ARG	-	expression tag	UNP Q9H0B6
B	215	GLY	-	expression tag	UNP Q9H0B6
B	216	SER	-	expression tag	UNP Q9H0B6
B	328	ASN	SER	engineered mutation	UNP Q9H0B6
D	198	MET	-	expression tag	UNP Q9H0B6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	199	GLY	-	expression tag	UNP Q9H0B6
D	200	SER	-	expression tag	UNP Q9H0B6
D	201	SER	-	expression tag	UNP Q9H0B6
D	202	HIS	-	expression tag	UNP Q9H0B6
D	203	HIS	-	expression tag	UNP Q9H0B6
D	204	HIS	-	expression tag	UNP Q9H0B6
D	205	HIS	-	expression tag	UNP Q9H0B6
D	206	HIS	-	expression tag	UNP Q9H0B6
D	207	HIS	-	expression tag	UNP Q9H0B6
D	208	SER	-	expression tag	UNP Q9H0B6
D	209	SER	-	expression tag	UNP Q9H0B6
D	210	GLY	-	expression tag	UNP Q9H0B6
D	211	LEU	-	expression tag	UNP Q9H0B6
D	212	VAL	-	expression tag	UNP Q9H0B6
D	213	PRO	-	expression tag	UNP Q9H0B6
D	214	ARG	-	expression tag	UNP Q9H0B6
D	215	GLY	-	expression tag	UNP Q9H0B6
D	216	SER	-	expression tag	UNP Q9H0B6
D	328	ASN	SER	engineered mutation	UNP Q9H0B6
F	198	MET	-	expression tag	UNP Q9H0B6
F	199	GLY	-	expression tag	UNP Q9H0B6
F	200	SER	-	expression tag	UNP Q9H0B6
F	201	SER	-	expression tag	UNP Q9H0B6
F	202	HIS	-	expression tag	UNP Q9H0B6
F	203	HIS	-	expression tag	UNP Q9H0B6
F	204	HIS	-	expression tag	UNP Q9H0B6
F	205	HIS	-	expression tag	UNP Q9H0B6
F	206	HIS	-	expression tag	UNP Q9H0B6
F	207	HIS	-	expression tag	UNP Q9H0B6
F	208	SER	-	expression tag	UNP Q9H0B6
F	209	SER	-	expression tag	UNP Q9H0B6
F	210	GLY	-	expression tag	UNP Q9H0B6
F	211	LEU	-	expression tag	UNP Q9H0B6
F	212	VAL	-	expression tag	UNP Q9H0B6
F	213	PRO	-	expression tag	UNP Q9H0B6
F	214	ARG	-	expression tag	UNP Q9H0B6
F	215	GLY	-	expression tag	UNP Q9H0B6
F	216	SER	-	expression tag	UNP Q9H0B6
F	328	ASN	SER	engineered mutation	UNP Q9H0B6
H	198	MET	-	expression tag	UNP Q9H0B6
H	199	GLY	-	expression tag	UNP Q9H0B6
H	200	SER	-	expression tag	UNP Q9H0B6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	201	SER	-	expression tag	UNP Q9H0B6
H	202	HIS	-	expression tag	UNP Q9H0B6
H	203	HIS	-	expression tag	UNP Q9H0B6
H	204	HIS	-	expression tag	UNP Q9H0B6
H	205	HIS	-	expression tag	UNP Q9H0B6
H	206	HIS	-	expression tag	UNP Q9H0B6
H	207	HIS	-	expression tag	UNP Q9H0B6
H	208	SER	-	expression tag	UNP Q9H0B6
H	209	SER	-	expression tag	UNP Q9H0B6
H	210	GLY	-	expression tag	UNP Q9H0B6
H	211	LEU	-	expression tag	UNP Q9H0B6
H	212	VAL	-	expression tag	UNP Q9H0B6
H	213	PRO	-	expression tag	UNP Q9H0B6
H	214	ARG	-	expression tag	UNP Q9H0B6
H	215	GLY	-	expression tag	UNP Q9H0B6
H	216	SER	-	expression tag	UNP Q9H0B6
H	328	ASN	SER	engineered mutation	UNP Q9H0B6

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).
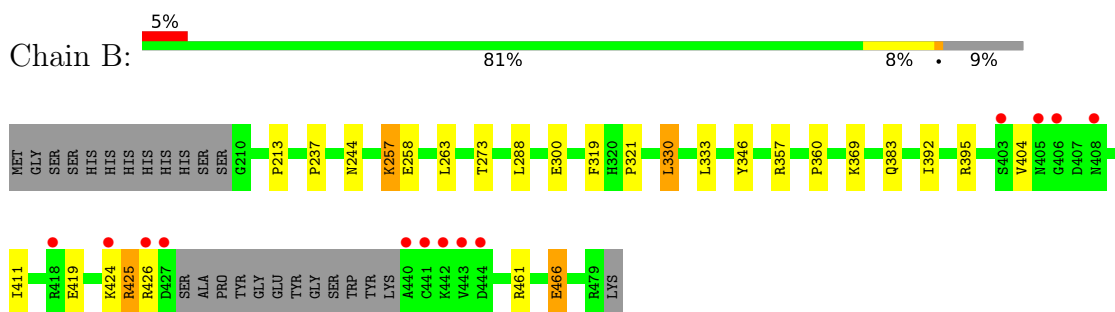
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	X 1	0	0

- Molecule 3 is water.

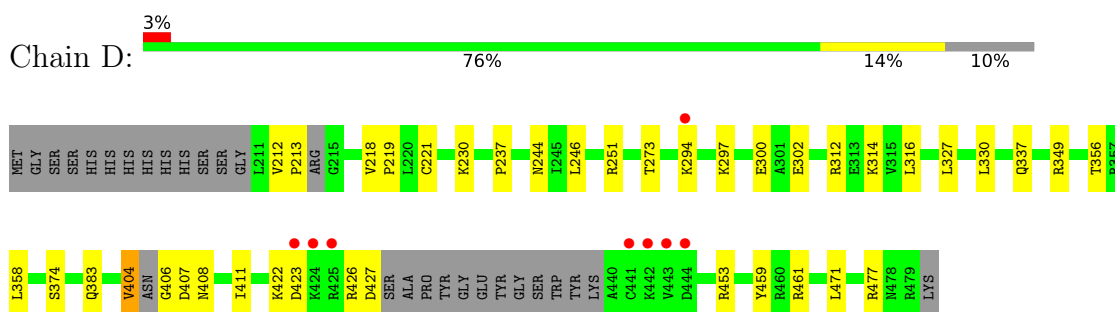| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	O 2	0	0
3	D	13	Total 13	O 13	0	0
3	H	2	Total 2	O 2	0	0

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.
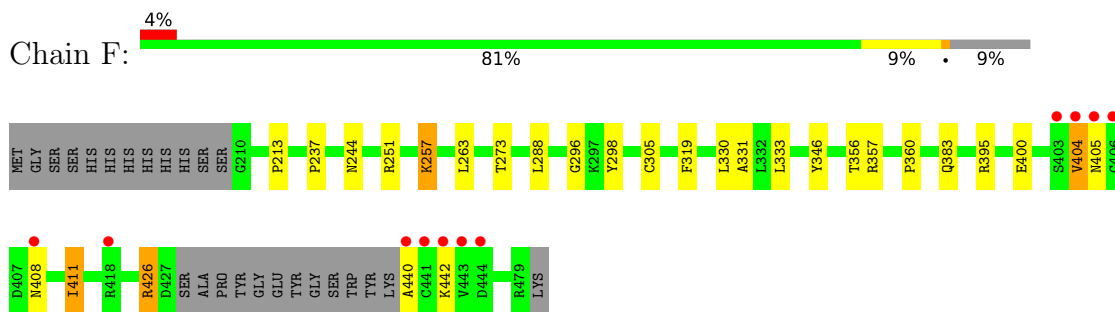
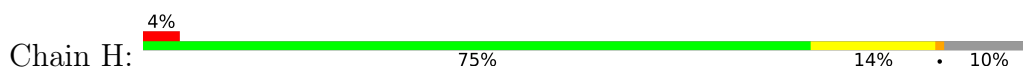• Molecule 1: Kinesin light chain 2
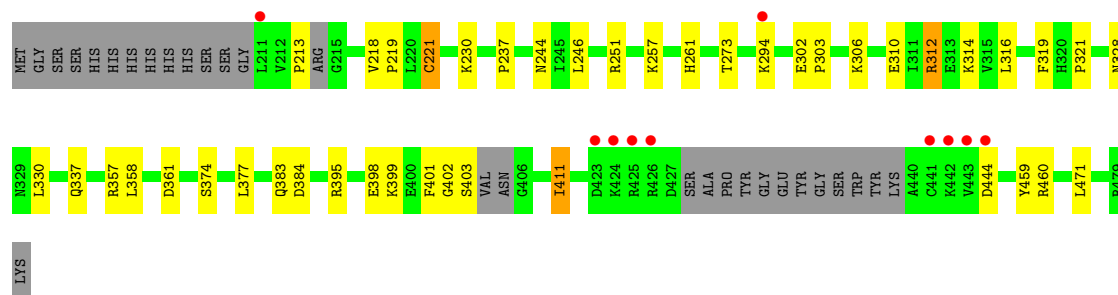
Chain B:

• Molecule 1: Kinesin light chain 2

Chain D:

• Molecule 1: Kinesin light chain 2

Chain F:

• Molecule 1: Kinesin light chain 2

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	101.20Å　101.20Å　115.63Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	25.00　–　2.70 24.72　–　2.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (25.00-2.70) 94.9 (24.72-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230　,　0.267 0.252　,　0.267	Depositor DCC
R_{free} test set	1733 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	51.2	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , -38.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l 0.487 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8095	wwPDB-VP
Average B, all atoms (Å^2)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: UNX

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	B	0.33	0/2061	0.52	1/2776 (0.0%)
1	D	0.34	0/2042	0.50	1/2747 (0.0%)
1	F	0.32	0/2060	0.51	1/2775 (0.0%)
1	H	0.35	0/2034	0.54	1/2736 (0.0%)
All	All	0.34	0/8197	0.52	4/11034 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	213	PRO	N-CA-CB	6.43	111.01	103.30
1	F	213	PRO	N-CA-CB	6.27	110.83	103.30
1	D	213	PRO	N-CA-CB	6.24	110.79	103.30
1	B	213	PRO	N-CA-CB	6.15	110.68	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2030	0	2026	14	0
1	D	2013	0	2013	17	0
1	F	2029	0	2023	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2005	0	2001	23	1
2	D	1	0	0	0	0
3	B	2	0	0	0	0
3	D	13	0	0	1	1
3	H	2	0	0	0	0
All	All	8095	0	8063	64	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 4.

All (64) 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:H:401:PHE:HB2	1:H:402:GLY:HA2	1.37	1.01
1:F:257:LYS:HE2	1:F:257:LYS:H	1.42	0.84
1:H:237:PRO:HD3	1:H:273:THR:HG21	1.78	0.66
1:H:401:PHE:CB	1:H:402:GLY:HA2	2.20	0.64
1:D:427:ASP:HB2	1:D:477:ARG:HH21	1.65	0.62
1:D:404:VAL:HG23	1:D:408:ASN:O	2.00	0.61
1:D:356:THR:O	1:F:404:VAL:HG11	2.01	0.61
1:B:319:PHE:O	1:B:357:ARG:HG3	2.01	0.60
1:F:426:ARG:HH22	1:H:460:ARG:NH1	1.98	0.60
1:B:330:LEU:HD12	1:B:346:TYR:CE1	2.37	0.60
1:F:426:ARG:HH12	1:H:460:ARG:HH22	1.49	0.59
1:F:426:ARG:HH22	1:H:460:ARG:HH12	1.51	0.58
1:H:218:VAL:HB	1:H:219:PRO:HD3	1.87	0.57
1:F:426:ARG:NH2	1:H:460:ARG:HH12	2.04	0.56
1:D:218:VAL:HB	1:D:219:PRO:HD3	1.87	0.56
1:B:237:PRO:HD3	1:B:273:THR:HG21	1.86	0.56
1:F:319:PHE:O	1:F:357:ARG:HG3	2.06	0.56
1:F:263:LEU:HB3	1:F:288:LEU:HD13	1.88	0.55
1:B:257:LYS:HE2	1:B:257:LYS:H	1.73	0.54
1:D:237:PRO:HD3	1:D:273:THR:HG21	1.90	0.53
1:B:424:LYS:N	1:B:425:ARG:HB3	2.23	0.53
1:D:212:VAL:CB	3:D:17:HOH:O	2.56	0.53
1:F:404:VAL:HA	1:F:408:ASN:HB3	1.92	0.52
1:D:404:VAL:HG22	1:F:356:THR:O	2.11	0.51
1:H:401:PHE:HB2	1:H:402:GLY:CA	2.26	0.51
1:B:263:LEU:HB3	1:B:288:LEU:HD13	1.93	0.51
1:D:404:VAL:CG2	1:D:408:ASN:O	2.58	0.51
1:F:237:PRO:HD3	1:F:273:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LYS:HG2	1:B:258:GLU:OE1	2.13	0.49
1:D:356:THR:O	1:F:404:VAL:CG1	2.61	0.49
1:D:459:TYR:HE1	1:D:471:LEU:HD11	1.79	0.48
1:B:360:PRO:HG2	1:B:395:ARG:HH21	1.80	0.46
1:D:312:ARG:HG3	1:D:316:LEU:HD12	1.95	0.46
1:H:395:ARG:O	1:H:399:LYS:N	2.48	0.45
1:F:331:ALA:HB2	1:F:346:TYR:HB2	1.99	0.45
1:B:321:PRO:HD3	1:B:357:ARG:NH1	2.31	0.44
1:H:374:SER:HA	1:H:377:LEU:HD12	1.98	0.44
1:H:459:TYR:HE1	1:H:471:LEU:HD11	1.82	0.44
1:D:302:GLU:OE1	1:D:337:GLN:NE2	2.50	0.44
1:D:406:GLY:HA3	1:D:407:ASP:HA	1.58	0.44
1:F:411:ILE:HG23	1:F:440:ALA:HB1	1.98	0.44
1:H:411:ILE:HD13	1:H:411:ILE:H	1.83	0.43
1:H:319:PHE:O	1:H:357:ARG:HG3	2.18	0.43
1:B:424:LYS:HB2	1:B:425:ARG:HA	2.01	0.43
1:H:302:GLU:HB3	1:H:303:PRO:HD3	2.01	0.43
1:F:305:CYS:HB3	1:F:330:LEU:HD13	2.00	0.43
1:B:426:ARG:HD3	1:D:426:ARG:HH11	1.83	0.43
1:H:302:GLU:OE1	1:H:337:GLN:NE2	2.48	0.43
1:H:302:GLU:HG2	1:H:306:LYS:HE2	2.01	0.43
1:F:360:PRO:HG2	1:F:395:ARG:HH21	1.85	0.42
1:H:221:CYS:HB3	1:H:246:LEU:HD13	2.01	0.42
1:H:312:ARG:HG3	1:H:316:LEU:HD12	2.00	0.42
1:D:218:VAL:HG13	1:D:246:LEU:HD11	2.02	0.42
1:B:369:LYS:HB3	1:B:392:ILE:HD11	2.02	0.42
1:F:296:GLY:HA2	1:F:298:TYR:CZ	2.55	0.41
1:H:398:GLU:HG2	1:H:403:SER:HA	2.01	0.41
1:F:405:ASN:H	1:F:408:ASN:HB3	1.85	0.41
1:B:300:GLU:CD	1:B:300:GLU:H	2.22	0.41
1:B:419:GLU:OE2	1:B:466:GLU:HG2	2.20	0.41
1:D:404:VAL:HG23	1:D:406:GLY:HA2	2.03	0.41
1:H:361:ASP:OD2	1:H:395:ARG:NH2	2.54	0.41
1:H:402:GLY:HA3	1:H:403:SER:HA	1.80	0.41
1:D:327:LEU:HD13	1:D:349:ARG:HB3	2.03	0.40
1:H:321:PRO:HD3	1:H:357:ARG:NH1	2.36	0.40

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:H:261:HIS:NE2	3:D:26:HOH:O[1_445]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	B	254/283 (90%)	245 (96%)	9 (4%)	0	100	100
1	D	247/283 (87%)	237 (96%)	10 (4%)	0	100	100
1	F	254/283 (90%)	245 (96%)	8 (3%)	1 (0%)	34	60
1	H	246/283 (87%)	236 (96%)	10 (4%)	0	100	100
All	All	1001/1132 (88%)	963 (96%)	37 (4%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	442	LYS

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	B	211/236 (89%)	201 (95%)	10 (5%)	26	54
1	D	210/236 (89%)	192 (91%)	18 (9%)	10	24
1	F	210/236 (89%)	201 (96%)	9 (4%)	29	57
1	H	208/236 (88%)	192 (92%)	16 (8%)	13	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	839/944 (89%)	786 (94%)	53 (6%)	18 40

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	244	ASN
1	B	257	LYS
1	B	330	LEU
1	B	333	LEU
1	B	383	GLN
1	B	404	VAL
1	B	411	ILE
1	B	425	ARG
1	B	461	ARG
1	B	466	GLU
1	D	221	CYS
1	D	230	LYS
1	D	244	ASN
1	D	251	ARG
1	D	294	LYS
1	D	297	LYS
1	D	300	GLU
1	D	314	LYS
1	D	330	LEU
1	D	358	LEU
1	D	374	SER
1	D	383	GLN
1	D	404	VAL
1	D	411	ILE
1	D	422	LYS
1	D	423	ASP
1	D	453	ARG
1	D	461	ARG
1	F	244	ASN
1	F	251	ARG
1	F	257	LYS
1	F	333	LEU
1	F	383	GLN
1	F	400	GLU
1	F	404	VAL
1	F	411	ILE
1	F	426	ARG

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Mol	Chain	Res	Type
1	H	221	CYS
1	H	230	LYS
1	H	244	ASN
1	H	251	ARG
1	H	257	LYS
1	H	294	LYS
1	H	310	GLU
1	H	312	ARG
1	H	314	LYS
1	H	328	ASN
1	H	330	LEU
1	H	358	LEU
1	H	383	GLN
1	H	384	ASP
1	H	411	ILE
1	H	444	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	D	326	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is unknown - 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	B	258/283 (91%)	0.56	13 (5%)	28	27	2, 2, 2, 16	1 (0%)
1	D	255/283 (90%)	0.55	8 (3%)	49	49	2, 2, 2, 2	1 (0%)
1	F	258/283 (91%)	0.51	11 (4%)	35	33	2, 2, 2, 16	2 (0%)
1	H	254/283 (89%)	0.53	10 (3%)	39	38	2, 2, 2, 16	0
All	All	1025/1132 (90%)	0.54	42 (4%)	37	36	2, 2, 2, 16	4 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	405	ASN	5.6
1	D	424	LYS	5.3
1	D	423	ASP	5.2
1	B	443	VAL	4.9
1	H	443	VAL	4.8
1	B	403	SER	3.9
1	H	423	ASP	3.9
1	D	443	VAL	3.6
1	H	441	CYS	3.6
1	F	403	SER	3.4
1	H	424	LYS	3.4
1	B	440	ALA	3.4
1	H	426	ARG	3.3
1	F	443	VAL	3.3
1	D	441	CYS	3.2
1	D	294	LYS	3.1
1	F	406	GLY	3.1
1	H	211	LEU	2.9
1	B	418	ARG	2.9
1	B	444	ASP	2.8
1	H	442	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	444	ASP	2.6
1	B	441	CYS	2.6
1	B	406	GLY	2.6
1	H	425	ARG	2.6
1	B	442	LYS	2.6
1	F	405	ASN	2.5
1	D	442	LYS	2.5
1	F	442	LYS	2.5
1	F	408	ASN	2.4
1	H	444	ASP	2.4
1	D	425	ARG	2.4
1	B	408	ASN	2.3
1	F	418	ARG	2.3
1	B	427	ASP	2.3
1	F	441	CYS	2.3
1	B	424	LYS	2.3
1	F	440	ALA	2.2
1	F	444	ASP	2.2
1	B	426	ARG	2.2
1	H	294	LYS	2.1
1	F	404	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	UNX	D	1	1/1	0.14	0.59	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.