



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:45 PM UTC

PDB ID : 5J3X / pdb_00005j3x
Title : Structure of c-CBL Y371F
Authors : Huang, D.T.; Buetow, L.; Dou, H.
Deposited on : 2016-03-31
Resolution : 2.82 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
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

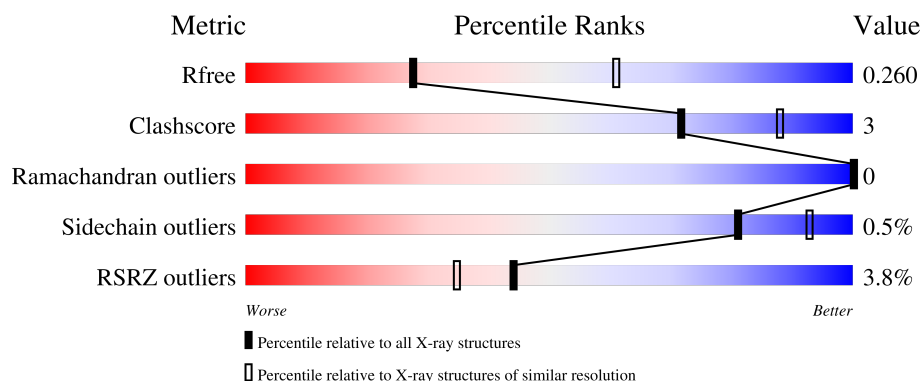
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	391	0% 92% 7%
1	B	391	3% 90% 9%
1	C	391	2% 89% 10%
1	D	391	4% 89% 10%
1	E	391	3% 87% 11%

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Mol	Chain	Length	Quality of chain
1	F	391	9% 90% 8% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18284 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 E3 ubiquitin-protein ligase CBL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3053	1962	513	553	25			
1	B	389	Total	C	N	O	S	0	0	0
			3055	1967	514	549	25			
1	C	389	Total	C	N	O	S	0	0	0
			3067	1975	516	551	25			
1	D	389	Total	C	N	O	S	0	0	0
			3031	1954	511	541	25			
1	E	381	Total	C	N	O	S	0	0	0
			2981	1921	500	535	25			
1	F	384	Total	C	N	O	S	0	0	0
			2985	1921	501	538	25			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLY	-	expression tag	UNP P22681
A	46	SER	-	expression tag	UNP P22681
A	371	PHE	TYR	engineered mutation	UNP P22681
B	45	GLY	-	expression tag	UNP P22681
B	46	SER	-	expression tag	UNP P22681
B	371	PHE	TYR	engineered mutation	UNP P22681
C	45	GLY	-	expression tag	UNP P22681
C	46	SER	-	expression tag	UNP P22681
C	371	PHE	TYR	engineered mutation	UNP P22681
D	45	GLY	-	expression tag	UNP P22681
D	46	SER	-	expression tag	UNP P22681
D	371	PHE	TYR	engineered mutation	UNP P22681
E	45	GLY	-	expression tag	UNP P22681
E	46	SER	-	expression tag	UNP P22681
E	371	PHE	TYR	engineered mutation	UNP P22681
F	45	GLY	-	expression tag	UNP P22681
F	46	SER	-	expression tag	UNP P22681

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Chain	Residue	Modelled	Actual	Comment	Reference
F	371	PHE	TYR	engineered mutation	UNP P22681

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	20	Total 20	O 20	0	0

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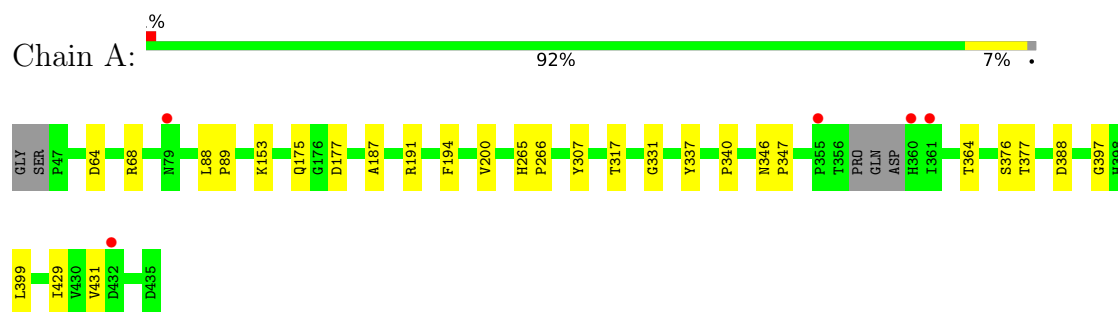
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	7	Total 7	O 7	0	0
4	D	7	Total 7	O 7	0	0
4	E	14	Total 14	O 14	0	0
4	F	16	Total 16	O 16	0	0

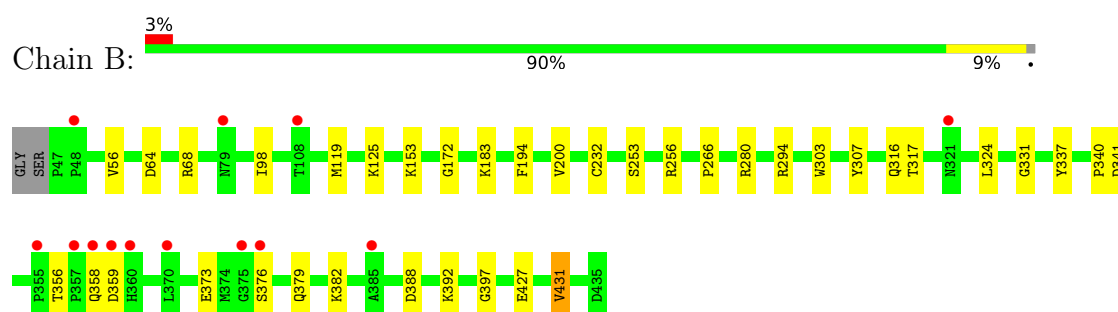
3 Residue-property plots [i](#)

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.

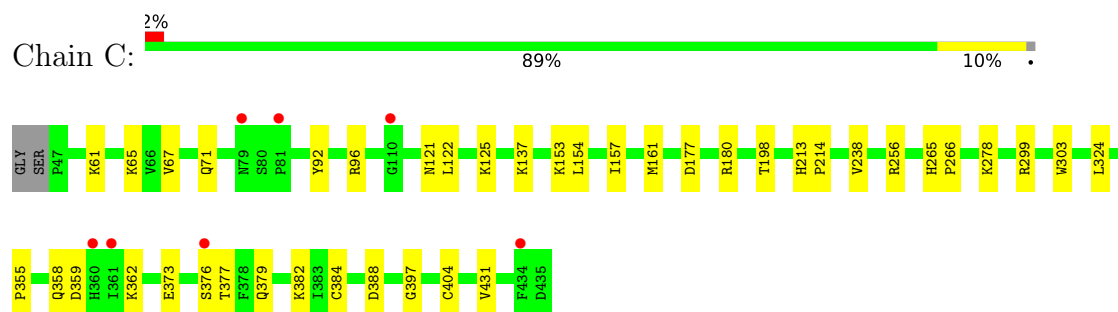
- Molecule 1: E3 ubiquitin-protein ligase CBL



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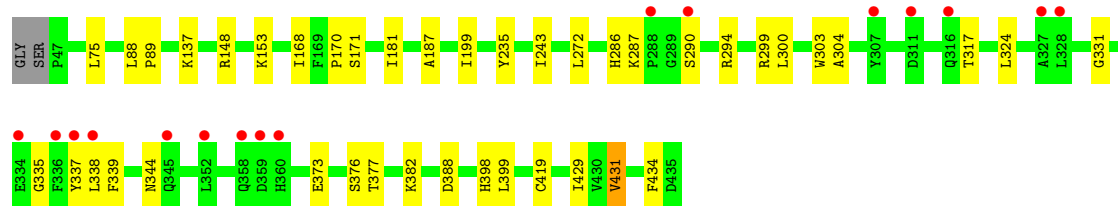


- Molecule 1: E3 ubiquitin-protein ligase CBL

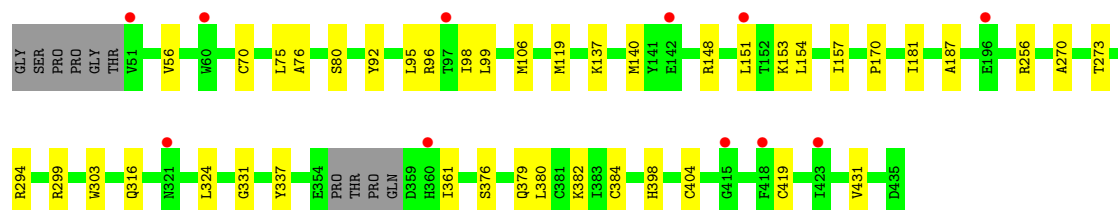
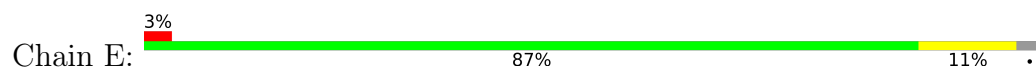


- Molecule 1: E3 ubiquitin-protein ligase CBL

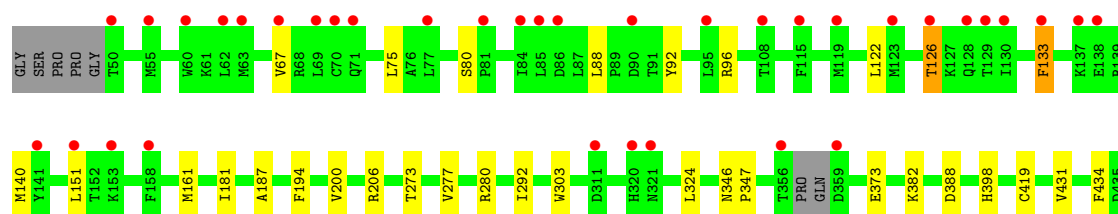
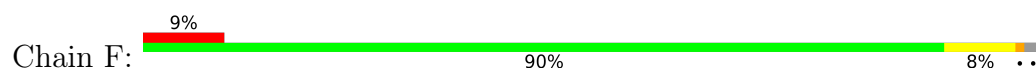




● Molecule 1: E3 ubiquitin-protein ligase CBL



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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	147.84Å 149.04Å 344.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.37 – 2.82 50.37 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.37-2.82) 91.5 (50.37-2.82)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.254 0.221 , 0.260	Depositor DCC
R_{free} test set	4540 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 86.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18284	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: ZN, CA

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	0.26	0/3133	0.67	0/4248
1	B	0.26	0/3136	0.69	2/4254 (0.0%)
1	C	0.26	0/3148	0.67	1/4267 (0.0%)
1	D	0.27	0/3112	0.68	1/4226 (0.0%)
1	E	0.26	0/3057	0.66	2/4146 (0.0%)
1	F	0.27	0/3063	0.67	0/4160
All	All	0.26	0/18649	0.67	6/25301 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	137	LYS	CB-CA-C	-5.80	109.90	116.63
1	B	356	THR	CA-C-N	5.46	126.67	119.84
1	B	356	THR	C-N-CA	5.46	126.67	119.84
1	D	137	LYS	CB-CA-C	-5.42	109.86	117.23
1	C	137	LYS	CB-CA-C	-5.39	109.90	117.23
1	E	270	ALA	CB-CA-C	-5.14	110.67	116.63

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	3053	0	2944	17	0
1	B	3055	0	2948	21	0
1	C	3067	0	2974	23	0
1	D	3031	0	2917	23	0
1	E	2981	0	2859	23	0
1	F	2985	0	2827	17	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	30	0	0	1	0
4	B	20	0	0	0	0
4	C	7	0	0	0	0
4	D	7	0	0	0	0
4	E	14	0	0	0	0
4	F	16	0	0	1	0
All	All	18284	0	17469	118	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 3.

All (118) 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:E:140:MET:HE1	1:E:151:LEU:HD22	1.73	0.69
1:E:256:ARG:HH12	1:E:361:ILE:H	1.41	0.69
1:A:388:ASP:HB2	1:A:431:VAL:HG11	1.81	0.62
1:D:75:LEU:O	1:D:148:ARG:NH2	2.33	0.60
1:E:76:ALA:O	1:E:148:ARG:NH2	2.35	0.59
1:E:95:LEU:HD23	1:E:98:ILE:HD12	1.85	0.58
1:E:99:LEU:HD22	1:E:106:MET:HE1	1.85	0.58
1:F:373:GLU:HA	1:F:382:LYS:HE2	1.85	0.58
1:E:379:GLN:HA	1:E:431:VAL:HG21	1.85	0.57
1:E:181:ILE:HD12	1:E:187:ALA:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ASP:HB3	1:B:431:VAL:HG11	1.87	0.56
1:B:266:PRO:HB2	1:B:340:PRO:HB2	1.87	0.56
1:F:140:MET:HE1	1:F:151:LEU:HD22	1.87	0.56
1:C:379:GLN:HA	1:C:431:VAL:HG21	1.88	0.55
1:C:373:GLU:HA	1:C:382:LYS:HE2	1.88	0.55
1:D:153:LYS:HD2	1:D:376:SER:HB2	1.88	0.55
1:C:388:ASP:HB3	1:C:431:VAL:HG11	1.88	0.54
1:C:121:ASN:OD1	1:C:125:LYS:NZ	2.40	0.54
1:F:92:TYR:CZ	1:F:96:ARG:HD2	2.43	0.54
1:B:397:GLY:O	1:C:299:ARG:NH1	2.35	0.54
1:C:397:GLY:O	1:D:299:ARG:NH1	2.35	0.54
1:D:373:GLU:HA	1:D:382:LYS:HE2	1.89	0.54
1:D:272:LEU:O	1:D:294:ARG:NH2	2.40	0.53
1:F:388:ASP:HB2	1:F:431:VAL:HG11	1.90	0.53
1:F:122:LEU:O	1:F:126:THR:OG1	2.24	0.53
1:F:80:SER:HB2	1:F:273:THR:HG21	1.92	0.52
1:E:398:HIS:HE1	1:E:419:CYS:HB3	1.75	0.52
1:F:67:VAL:HG23	1:F:88:LEU:HD12	1.92	0.52
1:E:384:CYS:HB3	1:E:404:CYS:SG	2.50	0.51
1:D:398:HIS:HE1	1:D:419:CYS:HB3	1.76	0.51
1:E:70:CYS:HA	1:E:75:LEU:HD12	1.92	0.51
1:C:256:ARG:HH22	1:C:355:PRO:HA	1.77	0.50
1:F:75:LEU:HD11	1:F:133:PHE:HZ	1.76	0.50
1:D:331:GLY:HA3	1:D:337:TYR:CD2	2.46	0.49
1:D:294:ARG:HG3	1:D:304:ALA:HB3	1.94	0.49
1:F:277:VAL:HG13	1:F:292:ILE:HD11	1.95	0.49
1:A:399:LEU:HD22	1:A:429:ILE:HD13	1.95	0.49
1:F:303:TRP:CE2	1:F:324:LEU:HD22	2.48	0.48
1:D:287:LYS:NZ	1:D:344:ASN:OD1	2.46	0.48
1:B:253:SER:HB2	1:B:256:ARG:HB3	1.96	0.48
1:B:280:ARG:NH1	1:B:341:ASP:OD2	2.46	0.48
1:B:98:ILE:HG12	1:B:172:GLY:HA2	1.96	0.48
1:D:388:ASP:HB2	1:D:431:VAL:HG11	1.95	0.48
1:E:80:SER:HB2	1:E:273:THR:HG21	1.95	0.47
1:B:358:GLN:HA	1:B:359:ASP:HA	1.60	0.47
1:E:303:TRP:CE2	1:E:324:LEU:HD22	2.49	0.47
1:F:280:ARG:HG2	1:F:292:ILE:HD13	1.97	0.47
1:B:294:ARG:NH2	1:B:316:GLN:OE1	2.40	0.47
1:C:153:LYS:HD2	1:C:376:SER:HB2	1.96	0.47
1:C:384:CYS:HB3	1:C:404:CYS:SG	2.54	0.47
1:E:331:GLY:HA3	1:E:337:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PRO:HB2	1:A:340:PRO:HB2	1.96	0.47
1:D:376:SER:OG	1:D:377:THR:N	2.47	0.47
1:D:317:THR:HG21	1:D:337:TYR:OH	2.15	0.46
1:E:153:LYS:HD2	1:E:376:SER:HB2	1.97	0.46
1:D:181:ILE:HB	1:D:187:ALA:HB2	1.97	0.46
1:A:376:SER:OG	1:A:377:THR:N	2.48	0.46
1:E:56:VAL:HG22	1:E:119:MET:HE2	1.98	0.46
1:A:307:TYR:HE1	1:A:317:THR:HG23	1.81	0.46
1:B:266:PRO:HG3	1:C:180:ARG:HD3	1.97	0.46
1:D:243:ILE:HD13	1:D:300:LEU:HB3	1.96	0.46
1:F:206:ARG:NH1	4:F:601:HOH:O	2.38	0.46
1:B:56:VAL:HG22	1:B:119:MET:HE2	1.99	0.45
1:D:335:GLY:HA2	1:D:338:LEU:HD21	1.98	0.45
1:C:154:LEU:HD23	1:C:157:ILE:HD12	1.99	0.45
1:A:153:LYS:NZ	4:A:603:HOH:O	2.48	0.45
1:A:397:GLY:O	1:E:299:ARG:NH1	2.40	0.45
1:C:92:TYR:CZ	1:C:96:ARG:HD2	2.52	0.45
1:D:290:SER:HA	1:D:339:PHE:HB2	1.99	0.45
1:F:122:LEU:HA	1:F:161:MET:HE1	1.99	0.44
1:A:153:LYS:HD2	1:A:376:SER:HB2	1.99	0.44
1:C:67:VAL:O	1:C:71:GLN:HG2	2.16	0.44
1:C:177:ASP:OD1	1:C:177:ASP:N	2.51	0.44
1:F:181:ILE:HD12	1:F:187:ALA:HA	1.98	0.44
1:C:61:LYS:O	1:C:65:LYS:HG3	2.17	0.44
1:C:122:LEU:HA	1:C:161:MET:HE1	2.00	0.44
1:C:358:GLN:HA	1:C:359:ASP:HA	1.59	0.44
1:E:294:ARG:NH1	1:E:316:GLN:OE1	2.50	0.44
1:B:64:ASP:O	1:B:68:ARG:HG2	2.17	0.44
1:B:331:GLY:HA3	1:B:337:TYR:CD2	2.53	0.44
1:B:303:TRP:CE2	1:B:324:LEU:HD22	2.54	0.43
1:B:379:GLN:HA	1:B:431:VAL:HG21	2.00	0.43
1:A:64:ASP:O	1:A:68:ARG:HG2	2.19	0.43
1:D:303:TRP:CD2	1:D:324:LEU:HD22	2.53	0.43
1:A:364:THR:HG22	1:E:170:PRO:HG3	1.99	0.43
1:F:346:ASN:HA	1:F:347:PRO:HD3	1.88	0.43
1:B:392:LYS:HB3	1:B:427:GLU:HG3	2.01	0.42
1:A:187:ALA:O	1:A:191:ARG:HG2	2.20	0.42
1:B:125:LYS:NZ	1:B:232:CYS:O	2.48	0.42
1:E:154:LEU:HD23	1:E:157:ILE:HD12	2.01	0.42
1:B:307:TYR:HE1	1:B:317:THR:HG23	1.85	0.42
1:B:373:GLU:HA	1:B:382:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:GLN:HE21	1:E:316:GLN:HB3	1.73	0.42
1:D:168:ILE:C	1:D:170:PRO:HD3	2.45	0.42
1:F:194:PHE:CD1	1:F:200:VAL:HG11	2.54	0.42
1:A:346:ASN:HA	1:A:347:PRO:HD3	1.82	0.42
1:E:181:ILE:HB	1:E:187:ALA:HB2	2.01	0.41
1:B:153:LYS:HD2	1:B:376:SER:HB2	2.02	0.41
1:E:92:TYR:CE2	1:E:96:ARG:HD2	2.55	0.41
1:B:183:LYS:HD3	1:B:183:LYS:HA	1.85	0.41
1:D:88:LEU:HB2	1:D:89:PRO:HD3	2.02	0.41
1:A:194:PHE:CD1	1:A:200:VAL:HG11	2.55	0.41
1:D:303:TRP:CE2	1:D:324:LEU:HD22	2.56	0.41
1:B:194:PHE:CD1	1:B:200:VAL:HG11	2.56	0.41
1:C:376:SER:OG	1:C:377:THR:N	2.52	0.41
1:F:398:HIS:HE1	1:F:419:CYS:HB3	1.86	0.41
1:A:88:LEU:HB2	1:A:89:PRO:HD3	2.03	0.41
1:C:213:HIS:HA	1:C:214:PRO:HD3	1.86	0.41
1:C:265:HIS:HA	1:C:266:PRO:HD3	1.87	0.41
1:D:199:ILE:HD11	1:D:235:TYR:HB3	2.02	0.41
1:A:177:ASP:OD1	1:A:177:ASP:N	2.54	0.41
1:A:331:GLY:HA3	1:A:337:TYR:CD2	2.56	0.41
1:C:362:LYS:HG3	1:D:171:SER:HB3	2.02	0.41
1:C:198:THR:O	1:C:238:VAL:HG23	2.20	0.40
1:C:303:TRP:CD2	1:C:324:LEU:HD22	2.56	0.40
1:D:399:LEU:HD22	1:D:429:ILE:HD13	2.03	0.40
1:A:265:HIS:CD2	1:A:347:PRO:HG2	2.57	0.40
1:E:380:LEU:O	1:E:382:LYS:NZ	2.48	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	382/391 (98%)	372 (97%)	10 (3%)	0	100	100
1	B	387/391 (99%)	373 (96%)	14 (4%)	0	100	100
1	C	387/391 (99%)	369 (95%)	18 (5%)	0	100	100
1	D	387/391 (99%)	367 (95%)	20 (5%)	0	100	100
1	E	377/391 (96%)	364 (97%)	13 (3%)	0	100	100
1	F	380/391 (97%)	371 (98%)	9 (2%)	0	100	100
All	All	2300/2346 (98%)	2216 (96%)	84 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	328/351 (93%)	327 (100%)	1 (0%)	86	95
1	B	325/351 (93%)	324 (100%)	1 (0%)	86	95
1	C	328/351 (93%)	327 (100%)	1 (0%)	86	95
1	D	320/351 (91%)	317 (99%)	3 (1%)	70	89
1	E	314/351 (90%)	314 (100%)	0	100	100
1	F	311/351 (89%)	308 (99%)	3 (1%)	68	88
All	All	1926/2106 (92%)	1917 (100%)	9 (0%)	81	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	B	431	VAL
1	C	278	LYS
1	D	286	HIS
1	D	431	VAL
1	D	434	PHE
1	F	126	THR

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Mol	Chain	Res	Type
1	F	133	PHE
1	F	434	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	259	ASN
1	A	365	GLN
1	A	379	GLN
1	B	128	GLN
1	B	146	GLN
1	B	365	GLN
1	C	387	ASN
1	D	360	HIS
1	E	286	HIS
1	F	259	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 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

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(Å ²)	Q<0.9
1	A	386/391 (98%)	0.13	5 (1%) 75 66	55, 82, 127, 184	0
1	B	389/391 (99%)	0.29	13 (3%) 49 39	67, 96, 140, 237	0
1	C	389/391 (99%)	0.36	7 (1%) 67 58	74, 104, 158, 255	0
1	D	389/391 (99%)	0.46	16 (4%) 41 32	66, 104, 156, 214	0
1	E	381/391 (97%)	0.40	11 (2%) 53 43	71, 111, 160, 201	0
1	F	384/391 (98%)	0.66	36 (9%) 14 10	64, 112, 181, 214	0
All	All	2318/2346 (98%)	0.38	88 (3%) 44 35	55, 101, 159, 255	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	130	ILE	6.1
1	F	359	ASP	3.8
1	C	361	ILE	3.6
1	B	357	PRO	3.5
1	F	77	LEU	3.5
1	F	67	VAL	3.5
1	F	119	MET	3.3
1	A	360	HIS	3.3
1	B	360	HIS	3.2
1	F	86	ASP	3.1
1	F	133	PHE	3.0
1	F	85	LEU	3.0
1	E	418	PHE	3.0
1	D	359	ASP	2.9
1	D	328	LEU	2.9
1	F	129	THR	2.9
1	F	141	TYR	2.9
1	E	196	GLU	2.8
1	F	95	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	62	LEU	2.8
1	F	356	THR	2.8
1	F	123	MET	2.8
1	C	434	PHE	2.8
1	D	337	TYR	2.7
1	B	321	ASN	2.7
1	E	142	GLU	2.7
1	B	375	GLY	2.7
1	A	355	PRO	2.6
1	D	352	LEU	2.6
1	F	321	ASN	2.6
1	B	355	PRO	2.6
1	E	321	ASN	2.6
1	E	360	HIS	2.5
1	B	48	PRO	2.5
1	A	79	ASN	2.5
1	A	361	ILE	2.5
1	D	334	GLU	2.5
1	F	81	PRO	2.5
1	F	138	GLU	2.5
1	D	316	GLN	2.5
1	F	70	CYS	2.5
1	B	370	LEU	2.4
1	B	358	GLN	2.4
1	F	108	THR	2.4
1	F	158	PHE	2.4
1	F	126	THR	2.4
1	D	338	LEU	2.4
1	D	336	PHE	2.4
1	B	79	ASN	2.4
1	D	311	ASP	2.4
1	B	385	ALA	2.4
1	F	151	LEU	2.4
1	F	63	MET	2.3
1	F	69	LEU	2.3
1	E	51	VAL	2.3
1	C	360	HIS	2.3
1	D	360	HIS	2.3
1	B	359	ASP	2.3
1	F	50	THR	2.3
1	C	110	GLY	2.3
1	F	128	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	153	LYS	2.3
1	F	84	ILE	2.3
1	D	307	TYR	2.3
1	D	358	GLN	2.2
1	B	376	SER	2.2
1	F	320	HIS	2.2
1	D	288	PRO	2.2
1	D	327	ALA	2.2
1	E	423	ILE	2.2
1	F	90	ASP	2.2
1	C	376	SER	2.2
1	B	108	THR	2.2
1	A	432	ASP	2.1
1	E	415	GLY	2.1
1	F	115	PHE	2.1
1	D	290	SER	2.1
1	C	81	PRO	2.1
1	E	151	LEU	2.1
1	E	60	TRP	2.1
1	F	311	ASP	2.1
1	D	345	GLN	2.1
1	F	71	GLN	2.1
1	C	79	ASN	2.1
1	F	60	TRP	2.1
1	F	137	LYS	2.0
1	E	97	THR	2.0
1	F	55	MET	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(Å ²)	Q<0.9
3	CA	A	503	1/1	0.87	0.12	160,160,160,160	0
2	ZN	E	501	1/1	0.89	0.15	221,221,221,221	0
3	CA	F	503	1/1	0.92	0.07	212,212,212,212	0
3	CA	E	503	1/1	0.93	0.06	177,177,177,177	0
3	CA	B	503	1/1	0.94	0.07	164,164,164,164	0
3	CA	C	503	1/1	0.94	0.06	197,197,197,197	0
3	CA	D	503	1/1	0.94	0.08	155,155,155,155	0
2	ZN	F	502	1/1	0.94	0.21	224,224,224,224	0
2	ZN	C	501	1/1	0.94	0.13	199,199,199,199	0
2	ZN	E	502	1/1	0.95	0.10	151,151,151,151	0
2	ZN	F	501	1/1	0.97	0.06	93,93,93,93	0
2	ZN	C	502	1/1	0.97	0.07	111,111,111,111	0
2	ZN	D	501	1/1	0.98	0.03	84,84,84,84	0
2	ZN	B	502	1/1	0.99	0.05	93,93,93,93	0
2	ZN	D	502	1/1	0.99	0.04	78,78,78,78	0
2	ZN	A	501	1/1	0.99	0.03	82,82,82,82	0
2	ZN	B	501	1/1	0.99	0.02	93,93,93,93	0
2	ZN	A	502	1/1	1.00	0.07	105,105,105,105	0

6.5 Other polymers

There are no such residues in this entry.