



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:00 AM UTC

PDB ID : 3BUW / pdb_00003buw
Title : Crystal structure of c-Cbl-TKB domain complexed with its binding motif in Syk
Authors : Ng, C.; Jackson, R.A.; Buschdorf, J.P.; Sun, Q.; Guy, G.R.; Sivaraman, J.
Deposited on : 2008-01-03
Resolution : 1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

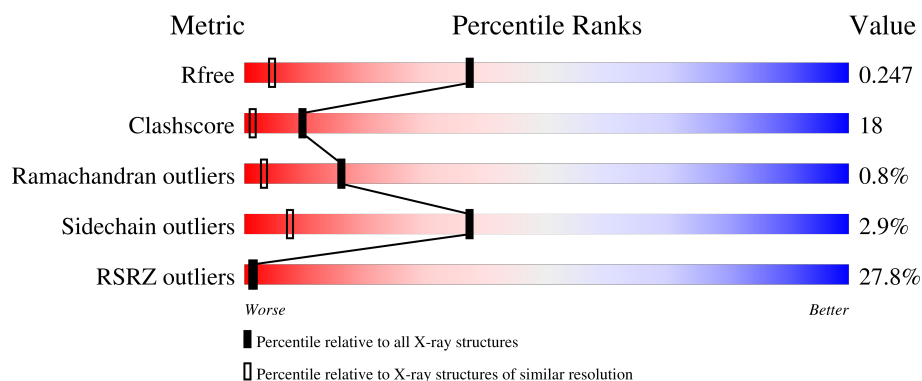
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	13	38% 31% 38% 31%
1	C	13	38% 15% 46% 8% 31%
2	B	329	26% 64% 27% 7%
2	D	329	24% 62% 29% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5731 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 13-meric peptide from Tyrosine-protein kinase SYK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	9	Total	C	N	O	P	0	0	0
			81	51	10	19	1			
1	C	9	Total	C	N	O	P	0	0	0
			81	51	10	19	1			

- Molecule 2 is a protein called E3 ubiquitin-protein ligase CBL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	305	Total	C	N	O	S	0	0	0
			2497	1617	425	442	13			
2	D	305	Total	C	N	O	S	0	0	0
			2497	1617	425	442	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	SER	GLY	cloning artifact	UNP P22681
D	24	SER	GLY	cloning artifact	UNP P22681

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	291	Total	O	0	0
			291	291		
3	C	14	Total	O	0	0
			14	14		
3	D	263	Total	O	0	0
			263	263		

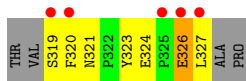
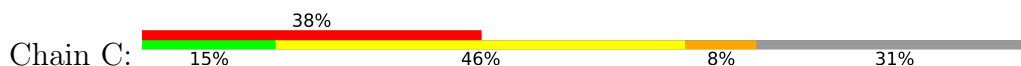
3 Residue-property plots [i](#)

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.

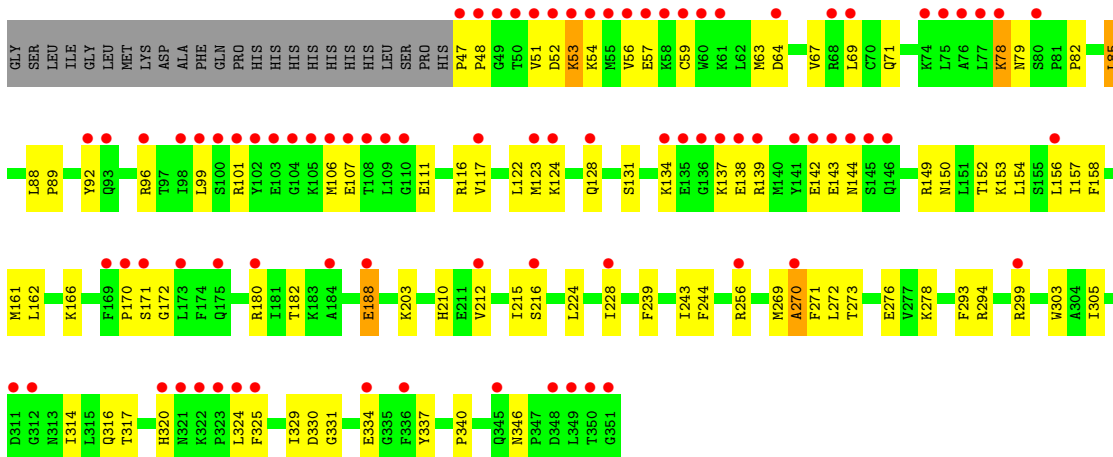
- Molecule 1: 13-meric peptide from Tyrosine-protein kinase SYK



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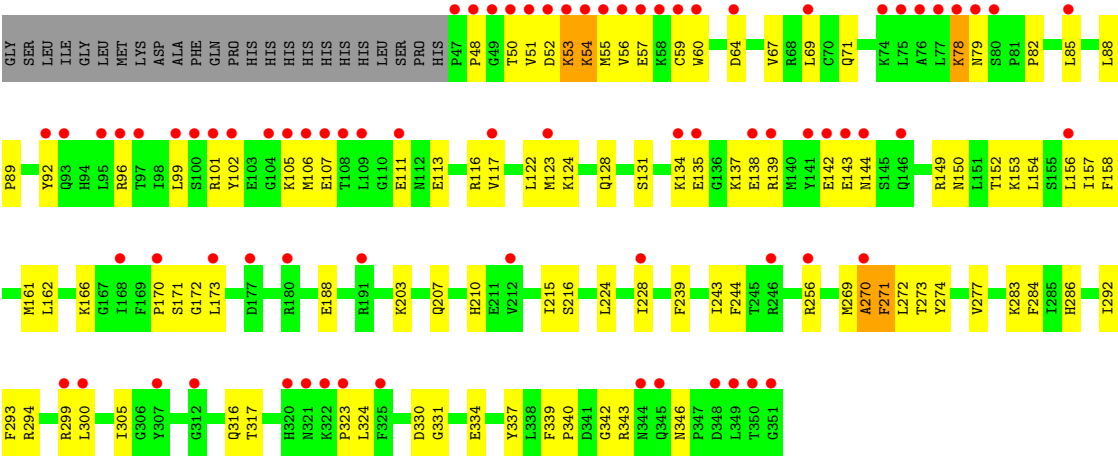


- Molecule 2: E3 ubiquitin-protein ligase CBL



- Molecule 2: E3 ubiquitin-protein ligase CBL





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.79Å 104.81Å 52.78Å 90.00° 89.83° 90.00°	Depositor
Resolution (Å)	20.00 – 1.45 20.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	79.8 (20.00-1.45) 92.4 (20.00-1.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.238 0.233 , 0.247	Depositor DCC
R_{free} test set	2546 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5731	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 43.82 % 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 1.6694e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PTR

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	0.39	0/66	0.92	0/88
1	C	0.42	0/66	0.87	0/88
2	B	0.48	0/2564	0.82	3/3461 (0.1%)
2	D	0.47	0/2564	0.81	2/3461 (0.1%)
All	All	0.47	0/5260	0.82	5/7098 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	216	SER	N-CA-C	6.58	119.45	111.82
2	D	216	SER	N-CA-C	6.43	119.28	111.82
2	B	137	LYS	CB-CA-C	-6.00	109.64	116.54
2	D	137	LYS	CB-CA-C	-6.00	109.64	116.54
2	B	182	THR	N-CA-C	5.39	117.60	111.02

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	81	0	63	3	0
1	C	81	0	63	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2497	0	2506	87	0
2	D	2497	0	2506	91	0
3	A	7	0	0	0	0
3	B	291	0	0	9	0
3	C	14	0	0	3	0
3	D	263	0	0	9	0
All	All	5731	0	5138	183	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 18.

All (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:ILE:HG22	2:B:161:MET:HE2	1.15	1.14
1:C:324:GLU:HB2	2:D:317:THR:HG22	1.32	1.11
2:D:157:ILE:HG22	2:D:161:MET:HE2	1.22	1.09
2:D:158:PHE:HA	2:D:161:MET:HE3	1.32	1.07
1:A:324:GLU:HB2	2:B:317:THR:HG22	1.35	1.06
2:B:158:PHE:HA	2:B:161:MET:HE3	1.31	1.05
2:B:149:ARG:HH12	2:B:153:LYS:HB2	1.28	0.99
2:D:149:ARG:HH12	2:D:153:LYS:HB2	1.28	0.95
2:B:156:LEU:HD11	2:B:273:THR:CG2	2.01	0.91
2:D:156:LEU:HD11	2:D:273:THR:CG2	2.04	0.87
2:B:92:TYR:CZ	2:B:96:ARG:HD2	2.12	0.85
2:B:210:HIS:HD2	2:B:215:ILE:H	1.25	0.84
2:D:150:ASN:O	2:D:154:LEU:HD23	1.80	0.81
2:B:156:LEU:HD11	2:B:273:THR:HG22	1.62	0.81
2:B:228:ILE:HG12	2:B:244:PHE:CD1	2.18	0.79
2:D:228:ILE:HG12	2:D:244:PHE:CD1	2.18	0.79
2:B:149:ARG:NH1	2:B:153:LYS:HB2	1.98	0.79
2:D:92:TYR:CZ	2:D:96:ARG:HD2	2.19	0.78
2:D:149:ARG:NH1	2:D:153:LYS:HB2	1.97	0.78
2:B:150:ASN:O	2:B:154:LEU:HD23	1.84	0.77
2:D:210:HIS:HD2	2:D:215:ILE:H	1.30	0.77
2:D:156:LEU:HD11	2:D:273:THR:HG22	1.66	0.76
2:B:158:PHE:CA	2:B:161:MET:HE3	2.12	0.76
2:B:157:ILE:HG22	2:B:161:MET:CE	2.09	0.76
2:D:82:PRO:HG3	2:D:156:LEU:HD12	1.66	0.75
2:D:124:LYS:O	2:D:128:GLN:HG3	1.85	0.75
2:B:210:HIS:CD2	2:B:215:ILE:H	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:LYS:O	2:B:57:GLU:HG2	1.89	0.72
2:B:269:MET:O	2:B:270:ALA:O	2.08	0.71
2:D:210:HIS:CD2	2:D:215:ILE:H	2.08	0.71
2:B:82:PRO:HG3	2:B:156:LEU:HD12	1.71	0.71
1:C:319:SER:HB2	3:D:650:HOH:O	1.89	0.71
2:B:56:VAL:HG11	2:B:99:LEU:HD11	1.72	0.70
2:D:53:LYS:O	2:D:57:GLU:HG2	1.92	0.70
2:D:157:ILE:HG22	2:D:161:MET:CE	2.13	0.70
2:D:59:CYS:HB2	2:D:123:MET:SD	2.32	0.69
2:D:158:PHE:CA	2:D:161:MET:HE3	2.16	0.68
2:B:293:PHE:HB3	2:B:305:ILE:HD13	1.75	0.68
2:B:92:TYR:OH	2:B:96:ARG:HD2	1.93	0.68
2:D:48:PRO:HG2	2:D:117:VAL:HA	1.75	0.68
2:B:157:ILE:CG2	2:B:161:MET:HE2	2.09	0.68
2:B:124:LYS:O	2:B:128:GLN:HG3	1.95	0.67
2:B:152:THR:O	2:B:156:LEU:HD13	1.95	0.67
2:D:269:MET:O	2:D:270:ALA:O	2.12	0.67
2:D:51:VAL:HG23	2:D:116:ARG:HG2	1.78	0.66
2:D:340:PRO:HD3	2:D:346:ASN:HD22	1.61	0.66
2:D:56:VAL:HG11	2:D:99:LEU:HD11	1.77	0.66
2:B:59:CYS:HB2	2:B:123:MET:SD	2.36	0.65
1:A:324:GLU:HB2	2:B:317:THR:CG2	2.21	0.65
2:B:203:LYS:H	2:B:203:LYS:CE	2.10	0.65
2:D:293:PHE:HB3	2:D:305:ILE:HD13	1.78	0.65
2:D:67:VAL:O	2:D:71:GLN:HG3	1.98	0.64
2:D:152:THR:O	2:D:156:LEU:HD13	1.98	0.63
2:B:293:PHE:CB	2:B:305:ILE:HD13	2.28	0.62
2:B:48:PRO:HG2	2:B:117:VAL:HA	1.80	0.62
2:D:203:LYS:H	2:D:203:LYS:CE	2.12	0.62
2:D:82:PRO:HG3	2:D:156:LEU:CD1	2.30	0.61
2:B:101:ARG:HD2	2:B:172:GLY:C	2.26	0.61
2:B:330:ASP:O	2:B:334:GLU:HG3	2.01	0.61
2:D:157:ILE:CG2	2:D:161:MET:HE2	2.15	0.60
2:B:340:PRO:HD3	2:B:346:ASN:HD22	1.66	0.60
2:D:293:PHE:CB	2:D:305:ILE:HD13	2.30	0.60
2:D:323:PRO:HB2	3:D:691:HOH:O	1.99	0.60
2:D:153:LYS:NZ	3:D:798:HOH:O	2.34	0.60
2:B:59:CYS:SG	2:B:122:LEU:HG	2.41	0.60
1:C:324:GLU:HB2	2:D:317:THR:CG2	2.18	0.59
2:D:92:TYR:OH	2:D:96:ARG:HD2	2.01	0.59
2:D:203:LYS:H	2:D:203:LYS:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:LYS:HD2	2:D:128:GLN:OE1	2.04	0.58
2:B:203:LYS:H	2:B:203:LYS:HE2	1.67	0.58
2:B:320:HIS:HA	3:B:469:HOH:O	2.03	0.58
2:B:124:LYS:HD3	3:B:470:HOH:O	2.04	0.58
2:B:67:VAL:O	2:B:71:GLN:HG3	2.04	0.57
2:B:294:ARG:HH21	2:B:316:GLN:NE2	2.03	0.57
2:D:286:HIS:HE1	3:D:812:HOH:O	1.87	0.56
2:B:203:LYS:H	2:B:203:LYS:CD	2.19	0.56
2:D:203:LYS:H	2:D:203:LYS:CD	2.18	0.55
2:D:330:ASP:O	2:D:334:GLU:HG3	2.06	0.55
2:B:294:ARG:HH21	2:B:316:GLN:HE22	1.54	0.55
2:B:157:ILE:O	2:B:161:MET:HG3	2.06	0.55
2:D:107:GLU:O	2:D:111:GLU:HG3	2.07	0.55
2:D:294:ARG:HH21	2:D:316:GLN:NE2	2.05	0.55
2:D:101:ARG:HD3	2:D:173:LEU:HB2	1.89	0.55
2:B:51:VAL:HG23	2:B:116:ARG:HG2	1.89	0.54
2:D:101:ARG:HD2	2:D:172:GLY:C	2.33	0.54
2:B:79:ASN:C	2:B:79:ASN:HD22	2.15	0.54
2:D:131:SER:HA	2:D:134:LYS:HG2	1.90	0.54
2:B:143:GLU:O	2:B:144:ASN:HB2	2.08	0.54
2:B:107:GLU:O	2:B:111:GLU:HG3	2.08	0.54
1:C:327:LEU:HD11	3:C:574:HOH:O	2.08	0.53
2:D:79:ASN:HD22	2:D:79:ASN:C	2.16	0.53
2:B:188:GLU:HG2	3:B:440:HOH:O	2.09	0.53
2:B:224:LEU:HD11	2:B:228:ILE:HD11	1.91	0.53
2:B:59:CYS:SG	2:B:123:MET:SD	3.06	0.53
2:D:162:LEU:HD11	2:D:166:LYS:HE3	1.91	0.52
2:D:243:ILE:CD1	2:D:300:LEU:HD13	2.39	0.52
2:B:212:VAL:HG11	3:B:598:HOH:O	2.09	0.52
2:D:293:PHE:HB3	2:D:305:ILE:CD1	2.40	0.52
2:B:59:CYS:CB	2:B:123:MET:SD	2.98	0.52
2:B:138:GLU:H	2:B:138:GLU:CD	2.18	0.52
2:B:99:LEU:HD22	2:B:106:MET:HE1	1.92	0.51
2:D:52:ASP:OD2	2:D:54:LYS:HB2	2.11	0.50
2:D:138:GLU:H	2:D:138:GLU:CD	2.20	0.50
2:D:143:GLU:O	2:D:144:ASN:HB2	2.11	0.50
2:B:331:GLY:HA3	2:B:337:TYR:CD2	2.46	0.50
2:D:134:LYS:HD3	3:D:818:HOH:O	2.12	0.50
2:D:99:LEU:HD22	2:D:106:MET:HE1	1.94	0.50
2:D:157:ILE:O	2:D:161:MET:HG3	2.11	0.50
2:B:269:MET:HB3	2:B:272:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:LYS:N	2:D:203:LYS:HD3	2.26	0.49
2:D:224:LEU:HD11	2:D:228:ILE:HD11	1.93	0.49
2:B:239:PHE:CE2	2:B:243:ILE:HD11	2.48	0.49
2:B:78:LYS:NZ	3:B:383:HOH:O	2.45	0.49
2:B:293:PHE:HB3	2:B:305:ILE:CD1	2.41	0.49
2:B:52:ASP:OD2	2:B:54:LYS:HB2	2.12	0.49
2:B:203:LYS:N	2:B:203:LYS:HD3	2.27	0.48
2:D:139:ARG:HA	2:D:142:GLU:OE1	2.13	0.48
2:B:82:PRO:HG3	2:B:156:LEU:CD1	2.41	0.48
2:D:294:ARG:HH21	2:D:316:GLN:HE22	1.60	0.48
2:B:256:ARG:HH11	2:B:256:ARG:HG2	1.79	0.48
2:B:170:PRO:O	2:B:171:SER:HB2	2.14	0.47
2:D:243:ILE:HD11	2:D:300:LEU:HD13	1.96	0.47
2:D:124:LYS:HD3	3:D:700:HOH:O	2.14	0.47
2:D:331:GLY:HA3	2:D:337:TYR:CD2	2.50	0.47
2:B:88:LEU:HB2	2:B:89:PRO:HD3	1.95	0.47
2:B:303:TRP:CE2	2:B:324:LEU:HD22	2.50	0.47
2:D:203:LYS:CD	2:D:203:LYS:N	2.78	0.47
2:D:59:CYS:CB	2:D:123:MET:SD	3.02	0.47
2:D:157:ILE:C	2:D:161:MET:HE2	2.39	0.47
2:D:59:CYS:SG	2:D:122:LEU:HD23	2.55	0.47
2:D:60:TRP:CD1	2:D:92:TYR:HD1	2.33	0.47
2:B:203:LYS:CD	2:B:203:LYS:N	2.79	0.46
2:D:153:LYS:NZ	2:D:271:PHE:CG	2.83	0.46
1:C:326:GLU:HA	3:C:572:HOH:O	2.15	0.46
2:D:59:CYS:SG	2:D:122:LEU:CD2	3.03	0.46
2:D:239:PHE:CE2	2:D:243:ILE:HD11	2.50	0.46
2:D:88:LEU:HB2	2:D:89:PRO:HD3	1.96	0.46
2:D:256:ARG:HG2	2:D:256:ARG:HH11	1.80	0.46
2:B:162:LEU:HD11	2:B:166:LYS:HE3	1.98	0.46
2:B:99:LEU:CD2	2:B:106:MET:HE1	2.46	0.45
2:B:139:ARG:HA	2:B:142:GLU:OE1	2.16	0.45
1:A:319:SER:OG	1:A:320:PHE:N	2.49	0.45
2:B:63:MET:HG2	2:B:88:LEU:HD22	1.98	0.45
1:C:320:PHE:HD2	3:C:193:HOH:O	2.00	0.45
1:C:321:ASN:HB3	2:D:274:TYR:CD2	2.51	0.45
2:D:78:LYS:NZ	3:D:627:HOH:O	2.49	0.44
2:B:278:LYS:HD3	2:B:314:ILE:HB	1.99	0.44
2:B:157:ILE:C	2:B:161:MET:HE2	2.43	0.44
2:D:283:LYS:HE2	2:D:284:PHE:CE2	2.52	0.44
2:B:293:PHE:HB2	2:B:305:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PRO:HB3	3:B:562:HOH:O	2.18	0.43
2:D:170:PRO:O	2:D:171:SER:HB2	2.17	0.43
2:D:270:ALA:O	2:D:272:LEU:N	2.51	0.43
2:B:131:SER:HA	2:B:134:LYS:HG2	2.00	0.43
2:B:270:ALA:O	2:B:272:LEU:N	2.52	0.43
2:B:149:ARG:CZ	3:B:361:HOH:O	2.66	0.42
2:D:203:LYS:H	2:D:203:LYS:HD3	1.81	0.42
2:D:203:LYS:O	2:D:207:GLN:HG3	2.19	0.42
2:B:89:PRO:HG3	3:B:636:HOH:O	2.19	0.42
2:B:124:LYS:HD2	2:B:128:GLN:OE1	2.19	0.42
2:B:153:LYS:HD3	3:B:560:HOH:O	2.18	0.42
2:B:85:LEU:HD12	2:B:85:LEU:HA	1.87	0.42
2:D:343:ARG:HD2	3:D:745:HOH:O	2.20	0.42
2:B:272:LEU:HD22	2:B:276:GLU:HB3	2.02	0.42
2:B:134:LYS:HE3	2:B:134:LYS:HB2	1.89	0.42
2:D:102:TYR:HA	2:D:105:LYS:HE3	2.00	0.42
2:D:284:PHE:CZ	2:D:342:GLY:HA3	2.55	0.41
2:B:101:ARG:HD2	2:B:172:GLY:CA	2.50	0.41
2:B:180:ARG:NH1	2:B:180:ARG:HG2	2.36	0.41
2:D:293:PHE:HB2	2:D:305:ILE:HD13	2.02	0.41
2:D:113:GLU:O	2:D:117:VAL:HG23	2.21	0.41
2:D:134:LYS:HG3	2:D:135:GLU:HG3	2.02	0.41
2:D:339:PHE:HA	2:D:340:PRO:HD2	1.98	0.41
2:B:79:ASN:C	2:B:79:ASN:ND2	2.78	0.41
2:B:143:GLU:OE1	2:B:143:GLU:HA	2.21	0.41
2:B:278:LYS:CD	2:B:314:ILE:HB	2.51	0.41
2:D:149:ARG:CZ	3:D:572:HOH:O	2.69	0.41
2:D:305:ILE:HD11	2:D:324:LEU:HD11	2.02	0.41
2:B:325:PHE:O	2:B:329:ILE:HG13	2.20	0.41
2:D:50:THR:O	2:D:55:MET:HE3	2.22	0.40
2:D:277:VAL:HG13	2:D:292:ILE:HD11	2.02	0.40
2:D:79:ASN:C	2:D:79:ASN:ND2	2.78	0.40
2:D:102:TYR:HA	2:D:105:LYS:CE	2.52	0.40

There are no symmetry-related clashes.

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	A	6/13 (46%)	4 (67%)	2 (33%)	0	100	100
1	C	6/13 (46%)	4 (67%)	2 (33%)	0	100	100
2	B	303/329 (92%)	287 (95%)	14 (5%)	2 (1%)	18	4
2	D	303/329 (92%)	289 (95%)	11 (4%)	3 (1%)	12	2
All	All	618/684 (90%)	584 (94%)	29 (5%)	5 (1%)	16	3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	270	ALA
2	D	270	ALA
2	B	271	PHE
2	D	271	PHE
2	D	54	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	A	8/11 (73%)	7 (88%)	1 (12%)	4	0
1	C	8/11 (73%)	7 (88%)	1 (12%)	4	0
2	B	272/293 (93%)	265 (97%)	7 (3%)	40	10
2	D	272/293 (93%)	265 (97%)	7 (3%)	40	10
All	All	560/608 (92%)	544 (97%)	16 (3%)	37	7

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	GLU
2	B	53	LYS
2	B	64	ASP
2	B	69	LEU
2	B	78	LYS
2	B	85	LEU
2	B	188	GLU
2	B	299	ARG
1	C	326	GLU
2	D	53	LYS
2	D	64	ASP
2	D	69	LEU
2	D	78	LYS
2	D	85	LEU
2	D	188	GLU
2	D	299	ARG

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

Mol	Chain	Res	Type
2	B	79	ASN
2	B	146	GLN
2	B	207	GLN
2	B	210	HIS
2	B	259	ASN
2	B	282	GLN
2	B	313	ASN
2	B	316	GLN
2	B	320	HIS
2	B	321	ASN
2	B	344	ASN
2	B	345	GLN
2	B	346	ASN
2	D	79	ASN
2	D	94	HIS
2	D	146	GLN
2	D	207	GLN
2	D	210	HIS
2	D	259	ASN
2	D	286	HIS
2	D	302	GLN

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Mol	Chain	Res	Type
2	D	316	GLN
2	D	320	HIS
2	D	321	ASN
2	D	326	GLN
2	D	344	ASN
2	D	345	GLN
2	D	346	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
1	PTR	C	323	1	15,16,17	1.57	3 (20%)	17,22,24	1.06	1 (5%)
1	PTR	A	323	1	15,16,17	1.61	2 (13%)	17,22,24	1.09	1 (5%)

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
1	PTR	C	323	1	-	0/10/11/13	0/1/1/1
1	PTR	A	323	1	-	0/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	PTR	P-OH	2.65	1.64	1.59
1	C	323	PTR	P-OH	2.22	1.63	1.59
1	C	323	PTR	CE2-CD2	2.17	1.42	1.38
1	A	323	PTR	CE2-CD2	2.02	1.42	1.38
1	C	323	PTR	CD1-CG	2.02	1.42	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	PTR	CD2-CE2-CZ	-2.50	116.87	119.73
1	C	323	PTR	CD2-CE2-CZ	-2.45	116.93	119.73

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 oligosaccharides 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

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	8/13 (61%)	3.92	5 (62%) 0 0	21, 34, 51, 52	0
1	C	8/13 (61%)	3.92	5 (62%) 0 0	21, 34, 51, 52	0
2	B	305/329 (92%)	1.20	86 (28%) 1 1	9, 18, 48, 57	0
2	D	305/329 (92%)	1.17	78 (25%) 1 1	9, 18, 48, 57	0
All	All	626/684 (91%)	1.26	174 (27%) 1 1	9, 19, 48, 57	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	47	PRO	9.4
1	C	319	SER	8.0
2	B	270	ALA	7.8
1	A	327	LEU	7.7
2	D	350	THR	7.6
2	D	270	ALA	6.9
1	C	320	PHE	6.8
2	B	104	GLY	6.8
2	B	51	VAL	6.7
2	D	47	PRO	6.6
2	B	321	ASN	6.5
2	B	101	ARG	6.5
1	C	327	LEU	6.4
2	B	320	HIS	6.4
2	D	321	ASN	6.3
2	B	141	TYR	6.2
2	B	350	THR	6.1
1	A	320	PHE	5.9
2	D	59	CYS	5.5
2	D	351	GLY	5.2
2	B	117	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
2	D	320	HIS	4.9
2	B	59	CYS	4.9
2	B	50	THR	4.6
1	A	319	SER	4.6
1	A	325	PRO	4.6
2	B	96	ARG	4.4
2	D	51	VAL	4.4
1	A	326	GLU	4.4
2	D	117	VAL	4.4
2	B	56	VAL	4.3
2	B	78	LYS	4.2
2	D	54	LYS	4.2
2	D	106	MET	4.2
2	B	58	LYS	4.1
2	D	104	GLY	4.1
2	B	142	GLU	4.1
2	D	78	LYS	4.1
2	B	351	GLY	4.1
2	B	171	SER	4.1
2	B	175	GLN	4.1
2	B	106	MET	4.0
1	C	325	PRO	4.0
2	B	48	PRO	4.0
2	D	108	THR	4.0
2	D	92	TYR	3.9
2	D	48	PRO	3.8
2	B	349	LEU	3.8
2	B	143	GLU	3.8
2	B	92	TYR	3.7
2	B	105	LYS	3.5
2	B	228	ILE	3.5
2	D	53	LYS	3.5
2	B	57	GLU	3.4
2	D	141	TYR	3.4
2	B	135	GLU	3.4
2	B	61	LYS	3.4
2	D	138	GLU	3.4
2	D	228	ILE	3.3
2	B	138	GLU	3.3
2	B	49	GLY	3.3
2	B	144	ASN	3.3
2	D	56	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	180	ARG	3.3
2	D	142	GLU	3.3
2	B	77	LEU	3.2
2	D	60	TRP	3.2
2	D	143	GLU	3.2
2	D	109	LEU	3.2
2	D	77	LEU	3.1
2	D	256	ARG	3.1
2	D	102	TYR	3.1
2	B	170	PRO	3.1
2	D	50	THR	3.0
2	D	349	LEU	3.0
2	D	312	GLY	3.0
2	D	101	ARG	3.0
2	D	99	LEU	3.0
2	B	60	TRP	3.0
2	D	58	LYS	3.0
2	B	53	LYS	2.9
2	B	173	LEU	2.9
2	B	134	LYS	2.9
2	D	134	LYS	2.9
2	D	322	LYS	2.9
2	B	256	ARG	2.9
2	D	135	GLU	2.9
2	B	146	GLN	2.9
2	B	107	GLU	2.8
2	D	146	GLN	2.8
2	D	180	ARG	2.8
2	D	74	LYS	2.8
2	D	139	ARG	2.8
2	B	52	ASP	2.8
2	D	123	MET	2.8
2	B	80	SER	2.7
2	B	311	ASP	2.7
2	D	49	GLY	2.7
2	D	348	ASP	2.7
1	C	326	GLU	2.7
2	D	156	LEU	2.7
2	B	55	MET	2.7
2	B	108	THR	2.6
2	D	80	SER	2.6
2	D	100	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	325	PHE	2.6
2	D	345	GLN	2.6
2	D	105	LYS	2.6
2	B	98	ILE	2.6
2	D	55	MET	2.6
2	D	75	LEU	2.6
2	B	334	GLU	2.6
2	B	102	TYR	2.5
2	D	57	GLU	2.5
2	B	322	LYS	2.5
2	B	123	MET	2.5
2	B	69	LEU	2.5
2	B	54	LYS	2.5
2	D	79	ASN	2.5
2	D	212	VAL	2.5
2	B	312	GLY	2.4
2	B	93	GLN	2.4
2	B	139	ARG	2.4
2	B	75	LEU	2.4
2	B	100	SER	2.4
2	B	216	SER	2.4
2	B	324	LEU	2.4
2	D	93	GLN	2.4
2	B	128	GLN	2.4
2	B	74	LYS	2.4
2	D	85	LEU	2.4
2	B	103	GLU	2.4
2	D	191	ARG	2.3
2	B	99	LEU	2.3
2	D	307	TYR	2.3
2	B	64	ASP	2.3
2	B	184	ALA	2.3
2	D	52	ASP	2.3
2	D	95	LEU	2.3
2	B	136	GLY	2.2
2	D	111	GLU	2.2
2	B	145	SER	2.2
2	D	168	ILE	2.2
2	D	64	ASP	2.2
2	D	177	ASP	2.2
2	D	246	ARG	2.2
2	B	110	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	299	ARG	2.2
2	D	144	ASN	2.2
2	D	170	PRO	2.2
2	B	336	PHE	2.2
2	D	325	PHE	2.2
2	D	107	GLU	2.2
2	B	323	PRO	2.1
2	D	76	ALA	2.1
2	D	96	ARG	2.1
2	B	348	ASP	2.1
2	B	68	ARG	2.1
2	B	156	LEU	2.1
2	B	345	GLN	2.1
2	B	137	LYS	2.1
2	B	212	VAL	2.1
2	D	323	PRO	2.1
2	D	97	THR	2.1
2	B	188	GLU	2.1
2	B	124	LYS	2.0
2	B	169	PHE	2.0
2	D	299	ARG	2.0
2	D	69	LEU	2.0
2	D	344	ASN	2.0
2	B	76	ALA	2.0
2	B	109	LEU	2.0
2	D	173	LEU	2.0
2	D	300	LEU	2.0

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
1	PTR	A	323	16/17	0.97	0.07	12,16,26,26	0
1	PTR	C	323	16/17	0.97	0.07	12,16,26,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.