



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:35 PM UTC

PDB ID : 3BUX / pdb_00003bux
Title : Crystal structure of c-Cbl-TKB domain complexed with its binding motif in c-Met
Authors : Ng, C.; Jackson, R.A.; Buschdorf, J.P.; Sun, Q.; Guy, G.R.; Sivaraman, J.
Deposited on : 2008-01-03
Resolution : 1.35 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

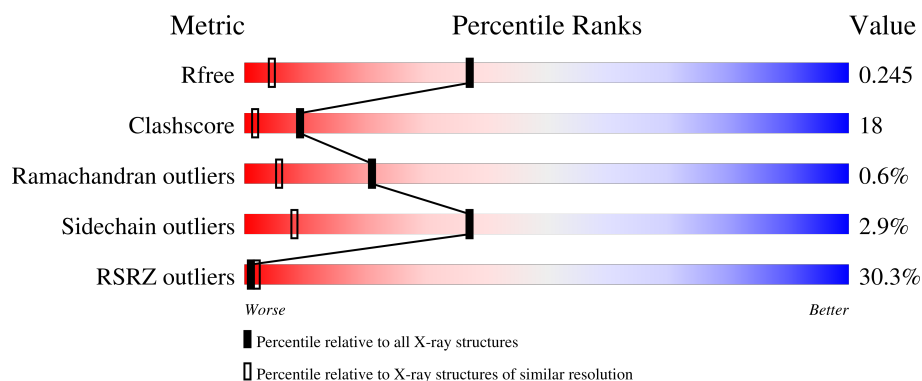
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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% 31% 38%
1	C	13	38% 31% 31% 38%
2	B	329	26% 63% 29% 7%
2	D	329	29% 62% 29% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5820 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 Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	8	Total	C	N	O	P	0	0	0
			70	39	12	18	1			
1	C	8	Total	C	N	O	P	0	0	0
			70	39	12	18	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	9	Total	O	0	0
			9	9		
3	B	317	Total	O	0	0
			317	317		
3	C	13	Total	O	0	0
			13	13		
3	D	347	Total	O	0	0
			347	347		

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.

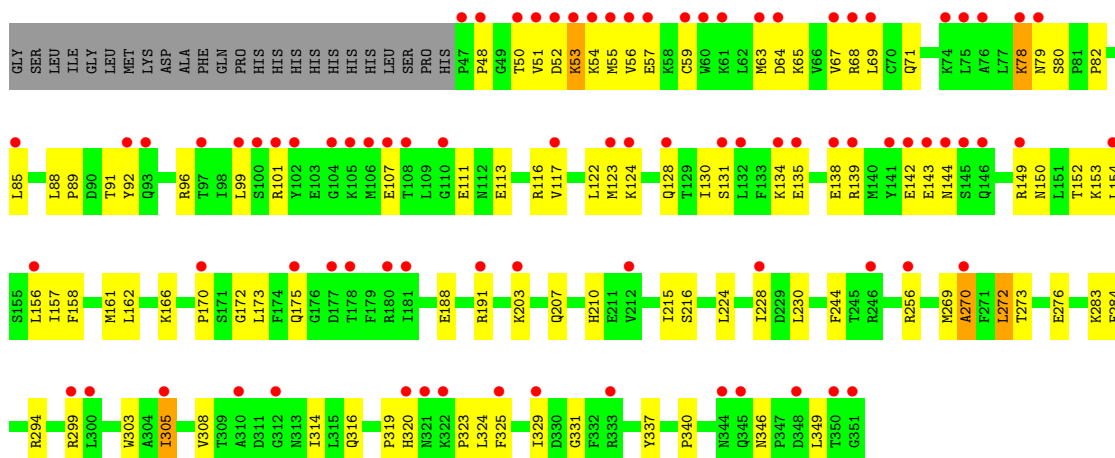
- Molecule 1: 13-meric peptide from Hepatocyte growth factor receptor



- Molecule 1: 13-meric peptide from Hepatocyte growth factor receptor

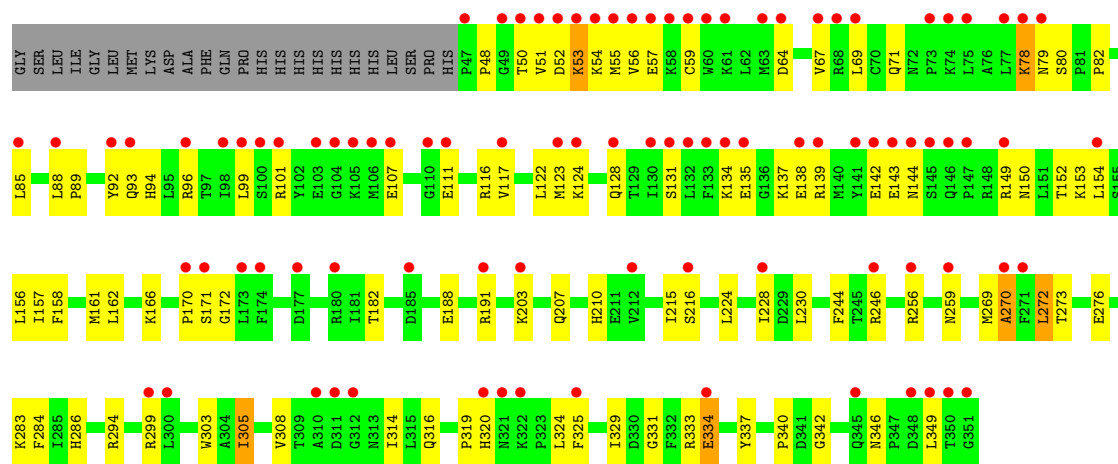


- Molecule 2: E3 ubiquitin-protein ligase CBL



- 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	63.17Å 104.80Å 52.60Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	20.00 – 1.35 20.00 – 1.35	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-1.35) 94.9 (20.00-1.35)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.35Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.240 0.230 , 0.245	Depositor DCC
R_{free} test set	2408 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5820	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 40.95 % 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 2.5369e-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	0.44	0/52	0.84	0/67
1	C	0.41	0/52	0.87	0/67
2	B	0.47	0/2564	0.79	1/3461 (0.0%)
2	D	0.49	2/2564 (0.1%)	0.82	3/3461 (0.1%)
All	All	0.48	2/5232 (0.0%)	0.80	4/7056 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	333	ARG	C-N	-5.68	1.26	1.34
2	D	334	GLU	C-N	-5.51	1.25	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	216	SER	N-CA-C	6.80	119.71	111.82
2	B	216	SER	N-CA-C	5.95	119.73	112.23
2	D	137	LYS	CB-CA-C	-5.95	109.70	116.54
2	D	182	THR	N-CA-C	5.51	116.97	110.97

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	70	0	54	3	0
1	C	70	0	54	3	0
2	B	2497	0	2506	93	0
2	D	2497	0	2506	92	0
3	A	9	0	0	0	0
3	B	317	0	0	12	0
3	C	13	0	0	0	0
3	D	347	0	0	13	0
All	All	5820	0	5120	187	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 (187) 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:158:PHE:HA	2:B:161:MET:HE3	1.30	1.13
2:B:157:ILE:HG22	2:B:161:MET:HE2	1.12	1.11
2:D:158:PHE:HA	2:D:161:MET:HE3	1.32	1.11
2:D:157:ILE:HG22	2:D:161:MET:HE2	1.09	1.05
1:C:998:ASN:HD21	2:D:320:HIS:HB2	1.33	0.94
2:B:156:LEU:HD11	2:B:273:THR:CG2	2.03	0.88
1:A:998:ASN:HD21	2:B:320:HIS:HB2	1.38	0.87
2:D:82:PRO:HG3	2:D:156:LEU:HD12	1.55	0.86
2:D:210:HIS:HD2	2:D:215:ILE:H	1.27	0.82
2:D:156:LEU:HD11	2:D:273:THR:CG2	2.10	0.82
2:D:158:PHE:CA	2:D:161:MET:HE3	2.09	0.81
2:D:157:ILE:HG22	2:D:161:MET:CE	2.04	0.81
2:B:158:PHE:CA	2:B:161:MET:HE3	2.09	0.80
2:D:157:ILE:CG2	2:D:161:MET:HE2	2.04	0.80
2:D:149:ARG:HH12	2:D:153:LYS:HB2	1.47	0.78
2:D:124:LYS:O	2:D:128:GLN:HG3	1.84	0.77
2:B:149:ARG:HH12	2:B:153:LYS:HB2	1.48	0.77
2:D:334:GLU:HG2	3:D:693:HOH:O	1.84	0.77
2:B:157:ILE:HG22	2:B:161:MET:CE	2.05	0.77
2:D:53:LYS:O	2:D:57:GLU:HG2	1.85	0.77
2:B:124:LYS:O	2:B:128:GLN:HG3	1.84	0.76
2:B:53:LYS:O	2:B:57:GLU:HG2	1.87	0.74
2:D:92:TYR:CZ	2:D:96:ARG:HD2	2.22	0.74
2:B:157:ILE:CG2	2:B:161:MET:HE2	2.06	0.72
2:B:82:PRO:HG3	2:B:156:LEU:HD12	1.71	0.72
2:D:156:LEU:HD11	2:D:273:THR:HG22	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:305:ILE:HD12	2:D:305:ILE:N	2.06	0.71
2:B:150:ASN:O	2:B:154:LEU:HD23	1.91	0.70
2:B:63:MET:SD	3:B:418:HOH:O	2.47	0.70
2:D:210:HIS:CD2	2:D:215:ILE:H	2.07	0.70
2:B:156:LEU:HD11	2:B:273:THR:HG22	1.71	0.69
2:D:152:THR:O	2:D:156:LEU:HD13	1.93	0.69
2:D:150:ASN:O	2:D:154:LEU:HD23	1.91	0.69
2:B:59:CYS:SG	2:B:122:LEU:HG	2.34	0.68
2:D:308:VAL:HG22	2:D:314:ILE:CD1	2.23	0.67
2:B:92:TYR:N	3:B:418:HOH:O	2.27	0.67
2:B:149:ARG:NH1	2:B:153:LYS:HB2	2.08	0.67
2:B:92:TYR:CZ	2:B:96:ARG:HD2	2.30	0.67
2:D:124:LYS:HD2	2:D:128:GLN:OE1	1.93	0.67
2:B:308:VAL:HG22	2:B:314:ILE:CD1	2.25	0.66
2:B:56:VAL:HG11	2:B:99:LEU:HD11	1.78	0.65
2:B:210:HIS:CD2	2:B:215:ILE:H	2.14	0.65
2:D:149:ARG:NH1	2:D:153:LYS:HB2	2.12	0.65
2:D:59:CYS:SG	2:D:122:LEU:HG	2.36	0.65
2:B:67:VAL:O	2:B:71:GLN:HG3	1.97	0.64
2:D:294:ARG:HH21	2:D:316:GLN:NE2	1.95	0.64
2:B:152:THR:O	2:B:156:LEU:HD13	1.97	0.64
2:B:228:ILE:HG12	2:B:244:PHE:CD1	2.33	0.64
2:B:305:ILE:N	2:B:305:ILE:HD12	2.12	0.63
2:B:48:PRO:HG2	2:B:117:VAL:HA	1.81	0.63
2:D:82:PRO:HG3	2:D:156:LEU:CD1	2.28	0.63
2:B:101:ARG:HD3	2:B:173:LEU:HB2	1.79	0.63
2:B:124:LYS:HD2	2:B:128:GLN:OE1	1.98	0.63
2:B:210:HIS:HD2	2:B:215:ILE:H	1.44	0.62
1:C:998:ASN:ND2	2:D:320:HIS:HB2	2.10	0.62
2:D:139:ARG:HA	2:D:142:GLU:OE1	1.99	0.62
2:B:203:LYS:H	2:B:203:LYS:CE	2.12	0.62
2:B:50:THR:HA	2:B:116:ARG:HD3	1.80	0.62
2:D:67:VAL:O	2:D:71:GLN:HG3	2.01	0.61
2:D:48:PRO:HG2	2:D:117:VAL:HA	1.83	0.61
2:D:203:LYS:H	2:D:203:LYS:CE	2.14	0.61
1:A:998:ASN:ND2	2:B:320:HIS:HB2	2.13	0.61
2:B:203:LYS:H	2:B:203:LYS:HE2	1.65	0.61
2:D:224:LEU:HD11	2:D:228:ILE:HD11	1.83	0.61
2:B:230:LEU:HD13	3:B:615:HOH:O	2.00	0.61
2:B:294:ARG:HH21	2:B:316:GLN:NE2	1.99	0.61
2:D:78:LYS:HD3	2:D:80:SER:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:ASP:HB2	3:D:389:HOH:O	2.01	0.60
2:D:92:TYR:OH	2:D:96:ARG:HD2	2.01	0.60
2:D:56:VAL:HG11	2:D:99:LEU:HD11	1.82	0.60
2:D:230:LEU:HD13	3:D:387:HOH:O	2.03	0.59
2:D:269:MET:O	2:D:270:ALA:O	2.21	0.58
2:B:138:GLU:H	2:B:138:GLU:CD	2.11	0.58
2:D:203:LYS:H	2:D:203:LYS:HE2	1.68	0.58
2:B:59:CYS:HB2	2:B:123:MET:SD	2.44	0.58
2:B:139:ARG:HA	2:B:142:GLU:OE1	2.04	0.57
2:B:308:VAL:HG22	2:B:314:ILE:HD11	1.85	0.57
2:B:79:ASN:C	2:B:79:ASN:HD22	2.12	0.57
2:B:124:LYS:HD3	3:B:530:HOH:O	2.04	0.57
2:D:286:HIS:HE1	3:D:442:HOH:O	1.87	0.57
2:D:50:THR:HA	2:D:116:ARG:HD3	1.85	0.57
2:D:203:LYS:H	2:D:203:LYS:CD	2.18	0.56
2:B:331:GLY:HA3	2:B:337:TYR:CD2	2.40	0.56
2:D:59:CYS:HB2	2:D:123:MET:SD	2.45	0.56
2:D:79:ASN:HD22	2:D:79:ASN:C	2.12	0.56
2:B:203:LYS:H	2:B:203:LYS:CD	2.18	0.56
2:B:340:PRO:HD3	2:B:346:ASN:HD22	1.71	0.56
2:D:308:VAL:HG22	2:D:314:ILE:HD11	1.88	0.56
2:B:224:LEU:HD11	2:B:228:ILE:HD11	1.88	0.55
2:D:131:SER:HA	2:D:134:LYS:HG2	1.89	0.55
2:D:228:ILE:HG12	2:D:244:PHE:CD1	2.42	0.55
2:B:305:ILE:HD13	2:B:319:PRO:HD3	1.89	0.55
2:D:224:LEU:CD1	2:D:228:ILE:HD11	2.36	0.54
2:D:138:GLU:H	2:D:138:GLU:CD	2.16	0.54
2:B:256:ARG:HG3	3:B:591:HOH:O	2.08	0.54
2:D:157:ILE:O	2:D:161:MET:HG3	2.07	0.54
2:B:283:LYS:HE2	2:B:284:PHE:CE2	2.44	0.53
2:B:92:TYR:OH	2:B:96:ARG:HD2	2.09	0.53
2:B:269:MET:O	2:B:270:ALA:O	2.27	0.53
2:D:52:ASP:OD2	2:D:54:LYS:HB2	2.08	0.52
2:D:331:GLY:HA3	2:D:337:TYR:CD2	2.44	0.52
2:D:64:ASP:HB2	3:D:503:HOH:O	2.10	0.52
2:B:78:LYS:HD3	2:B:80:SER:HB3	1.91	0.52
2:B:64:ASP:HB2	3:B:407:HOH:O	2.08	0.52
2:B:131:SER:HA	2:B:134:LYS:HG2	1.92	0.52
2:B:157:ILE:O	2:B:161:MET:HG3	2.10	0.51
2:D:124:LYS:HZ3	2:D:128:GLN:HG2	1.75	0.51
2:B:52:ASP:OD2	2:B:54:LYS:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:GLU:O	2:D:144:ASN:HB2	2.11	0.51
2:B:143:GLU:O	2:B:144:ASN:HB2	2.12	0.50
2:D:162:LEU:HD11	2:D:166:LYS:HE3	1.92	0.50
2:D:340:PRO:HD3	2:D:346:ASN:HD22	1.75	0.50
2:D:305:ILE:HD13	2:D:319:PRO:HD3	1.93	0.50
2:B:65:LYS:HD3	2:B:130:ILE:HD13	1.93	0.50
2:B:256:ARG:HH11	2:B:256:ARG:HG2	1.76	0.50
2:B:323:PRO:HB2	3:B:481:HOH:O	2.11	0.50
2:B:203:LYS:N	2:B:203:LYS:HD3	2.27	0.49
2:D:88:LEU:HB2	2:D:89:PRO:HD3	1.93	0.49
2:B:162:LEU:HD11	2:B:166:LYS:HE3	1.94	0.49
2:B:88:LEU:HB2	2:B:89:PRO:HD3	1.93	0.49
2:D:134:LYS:HD3	3:D:474:HOH:O	2.13	0.49
2:D:50:THR:HA	2:D:116:ARG:CD	2.43	0.48
2:B:91:THR:HB	3:B:418:HOH:O	2.12	0.48
2:D:101:ARG:HD2	2:D:172:GLY:HA3	1.96	0.48
2:D:149:ARG:CZ	3:D:422:HOH:O	2.60	0.48
2:B:50:THR:HA	2:B:116:ARG:CD	2.42	0.48
2:B:82:PRO:HG3	2:B:156:LEU:CD1	2.42	0.48
2:D:203:LYS:N	2:D:203:LYS:HD3	2.28	0.48
2:D:101:ARG:HD2	2:D:172:GLY:C	2.39	0.47
2:B:101:ARG:HD2	2:B:172:GLY:C	2.39	0.47
2:B:59:CYS:SG	2:B:122:LEU:CD2	3.02	0.47
2:B:325:PHE:HE1	2:B:349:LEU:HD22	1.79	0.47
2:D:256:ARG:HG2	2:D:256:ARG:HH11	1.79	0.47
2:D:303:TRP:CE2	2:D:324:LEU:HD22	2.50	0.47
2:B:149:ARG:CZ	3:B:386:HOH:O	2.62	0.47
2:D:191:ARG:HB2	2:D:191:ARG:NH1	2.30	0.47
2:D:228:ILE:O	2:D:230:LEU:HD13	2.14	0.47
2:D:259:ASN:HB2	3:D:440:HOH:O	2.14	0.46
2:D:283:LYS:HE2	2:D:284:PHE:CE2	2.50	0.46
2:B:78:LYS:HG2	3:B:628:HOH:O	2.15	0.46
2:D:203:LYS:CD	2:D:203:LYS:N	2.79	0.46
2:D:294:ARG:HH21	2:D:316:GLN:HE22	1.62	0.46
2:B:51:VAL:HG22	2:B:55:MET:SD	2.56	0.45
2:B:294:ARG:HH21	2:B:316:GLN:HE22	1.63	0.45
2:B:59:CYS:SG	2:B:122:LEU:CG	3.04	0.45
2:B:157:ILE:C	2:B:161:MET:HE2	2.42	0.45
2:B:303:TRP:CE2	2:B:324:LEU:HD22	2.52	0.45
2:B:203:LYS:CD	2:B:203:LYS:N	2.78	0.44
2:D:230:LEU:HD12	2:D:230:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:ASN:O	1:A:1000:SER:N	2.51	0.44
2:B:224:LEU:CD1	2:B:228:ILE:HD11	2.47	0.43
2:D:284:PHE:CZ	2:D:342:GLY:HA3	2.54	0.43
2:B:131:SER:O	2:B:134:LYS:HG2	2.18	0.43
2:D:170:PRO:O	2:D:171:SER:HB2	2.18	0.43
2:D:203:LYS:O	2:D:207:GLN:HG3	2.18	0.43
2:D:107:GLU:O	2:D:111:GLU:HG3	2.19	0.43
2:D:272:LEU:HD22	2:D:276:GLU:HB3	2.00	0.43
2:B:305:ILE:N	2:B:305:ILE:CD1	2.81	0.43
2:B:203:LYS:HG3	3:B:644:HOH:O	2.19	0.43
2:B:272:LEU:HD22	2:B:276:GLU:CB	2.49	0.43
2:D:51:VAL:HG22	2:D:55:MET:SD	2.59	0.42
2:B:64:ASP:OD1	2:B:68:ARG:NH2	2.50	0.42
2:B:188:GLU:HG2	3:B:495:HOH:O	2.19	0.42
2:B:203:LYS:H	2:B:203:LYS:HD3	1.80	0.42
2:D:188:GLU:HG2	3:D:644:HOH:O	2.19	0.42
1:C:998:ASN:O	1:C:1000:SER:N	2.53	0.42
2:D:101:ARG:HD2	2:D:172:GLY:CA	2.49	0.42
2:B:228:ILE:O	2:B:230:LEU:HD13	2.19	0.42
2:D:272:LEU:HD22	2:D:276:GLU:CB	2.49	0.42
2:B:191:ARG:HB2	2:B:191:ARG:NH1	2.34	0.42
2:B:170:PRO:HG2	2:B:175:GLN:HG3	2.03	0.41
2:D:305:ILE:N	2:D:305:ILE:CD1	2.75	0.41
2:D:94:HIS:HD2	3:D:535:HOH:O	2.03	0.41
2:B:230:LEU:HD12	2:B:230:LEU:N	2.36	0.41
2:D:246:ARG:HD3	3:D:487:HOH:O	2.20	0.41
2:D:154:LEU:CD2	3:D:492:HOH:O	2.68	0.41
2:D:203:LYS:H	2:D:203:LYS:HD3	1.81	0.41
2:D:93:GLN:HG2	3:D:586:HOH:O	2.21	0.41
2:D:305:ILE:CD1	2:D:319:PRO:HD3	2.51	0.41
2:D:325:PHE:O	2:D:329:ILE:HG13	2.21	0.41
2:D:158:PHE:N	2:D:161:MET:HE3	2.37	0.40
2:D:325:PHE:HE1	2:D:349:LEU:HD22	1.86	0.40
2:B:113:GLU:O	2:B:117:VAL:HG23	2.21	0.40
2:B:325:PHE:O	2:B:329:ILE:HG13	2.21	0.40
2:B:203:LYS:O	2:B:207:GLN:HG3	2.21	0.40
2:B:107:GLU:O	2:B:111:GLU:HG3	2.22	0.40
2:B:305:ILE:CD1	2:B:319:PRO:HD3	2.51	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	5/13 (38%)	4 (80%)	0	1 (20%)	0	0
1	C	5/13 (38%)	4 (80%)	0	1 (20%)	0	0
2	B	303/329 (92%)	294 (97%)	8 (3%)	1 (0%)	36	16
2	D	303/329 (92%)	293 (97%)	9 (3%)	1 (0%)	36	16
All	All	616/684 (90%)	595 (97%)	17 (3%)	4 (1%)	21	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	270	ALA
2	D	270	ALA
1	A	999	GLU
1	C	999	GLU

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	6/11 (54%)	6 (100%)	0	100	100
1	C	6/11 (54%)	6 (100%)	0	100	100
2	B	272/293 (93%)	264 (97%)	8 (3%)	37	8
2	D	272/293 (93%)	264 (97%)	8 (3%)	37	8
All	All	556/608 (91%)	540 (97%)	16 (3%)	37	8

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

Mol	Chain	Res	Type
2	B	53	LYS
2	B	69	LEU
2	B	78	LYS
2	B	85	LEU
2	B	135	GLU
2	B	272	LEU
2	B	299	ARG
2	B	305	ILE
2	D	53	LYS
2	D	69	LEU
2	D	78	LYS
2	D	85	LEU
2	D	135	GLU
2	D	272	LEU
2	D	299	ARG
2	D	305	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	998	ASN
2	B	79	ASN
2	B	94	HIS
2	B	146	GLN
2	B	207	GLN
2	B	210	HIS
2	B	249	GLN
2	B	259	ASN
2	B	302	GLN
2	B	316	GLN
2	B	321	ASN
2	B	344	ASN
2	B	345	GLN
2	B	346	ASN
1	C	998	ASN
2	D	79	ASN
2	D	94	HIS
2	D	146	GLN
2	D	207	GLN
2	D	210	HIS
2	D	282	GLN

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Mol	Chain	Res	Type
2	D	286	HIS
2	D	302	GLN
2	D	316	GLN
2	D	320	HIS
2	D	321	ASN
2	D	344	ASN
2	D	345	GLN
2	D	346	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](#)

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	A	1003	1	15,16,17	1.56	3 (20%)	17,22,24	1.03	1 (5%)
1	PTR	C	1003	1	15,16,17	1.54	3 (20%)	17,22,24	1.02	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	A	1003	1	-	0/10/11/13	0/1/1/1
1	PTR	C	1003	1	-	0/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1003	PTR	P-OH	2.35	1.64	1.59
1	C	1003	PTR	P-OH	2.26	1.63	1.59
1	C	1003	PTR	CE2-CD2	2.10	1.42	1.38
1	A	1003	PTR	CE2-CD2	2.08	1.42	1.38
1	C	1003	PTR	CD2-CG	2.08	1.43	1.38
1	A	1003	PTR	CD2-CG	2.05	1.43	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1003	PTR	CD2-CE2-CZ	-2.45	116.94	119.73
1	C	1003	PTR	CD2-CE2-CZ	-2.39	117.00	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	7/13 (53%)	3.13	5 (71%) 0 0	16, 24, 34, 34	0
1	C	7/13 (53%)	3.31	5 (71%) 0 0	16, 24, 34, 34	0
2	B	305/329 (92%)	1.36	85 (27%) 1 2	8, 15, 30, 34	0
2	D	305/329 (92%)	1.50	94 (30%) 1 2	8, 15, 30, 34	0
All	All	624/684 (91%)	1.47	189 (30%) 1 2	8, 16, 31, 34	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	270	ALA	9.1
2	B	47	PRO	8.8
2	B	351	GLY	8.4
2	B	270	ALA	8.3
2	D	47	PRO	8.3
2	D	350	THR	8.2
2	B	350	THR	8.1
2	D	351	GLY	7.2
1	C	998	ASN	6.7
2	D	101	ARG	6.2
1	A	998	ASN	5.9
2	D	64	ASP	5.6
2	D	104	GLY	5.5
2	D	96	ARG	5.5
2	B	59	CYS	5.3
1	A	999	GLU	5.2
2	D	321	ASN	5.2
2	D	59	CYS	5.1
1	C	1005	ALA	4.9
2	D	141	TYR	4.8
2	D	54	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	78	LYS	4.7
2	B	141	TYR	4.6
2	D	143	GLU	4.6
2	D	134	LYS	4.4
2	B	104	GLY	4.4
2	D	92	TYR	4.3
2	D	117	VAL	4.3
2	D	173	LEU	4.1
2	B	54	LYS	4.1
2	B	117	VAL	4.1
2	D	107	GLU	4.1
2	D	310	ALA	4.1
1	C	1001	VAL	4.0
2	B	321	ASN	4.0
2	D	170	PRO	4.0
2	D	123	MET	4.0
2	B	64	ASP	3.9
2	B	123	MET	3.9
2	D	69	LEU	3.9
2	D	135	GLU	3.9
2	D	349	LEU	3.9
2	B	106	MET	3.9
2	B	142	GLU	3.8
2	D	50	THR	3.8
1	A	1005	ALA	3.8
2	B	312	GLY	3.7
2	D	142	GLU	3.7
2	D	334	GLU	3.7
2	B	134	LYS	3.7
2	B	310	ALA	3.7
2	B	48	PRO	3.7
2	B	143	GLU	3.7
2	D	57	GLU	3.6
2	D	146	GLN	3.6
2	D	61	LYS	3.6
2	B	145	SER	3.5
2	B	56	VAL	3.5
2	B	52	ASP	3.5
2	D	106	MET	3.5
2	D	180	ARG	3.5
2	D	144	ASN	3.5
2	D	124	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	999	GLU	3.5
2	B	107	GLU	3.5
2	B	144	ASN	3.4
2	B	108	THR	3.4
2	D	325	PHE	3.3
1	A	1001	VAL	3.3
2	B	61	LYS	3.3
2	B	135	GLU	3.3
2	D	51	VAL	3.3
2	B	146	GLN	3.3
2	B	51	VAL	3.3
2	D	311	ASP	3.3
2	D	131	SER	3.3
2	D	348	ASP	3.2
2	D	85	LEU	3.2
2	B	74	LYS	3.2
2	B	344	ASN	3.2
2	B	154	LEU	3.2
2	D	56	VAL	3.2
2	B	101	ARG	3.2
2	B	348	ASP	3.2
2	B	99	LEU	3.2
2	B	180	ARG	3.1
2	B	100	SER	3.1
2	B	85	LEU	3.1
2	D	154	LEU	3.1
2	D	49	GLY	3.1
2	B	78	LYS	3.0
2	D	53	LYS	3.0
2	B	50	THR	3.0
2	B	92	TYR	3.0
2	D	149	ARG	3.0
2	B	138	GLU	3.0
2	D	171	SER	3.0
2	D	130	ILE	3.0
2	B	177	ASP	2.9
2	B	63	MET	2.9
2	D	128	GLN	2.9
2	D	52	ASP	2.9
2	B	345	GLN	2.9
2	D	312	GLY	2.9
2	D	322	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	93	GLN	2.9
2	B	149	ARG	2.9
2	D	68	ARG	2.9
2	D	58	LYS	2.9
2	B	69	LEU	2.8
2	D	55	MET	2.8
2	D	99	LEU	2.8
2	B	55	MET	2.8
2	D	138	GLU	2.8
2	D	60	TRP	2.8
2	D	100	SER	2.7
2	D	75	LEU	2.7
2	D	299	ARG	2.7
2	B	228	ILE	2.7
1	C	1000	SER	2.7
2	B	97	THR	2.7
2	D	103	GLU	2.7
2	D	98	ILE	2.6
2	D	256	ARG	2.6
2	D	345	GLN	2.6
2	D	63	MET	2.6
2	D	145	SER	2.6
2	B	53	LYS	2.6
2	B	76	ALA	2.6
2	D	191	ARG	2.5
2	B	246	ARG	2.5
2	D	271	PHE	2.5
2	D	110	GLY	2.5
2	B	191	ARG	2.5
2	B	300	LEU	2.5
2	B	329	ILE	2.5
2	D	177	ASP	2.5
2	D	77	LEU	2.5
1	A	1000	SER	2.4
2	B	139	ARG	2.4
2	B	325	PHE	2.4
2	D	105	LYS	2.4
2	D	133	PHE	2.4
2	B	203	LYS	2.4
2	B	57	GLU	2.4
2	D	73	PRO	2.4
2	B	256	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	88	LEU	2.3
2	B	131	SER	2.3
2	D	79	ASN	2.3
2	B	105	LYS	2.3
2	D	174	PHE	2.3
2	D	320	HIS	2.3
2	D	185	ASP	2.3
2	D	132	LEU	2.3
2	B	79	ASN	2.3
2	B	299	ARG	2.3
2	B	67	VAL	2.3
2	B	212	VAL	2.3
2	D	67	VAL	2.3
2	D	74	LYS	2.3
2	D	216	SER	2.3
2	B	75	LEU	2.3
2	D	246	ARG	2.2
2	B	128	GLN	2.2
2	B	178	THR	2.2
2	B	320	HIS	2.2
2	B	156	LEU	2.2
2	D	228	ILE	2.2
2	D	111	GLU	2.2
2	B	110	GLY	2.2
2	D	139	ARG	2.2
2	D	259	ASN	2.2
2	B	93	GLN	2.2
2	B	175	GLN	2.1
2	B	102	TYR	2.1
2	B	322	LYS	2.1
2	D	203	LYS	2.1
2	B	68	ARG	2.1
2	B	170	PRO	2.1
2	B	60	TRP	2.1
2	B	333	ARG	2.1
2	D	300	LEU	2.1
2	D	147	PRO	2.1
2	B	132	LEU	2.0
2	B	124	LYS	2.0
2	B	181	ILE	2.0
2	B	305	ILE	2.0
2	D	212	VAL	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($\text{\AA}^2$)	Q<0.9
1	PTR	A	1003	16/17	0.97	0.07	10,12,18,18	0
1	PTR	C	1003	16/17	0.97	0.07	10,12,18,18	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.