



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:05 PM UTC

PDB ID : 3E5X / pdb_00003e5x
Title : OCPA complexed CprK
Authors : Levy, C.
Deposited on : 2008-08-14
Resolution : 2.00 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

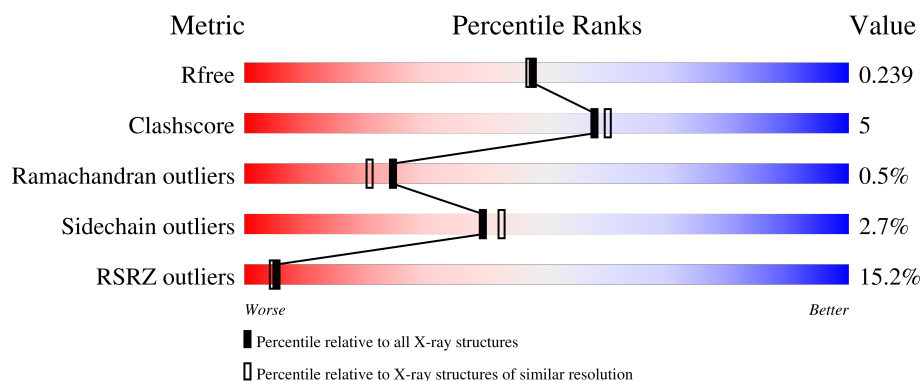
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	250	
1	B	250	
1	C	250	
1	D	250	

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	3C4	A	501	-	X	-	-

2 Entry composition [i](#)

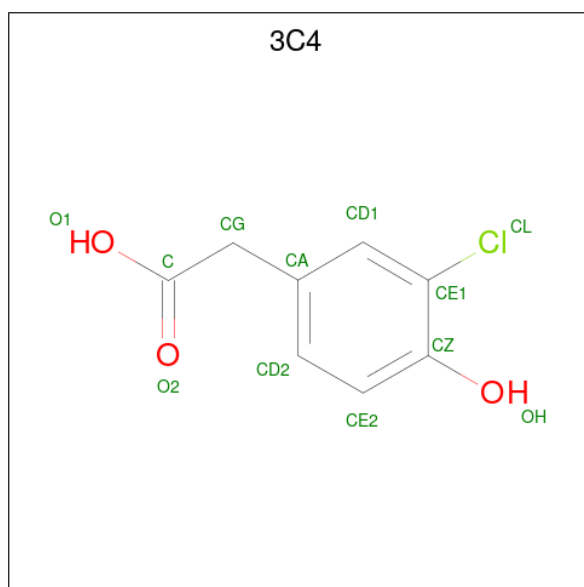
There are 3 unique types of molecules in this entry. The entry contains 7584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cyclic nucleotide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1719	1108	283	317	11			
1	C	214	Total	C	N	O	S	0	0	0
			1719	1108	283	317	11			
1	B	219	Total	C	N	O	S	0	0	0
			1758	1133	291	323	11			
1	D	220	Total	C	N	O	S	0	1	0
			1775	1143	294	327	11			

- Molecule 2 is (3-CHLORO-4-HYDROXYPHENYL)ACETIC ACID (CCD ID: 3C4) (formula: C₈H₇ClO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			12	8	1	3		
2	C	1	Total	C	Cl	O	0	0
			12	8	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Cl	O	0	0
			12	8	1	3		
2	B	1	Total	C	Cl	O	0	0
			12	8	1	3		
2	D	1	Total	C	Cl	O	0	0
			12	8	1	3		

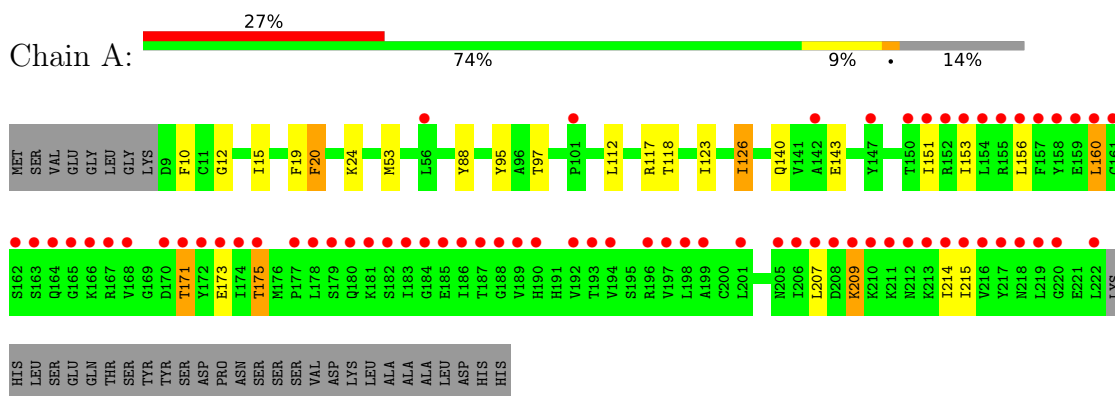
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total	O	0	0
			121	121		
3	C	130	Total	O	0	0
			130	130		
3	B	151	Total	O	0	0
			151	151		
3	D	151	Total	O	0	0
			151	151		

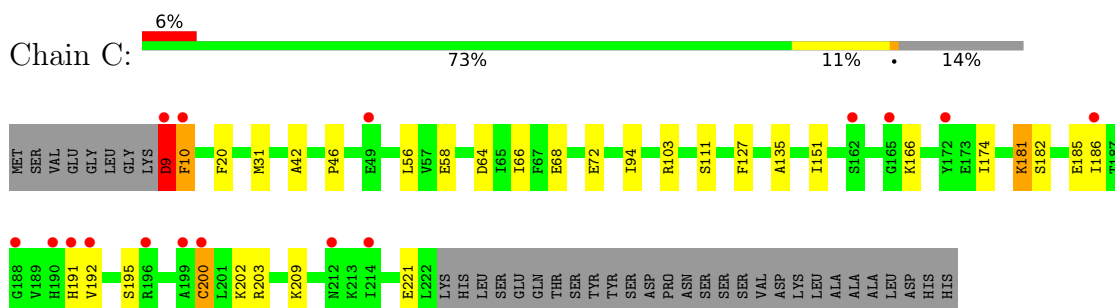
3 Residue-property plots

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.

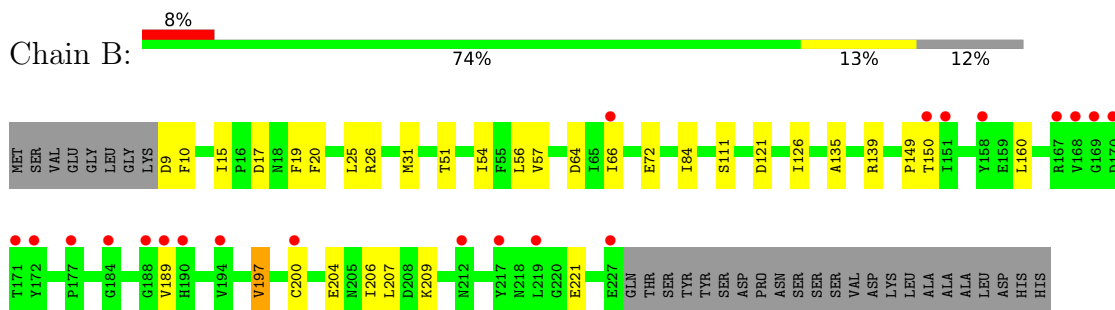
- Molecule 1: Cyclic nucleotide-binding protein



- Molecule 1: Cyclic nucleotide-binding protein

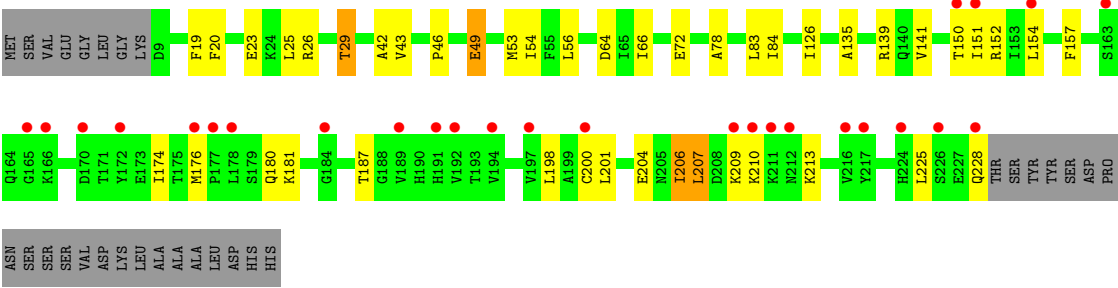


- Molecule 1: Cyclic nucleotide-binding protein



- Molecule 1: Cyclic nucleotide-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.70Å 118.38Å 87.46Å 90.00° 95.68° 90.00°	Depositor
Resolution (Å)	35.94 – 2.00 35.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (35.94-2.00) 96.2 (35.94-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.238 0.196 , 0.239	Depositor DCC
R_{free} test set	3754 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7584	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: 3C4

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	1.35	8/1752 (0.5%)	1.06	2/2362 (0.1%)
1	B	1.41	6/1792 (0.3%)	1.14	1/2415 (0.0%)
1	C	1.34	6/1752 (0.3%)	1.14	4/2362 (0.2%)
1	D	1.33	6/1813 (0.3%)	1.15	2/2444 (0.1%)
All	All	1.36	26/7109 (0.4%)	1.13	9/9583 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	THR	CB-OG1	21.79	1.78	1.43
1	B	221	GLU	C-N	19.22	1.57	1.33
1	A	171	THR	CB-CG2	10.29	1.86	1.52
1	B	135	ALA	CA-CB	8.72	1.67	1.53
1	A	126	ILE	CA-CB	6.59	1.62	1.54
1	D	135	ALA	CA-CB	6.35	1.63	1.53
1	C	42	ALA	CA-CB	6.29	1.60	1.53
1	D	126	ILE	N-CA	-6.12	1.39	1.46
1	A	112	LEU	C-O	-6.06	1.17	1.24
1	C	135	ALA	CA-CB	5.99	1.63	1.53
1	A	153	ILE	CA-CB	5.65	1.61	1.54
1	C	127	PHE	CA-C	5.62	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	200	CYS	CB-SG	-5.60	1.62	1.81
1	D	42	ALA	C-O	-5.43	1.17	1.24
1	D	78	ALA	C-O	-5.36	1.17	1.24
1	A	88	TYR	C-O	5.29	1.28	1.24
1	D	141	VAL	CA-CB	5.23	1.60	1.54
1	C	94	ILE	N-CA	-5.22	1.40	1.46
1	B	126	ILE	C-O	-5.16	1.18	1.24
1	B	51	THR	CA-CB	5.06	1.60	1.53
1	A	175	THR	CA-CB	5.06	1.59	1.52
1	B	200	CYS	CB-SG	-5.05	1.64	1.81
1	A	117	ARG	CA-C	5.04	1.59	1.52
1	B	197	VAL	CA-CB	5.03	1.60	1.54
1	C	174	ILE	CA-CB	5.03	1.60	1.53
1	D	29	THR	CA-CB	5.03	1.61	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	PHE	N-CA-C	-8.22	95.81	109.46
1	A	123	ILE	CB-CA-C	-6.14	103.85	112.14
1	C	10	PHE	N-CA-C	5.97	123.51	110.80
1	C	186	ILE	CB-CA-C	-5.54	104.82	112.24
1	C	195	SER	N-CA-C	5.34	117.10	111.28
1	D	43	VAL	N-CA-C	-5.20	105.47	110.72
1	C	202	LYS	N-CA-C	5.17	116.72	111.14
1	A	24	LYS	N-CA-C	5.13	118.64	112.38
1	D	206	ILE	N-CA-C	-5.05	106.87	111.67

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	9	ASP	Peptide
1	C	9	ASP	Peptide

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	A	1719	0	1748	15	0
1	B	1758	0	1788	12	0
1	C	1719	0	1748	13	0
1	D	1775	0	1798	25	0
2	A	12	0	6	0	0
2	B	24	0	12	0	0
2	C	12	0	6	0	0
2	D	12	0	6	0	0
3	A	121	0	0	2	0
3	B	151	0	0	3	0
3	C	130	0	0	3	0
3	D	151	0	0	6	0
All	All	7584	0	7112	64	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 5.

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:A:171:THR:CB	1:A:171:THR:CG2	1.86	1.50
1:A:171:THR:CB	1:A:171:THR:OG1	1.78	1.30
1:B:121:ASP:OD2	3:B:1594:HOH:O	1.90	0.89
1:D:23:GLU:O	1:D:26:ARG:HG2	1.78	0.82
1:C:151:ILE:HD12	3:C:1099:HOH:O	1.80	0.80
1:B:139:ARG:NH1	3:B:1318:HOH:O	2.21	0.72
1:D:152:ARG:NH1	1:D:187:THR:O	2.33	0.61
1:D:157:PHE:CZ	1:D:198:LEU:HD21	2.38	0.58
1:D:150:THR:HG21	3:D:1116:HOH:O	2.04	0.57
1:C:68:GLU:H	1:C:68:GLU:CD	2.13	0.57
1:D:49:GLU:HG2	3:D:1305:HOH:O	2.06	0.56
1:B:19:PHE:O	1:B:20:PHE:C	2.49	0.56
1:B:56:LEU:HD12	3:B:1575:HOH:O	2.06	0.56
1:D:174:ILE:HG22	1:D:176:MET:HG2	1.89	0.54
1:C:9:ASP:N	1:C:9:ASP:OD1	2.36	0.54
1:A:173:GLU:HG2	1:A:215:ILE:HD12	1.89	0.53
1:D:204:GLU:HB2	1:D:206:ILE:HD12	1.89	0.53
1:D:209:LYS:O	1:D:213:LYS:O	2.26	0.53
1:A:151:ILE:HD12	3:A:1258:HOH:O	2.09	0.53
1:D:157:PHE:HZ	1:D:198:LEU:HD21	1.74	0.53
1:D:228:GLN:C	3:D:1130:HOH:O	2.53	0.52
1:D:154:LEU:CD2	1:D:201:LEU:HD21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLU:HG2	1:C:103:ARG:HB3	1.92	0.51
1:C:182:SER:HA	1:C:185:GLU:HG2	1.93	0.51
1:D:46:PRO:HB3	1:D:66:ILE:HD12	1.93	0.51
1:A:171:THR:CG2	1:A:171:THR:CA	2.84	0.50
1:D:180:GLN:HG2	1:D:198:LEU:HD12	1.94	0.48
1:C:191:HIS:HD2	3:C:1133:HOH:O	1.96	0.47
1:D:228:GLN:HB2	3:D:1583:HOH:O	2.13	0.47
1:D:200:CYS:O	1:D:204:GLU:HG3	2.15	0.46
1:D:206:ILE:HD13	1:D:225:LEU:CD1	2.46	0.45
1:A:209:LYS:HG2	1:A:214:ILE:CD1	2.46	0.45
1:A:15:ILE:HD11	1:A:156:LEU:HD11	1.98	0.45
1:A:53:MET:HE1	1:A:126:ILE:HG21	1.99	0.45
1:B:26:ARG:NH2	1:B:57:VAL:O	2.50	0.44
1:B:31:MET:O	1:B:111:SER:HB2	2.16	0.44
1:D:207:LEU:C	1:D:207:LEU:HD23	2.43	0.44
1:C:181:LYS:O	1:C:185:GLU:HG2	2.17	0.44
1:B:150:THR:HG22	1:B:197:VAL:HG21	1.99	0.44
1:C:46:PRO:HB3	1:C:66:ILE:HD12	2.01	0.43
1:B:149:PRO:HB3	1:B:189:VAL:HG22	2.00	0.43
1:D:139:ARG:CZ	3:D:1502:HOH:O	2.67	0.43
1:C:31:MET:O	1:C:111:SER:HB2	2.19	0.42
1:B:64:ASP:OD2	1:B:72:GLU:OE2	2.37	0.42
1:D:151:ILE:HD13	1:D:151:ILE:HA	1.86	0.42
1:C:64:ASP:OD2	1:C:72:GLU:OE2	2.37	0.42
1:B:15:ILE:HD12	1:B:17:ASP:HB3	2.00	0.42
1:D:53:MET:HB3	1:D:83:LEU:HD11	2.01	0.42
1:A:95:TYR:CZ	1:A:97:THR:CG2	3.02	0.42
1:B:204:GLU:HB2	1:B:206:ILE:HD12	2.01	0.42
1:D:150:THR:HG23	3:D:1208:HOH:O	2.19	0.41
1:C:192:VAL:HG12	3:C:1343:HOH:O	2.20	0.41
1:A:140:GLN:HG3	3:A:1263:HOH:O	2.21	0.41
1:D:26:ARG:HA	1:D:29:THR:HG23	2.03	0.41
1:B:54:ILE:HB	1:B:84:ILE:HB	2.03	0.41
1:A:10:PHE:CE2	1:A:12:GLY:HA3	2.56	0.41
1:D:19:PHE:O	1:D:20:PHE:C	2.64	0.41
1:A:118:THR:O	1:C:166:LYS:HB3	2.21	0.41
1:C:221:GLU:HA	1:C:221:GLU:OE1	2.20	0.41
1:A:209:LYS:HE2	1:A:209:LYS:O	2.21	0.41
1:A:19:PHE:O	1:A:20:PHE:C	2.63	0.40
1:D:54:ILE:HB	1:D:84:ILE:HB	2.03	0.40
1:A:160:LEU:HD12	1:A:160:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ASP:OD2	1:D:72:GLU:OE2	2.38	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	212/250 (85%)	206 (97%)	5 (2%)	1 (0%)	24	21
1	B	217/250 (87%)	211 (97%)	6 (3%)	0	100	100
1	C	212/250 (85%)	204 (96%)	6 (3%)	2 (1%)	14	9
1	D	219/250 (88%)	214 (98%)	4 (2%)	1 (0%)	24	21
All	All	860/1000 (86%)	835 (97%)	21 (2%)	4 (0%)	24	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	210	LYS
1	C	10	PHE
1	C	20	PHE
1	A	20	PHE

5.3.2 Protein sidechains [i](#)

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	189/220 (86%)	184 (97%)	5 (3%)	40	44
1	B	193/220 (88%)	188 (97%)	5 (3%)	40	44
1	C	189/220 (86%)	183 (97%)	6 (3%)	34	35
1	D	195/220 (89%)	190 (97%)	5 (3%)	40	44
All	All	766/880 (87%)	745 (97%)	21 (3%)	39	42

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLU
1	A	160	LEU
1	A	175	THR
1	A	207	LEU
1	A	209	LYS
1	C	9	ASP
1	C	56	LEU
1	C	181	LYS
1	C	200	CYS
1	C	203	ARG
1	C	209	LYS
1	B	25	LEU
1	B	66	ILE
1	B	160	LEU
1	B	207	LEU
1	B	209	LYS
1	D	25	LEU
1	D	49	GLU
1	D	56	LEU
1	D	181	LYS
1	D	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	140	GLN
1	A	180	GLN
1	B	212	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	3C4	C	502	-	12,12,12	4.26	4 (33%)	16,16,16	2.25	4 (25%)
2	3C4	B	505	-	12,12,12	4.16	7 (58%)	16,16,16	3.29	6 (37%)
2	3C4	D	503	-	12,12,12	4.67	6 (50%)	16,16,16	2.35	3 (18%)
2	3C4	A	501	-	12,12,12	4.59	5 (41%)	16,16,16	2.58	8 (50%)
2	3C4	B	504	-	12,12,12	4.14	5 (41%)	16,16,16	2.40	5 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3C4	C	502	-	-	2/4/4/4	0/1/1/1
2	3C4	B	505	-	-	0/4/4/4	0/1/1/1
2	3C4	D	503	-	-	2/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3C4	A	501	-	-	2/4/4/4	0/1/1/1
2	3C4	B	504	-	-	2/4/4/4	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	3C4	CZ-CE1	12.39	1.51	1.39
2	D	503	3C4	CZ-CE1	12.35	1.51	1.39
2	C	502	3C4	CZ-CE1	11.25	1.50	1.39
2	B	504	3C4	CZ-CE1	11.21	1.50	1.39
2	B	505	3C4	CZ-CE1	8.80	1.48	1.39
2	B	505	3C4	CE2-CD2	-8.29	1.25	1.38
2	D	503	3C4	CE2-CD2	-7.43	1.26	1.38
2	A	501	3C4	CE2-CD2	-7.16	1.27	1.38
2	C	502	3C4	CE2-CZ	6.46	1.50	1.39
2	B	504	3C4	CE2-CD2	-5.76	1.29	1.38
2	C	502	3C4	CE2-CD2	-5.19	1.30	1.38
2	B	504	3C4	CE2-CZ	5.05	1.48	1.39
2	B	505	3C4	CD1-CA	-4.45	1.31	1.39
2	D	503	3C4	CD1-CA	-4.33	1.32	1.39
2	A	501	3C4	OH-CZ	4.33	1.45	1.36
2	D	503	3C4	CE2-CZ	3.86	1.46	1.39
2	A	501	3C4	CE2-CZ	3.82	1.46	1.39
2	B	505	3C4	CE2-CZ	3.58	1.45	1.39
2	B	505	3C4	CD1-CE1	-3.25	1.33	1.38
2	B	504	3C4	CD1-CA	-3.11	1.34	1.39
2	B	505	3C4	OH-CZ	3.03	1.42	1.36
2	D	503	3C4	O1-C	-2.86	1.21	1.30
2	C	502	3C4	CG-CA	2.63	1.55	1.51
2	A	501	3C4	O1-C	-2.35	1.23	1.30
2	D	503	3C4	CD2-CA	-2.15	1.34	1.38
2	B	505	3C4	CD2-CA	-2.07	1.34	1.38
2	B	504	3C4	OH-CZ	2.05	1.40	1.36

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	505	3C4	CE2-CZ-CE1	-9.70	109.37	118.49
2	D	503	3C4	CE2-CZ-CE1	-7.51	111.42	118.49
2	B	504	3C4	CE2-CZ-CE1	-7.22	111.70	118.49
2	C	502	3C4	CE2-CZ-CE1	-7.06	111.85	118.49
2	A	501	3C4	CE2-CZ-CE1	-7.04	111.87	118.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	505	3C4	CD1-CE1-CZ	5.73	124.27	120.92
2	B	505	3C4	OH-CZ-CE2	3.75	129.43	119.36
2	B	505	3C4	CE2-CD2-CA	3.06	125.02	121.00
2	A	501	3C4	OH-CZ-CE2	2.97	127.32	119.36
2	C	502	3C4	OH-CZ-CE2	2.79	126.85	119.36
2	A	501	3C4	CD2-CE2-CZ	2.74	123.24	120.50
2	A	501	3C4	CE1-CD1-CA	-2.74	118.69	120.46
2	B	504	3C4	CD2-CA-CD1	2.50	121.99	118.55
2	A	501	3C4	CD2-CA-CD1	2.45	121.92	118.55
2	D	503	3C4	OH-CZ-CE2	2.45	125.92	119.36
2	B	504	3C4	O2-C-CG	-2.41	115.66	122.94
2	A	501	3C4	CG-CA-CD2	-2.40	117.37	120.89
2	B	505	3C4	CZ-CE1-CL	-2.37	115.22	119.43
2	A	501	3C4	O1-C-CG	2.34	122.91	113.98
2	B	505	3C4	CE1-CD1-CA	-2.27	118.99	120.46
2	D	503	3C4	CD2-CA-CD1	2.27	121.68	118.55
2	A	501	3C4	CD1-CE1-CL	2.23	122.10	118.45
2	B	504	3C4	OH-CZ-CE2	2.21	125.29	119.36
2	B	504	3C4	O1-C-CG	2.11	122.04	113.98
2	C	502	3C4	O1-C-CG	2.09	121.94	113.98
2	C	502	3C4	CD2-CA-CD1	2.04	121.36	118.55

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	3C4	O2-C-CG-CA
2	A	501	3C4	O1-C-CG-CA
2	C	502	3C4	O2-C-CG-CA
2	C	502	3C4	O1-C-CG-CA
2	B	504	3C4	O1-C-CG-CA
2	B	504	3C4	O2-C-CG-CA
2	D	503	3C4	O2-C-CG-CA
2	D	503	3C4	O1-C-CG-CA

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	214/250 (85%)	1.58	68 (31%) 1 1	20, 29, 62, 69	0
1	B	219/250 (87%)	0.82	21 (9%) 13 12	18, 27, 44, 49	0
1	C	214/250 (85%)	0.94	16 (7%) 20 19	22, 29, 44, 50	0
1	D	220/250 (88%)	0.97	27 (12%) 8 7	18, 27, 45, 57	1 (0%)
All	All	867/1000 (86%)	1.08	132 (15%) 5 5	18, 28, 55, 69	1 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	LEU	6.3
1	D	209	LYS	6.3
1	A	171	THR	5.6
1	A	172	TYR	5.5
1	A	190	HIS	5.1
1	A	151	ILE	5.0
1	A	166	LYS	4.7
1	A	157	PHE	4.6
1	A	184	GLY	4.5
1	A	206	ILE	4.4
1	A	201	LEU	4.3
1	A	188	GLY	4.3
1	A	212	ASN	4.3
1	D	170	ASP	4.2
1	A	197	VAL	4.2
1	A	193	THR	4.1
1	A	189	VAL	4.1
1	A	192	VAL	4.0
1	A	219	LEU	4.0
1	A	155	ARG	3.9
1	A	152	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	215	ILE	3.9
1	A	220	GLY	3.7
1	A	175	THR	3.7
1	A	186	ILE	3.7
1	A	183	ILE	3.7
1	A	165	GLY	3.6
1	D	192	VAL	3.6
1	A	170	ASP	3.6
1	A	158	TYR	3.6
1	C	192	VAL	3.6
1	A	209	LYS	3.5
1	B	168	VAL	3.5
1	A	198	LEU	3.5
1	D	210	LYS	3.5
1	A	167	ARG	3.3
1	A	181	LYS	3.3
1	D	150	THR	3.3
1	A	205	ASN	3.3
1	D	212	ASN	3.3
1	A	168	VAL	3.2
1	A	156	LEU	3.2
1	D	211	LYS	3.2
1	A	214	ILE	3.1
1	A	222	LEU	3.1
1	A	217	TYR	3.1
1	A	150	THR	3.1
1	A	163	SER	3.1
1	A	187	THR	3.1
1	D	191[A]	HIS	3.1
1	C	199	ALA	3.1
1	D	224	HIS	3.0
1	D	166	LYS	3.0
1	B	151	ILE	3.0
1	A	173	GLU	3.0
1	C	200	CYS	3.0
1	A	199	ALA	3.0
1	D	177	PRO	2.9
1	C	191	HIS	2.9
1	D	172	TYR	2.9
1	A	208	ASP	2.9
1	B	189	VAL	2.8
1	C	9	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	212	ASN	2.8
1	D	151	ILE	2.8
1	C	188	GLY	2.8
1	B	177	PRO	2.8
1	D	226	SER	2.8
1	A	159	GLU	2.8
1	A	179	SER	2.7
1	A	216	VAL	2.7
1	A	213	LYS	2.7
1	B	188	GLY	2.7
1	B	171	THR	2.7
1	A	162	SER	2.7
1	D	163	SER	2.7
1	B	184	GLY	2.7
1	B	150	THR	2.7
1	A	153	ILE	2.6
1	D	165	GLY	2.6
1	A	174	ILE	2.6
1	C	212	ASN	2.6
1	C	49	GLU	2.6
1	B	227	GLU	2.6
1	A	218	ASN	2.6
1	B	217	TYR	2.5
1	D	200	CYS	2.5
1	A	164	GLN	2.5
1	C	186	ILE	2.5
1	B	200	CYS	2.5
1	A	178	LEU	2.5
1	C	214	ILE	2.5
1	A	182	SER	2.5
1	D	154	LEU	2.5
1	B	66	ILE	2.4
1	A	160	LEU	2.4
1	A	142	ALA	2.4
1	D	184	GLY	2.4
1	C	196	ARG	2.4
1	A	194	VAL	2.4
1	D	189	VAL	2.4
1	A	161	CYS	2.4
1	A	196	ARG	2.3
1	B	190	HIS	2.3
1	D	216	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	56	LEU	2.3
1	B	169	GLY	2.3
1	C	162	SER	2.3
1	D	178	LEU	2.3
1	C	190	HIS	2.3
1	A	210	LYS	2.3
1	A	101	PRO	2.3
1	A	154	LEU	2.3
1	A	177	PRO	2.2
1	D	228	GLN	2.2
1	B	194	VAL	2.2
1	A	211	LYS	2.2
1	A	185	GLU	2.1
1	B	158	TYR	2.1
1	A	180	GLN	2.1
1	C	165	GLY	2.1
1	A	147	TYR	2.1
1	B	172	TYR	2.1
1	B	167	ARG	2.1
1	D	194	VAL	2.1
1	C	10	PHE	2.0
1	C	172	TYR	2.0
1	D	217	TYR	2.0
1	D	176	MET	2.0
1	D	197	VAL	2.0
1	B	219	LEU	2.0
1	B	170	ASP	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
2	3C4	B	505	12/12	0.75	0.19	47,48,49,54	0
2	3C4	C	502	12/12	0.96	0.10	16,19,21,22	0
2	3C4	B	504	12/12	0.96	0.11	17,20,21,22	0
2	3C4	A	501	12/12	0.97	0.10	17,19,21,21	0
2	3C4	D	503	12/12	0.98	0.17	17,18,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.