



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:19 AM GMT

PDB ID : 3E5U
Title : OCPA complexed CprK (C200S)
Authors : Levy, C.
Deposited on : 2008-08-14
Resolution : 1.83 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

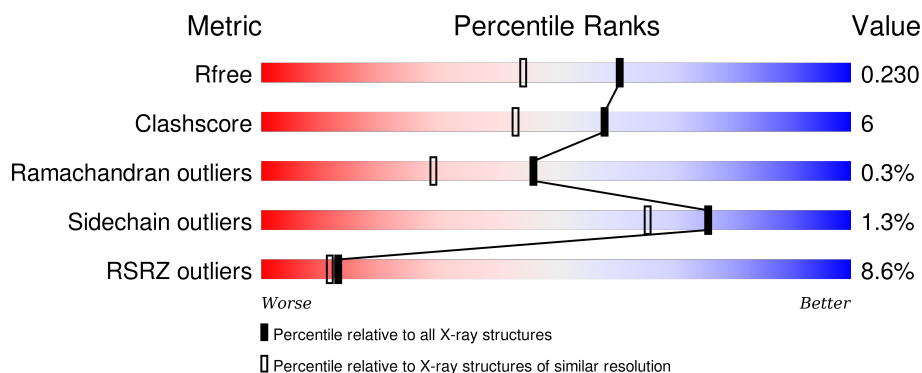
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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}	91344	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>8%</div> <div>74%</div> <div>11%</div> <div>•</div> <div>14%</div> </div>
1	B	250	<div> <div>8%</div> <div>76%</div> <div>10%</div> <div>•</div> <div>13%</div> </div>
1	C	250	<div> <div>8%</div> <div>74%</div> <div>11%</div> <div>•</div> <div>12%</div> </div>
1	D	250	<div> <div>6%</div> <div>77%</div> <div>10%</div> <div>•</div> <div>12%</div> </div>

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
3	PO4	C	603	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7860 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	C	219	Total	C	N	O	S	0	2	0
			1757	1132	289	325	11			
1	A	215	Total	C	N	O	S	0	2	0
			1720	1110	282	317	11			
1	D	220	Total	C	N	O	S	0	2	0
			1749	1128	285	325	11			
1	B	218	Total	C	N	O	S	0	2	0
			1754	1130	289	326	9			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	200	SER	CYS	ENGINEERED	UNP Q18R04
C	233	SER	-	EXPRESSION TAG	UNP Q18R04
C	234	ASP	-	EXPRESSION TAG	UNP Q18R04
C	235	PRO	-	EXPRESSION TAG	UNP Q18R04
C	236	ASN	-	EXPRESSION TAG	UNP Q18R04
C	237	SER	-	EXPRESSION TAG	UNP Q18R04
C	238	SER	-	EXPRESSION TAG	UNP Q18R04
C	239	SER	-	EXPRESSION TAG	UNP Q18R04
C	240	VAL	-	EXPRESSION TAG	UNP Q18R04
C	241	ASP	-	EXPRESSION TAG	UNP Q18R04
C	242	LYS	-	EXPRESSION TAG	UNP Q18R04
C	243	LEU	-	EXPRESSION TAG	UNP Q18R04
C	244	ALA	-	EXPRESSION TAG	UNP Q18R04
C	245	ALA	-	EXPRESSION TAG	UNP Q18R04
C	246	ALA	-	EXPRESSION TAG	UNP Q18R04
C	247	LEU	-	EXPRESSION TAG	UNP Q18R04
C	248	ASP	-	EXPRESSION TAG	UNP Q18R04
C	249	HIS	-	EXPRESSION TAG	UNP Q18R04
C	250	HIS	-	EXPRESSION TAG	UNP Q18R04
A	200	SER	CYS	ENGINEERED	UNP Q18R04
A	233	SER	-	EXPRESSION TAG	UNP Q18R04

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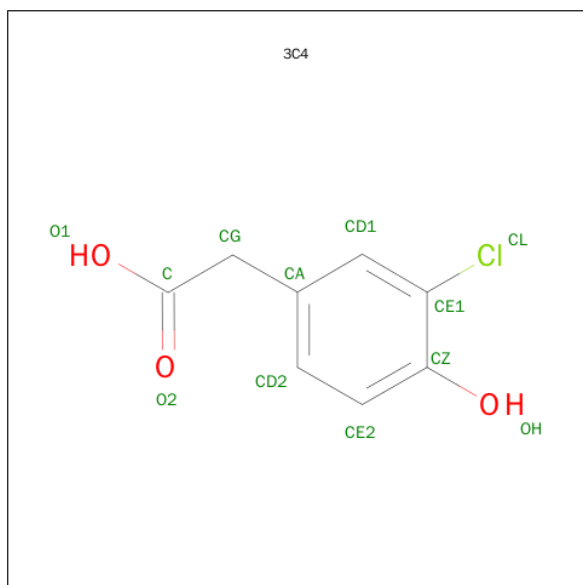
Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ASP	-	EXPRESSION TAG	UNP Q18R04
A	235	PRO	-	EXPRESSION TAG	UNP Q18R04
A	236	ASN	-	EXPRESSION TAG	UNP Q18R04
A	237	SER	-	EXPRESSION TAG	UNP Q18R04
A	238	SER	-	EXPRESSION TAG	UNP Q18R04
A	239	SER	-	EXPRESSION TAG	UNP Q18R04
A	240	VAL	-	EXPRESSION TAG	UNP Q18R04
A	241	ASP	-	EXPRESSION TAG	UNP Q18R04
A	242	LYS	-	EXPRESSION TAG	UNP Q18R04
A	243	LEU	-	EXPRESSION TAG	UNP Q18R04
A	244	ALA	-	EXPRESSION TAG	UNP Q18R04
A	245	ALA	-	EXPRESSION TAG	UNP Q18R04
A	246	ALA	-	EXPRESSION TAG	UNP Q18R04
A	247	LEU	-	EXPRESSION TAG	UNP Q18R04
A	248	ASP	-	EXPRESSION TAG	UNP Q18R04
A	249	HIS	-	EXPRESSION TAG	UNP Q18R04
A	250	HIS	-	EXPRESSION TAG	UNP Q18R04
D	200	SER	CYS	ENGINEERED	UNP Q18R04
D	233	SER	-	EXPRESSION TAG	UNP Q18R04
D	234	ASP	-	EXPRESSION TAG	UNP Q18R04
D	235	PRO	-	EXPRESSION TAG	UNP Q18R04
D	236	ASN	-	EXPRESSION TAG	UNP Q18R04
D	237	SER	-	EXPRESSION TAG	UNP Q18R04
D	238	SER	-	EXPRESSION TAG	UNP Q18R04
D	239	SER	-	EXPRESSION TAG	UNP Q18R04
D	240	VAL	-	EXPRESSION TAG	UNP Q18R04
D	241	ASP	-	EXPRESSION TAG	UNP Q18R04
D	242	LYS	-	EXPRESSION TAG	UNP Q18R04
D	243	LEU	-	EXPRESSION TAG	UNP Q18R04
D	244	ALA	-	EXPRESSION TAG	UNP Q18R04
D	245	ALA	-	EXPRESSION TAG	UNP Q18R04
D	246	ALA	-	EXPRESSION TAG	UNP Q18R04
D	247	LEU	-	EXPRESSION TAG	UNP Q18R04
D	248	ASP	-	EXPRESSION TAG	UNP Q18R04
D	249	HIS	-	EXPRESSION TAG	UNP Q18R04
D	250	HIS	-	EXPRESSION TAG	UNP Q18R04
B	200	SER	CYS	ENGINEERED	UNP Q18R04
B	233	SER	-	EXPRESSION TAG	UNP Q18R04
B	234	ASP	-	EXPRESSION TAG	UNP Q18R04
B	235	PRO	-	EXPRESSION TAG	UNP Q18R04
B	236	ASN	-	EXPRESSION TAG	UNP Q18R04
B	237	SER	-	EXPRESSION TAG	UNP Q18R04

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Chain	Residue	Modelled	Actual	Comment	Reference
B	238	SER	-	EXPRESSION TAG	UNP Q18R04
B	239	SER	-	EXPRESSION TAG	UNP Q18R04
B	240	VAL	-	EXPRESSION TAG	UNP Q18R04
B	241	ASP	-	EXPRESSION TAG	UNP Q18R04
B	242	LYS	-	EXPRESSION TAG	UNP Q18R04
B	243	LEU	-	EXPRESSION TAG	UNP Q18R04
B	244	ALA	-	EXPRESSION TAG	UNP Q18R04
B	245	ALA	-	EXPRESSION TAG	UNP Q18R04
B	246	ALA	-	EXPRESSION TAG	UNP Q18R04
B	247	LEU	-	EXPRESSION TAG	UNP Q18R04
B	248	ASP	-	EXPRESSION TAG	UNP Q18R04
B	249	HIS	-	EXPRESSION TAG	UNP Q18R04
B	250	HIS	-	EXPRESSION TAG	UNP Q18R04

- Molecule 2 is (3-CHLORO-4-HYDROXYPHENYL)ACETIC ACID (three-letter code: 3C4) (formula: $C_8H_7ClO_3$).



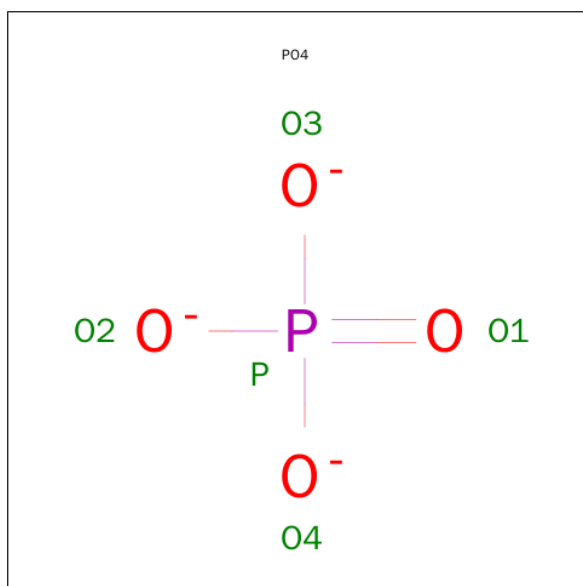
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Cl	O	0	0
			12	8	1	3		
2	A	1	Total	C	Cl	O	0	0
			12	8	1	3		
2	A	1	Total	C	Cl	O	0	0
			12	8	1	3		
2	D	1	Total	C	Cl	O	0	0
			12	8	1	3		

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	219	Total	O	0	0
			219	219		
5	A	197	Total	O	0	0
			197	197		

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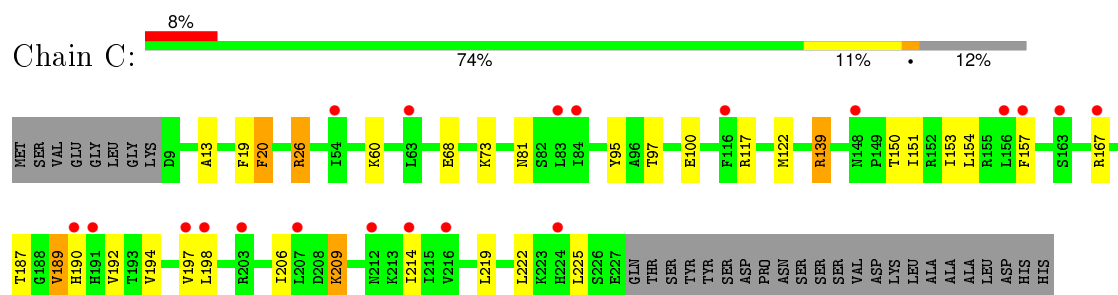
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	178	Total 178	O 178	0	0
5	B	210	Total 210	O 210	0	0

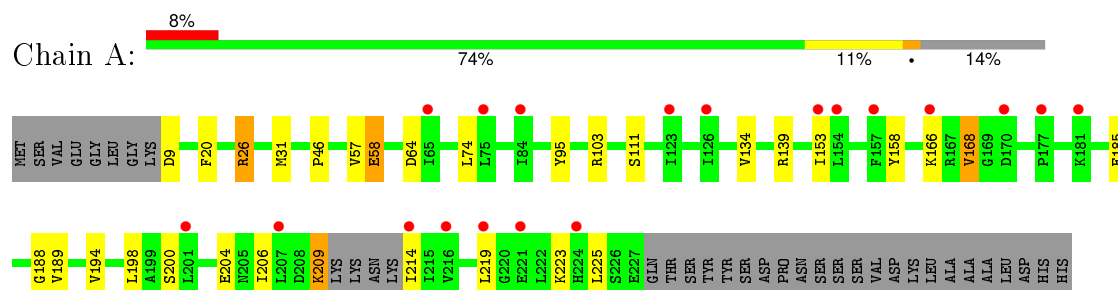
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

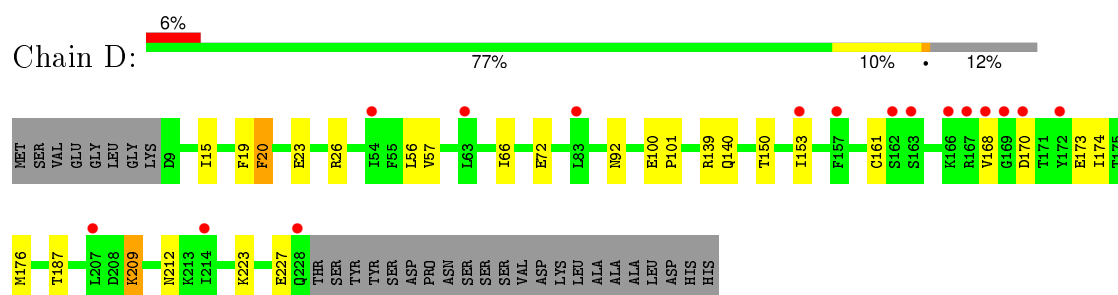
- Molecule 1: Cyclic nucleotide-binding protein



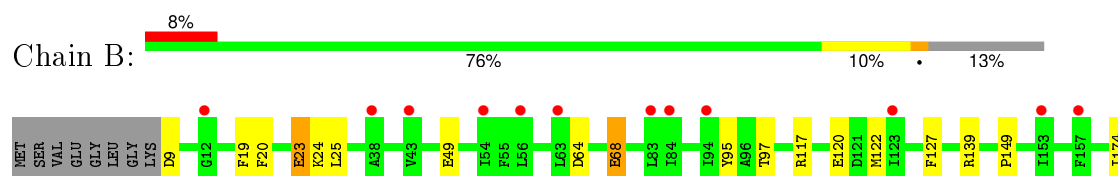
- Molecule 1: Cyclic nucleotide-binding protein

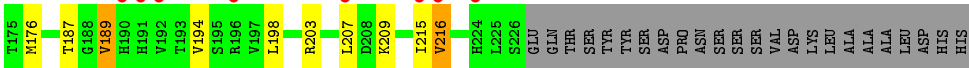


- Molecule 1: Cyclic nucleotide-binding protein



- 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	56.14Å 117.17Å 84.88Å 90.00° 94.65° 90.00°	Depositor
Resolution (Å)	19.21 – 1.83 19.21 – 1.83	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.21-1.83) 97.1 (19.21-1.83)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.182 , 0.227 0.187 , 0.230	Depositor DCC
R_{free} test set	4666 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 93327 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7860	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, PO4, 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	1.06	3/1761 (0.2%)	0.93	5/2375 (0.2%)
1	B	1.10	3/1795 (0.2%)	0.97	7/2421 (0.3%)
1	C	1.05	2/1799 (0.1%)	0.96	7/2426 (0.3%)
1	D	1.03	0/1789	0.92	2/2413 (0.1%)
All	All	1.06	8/7144 (0.1%)	0.95	21/9635 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	GLU	CG-CD	7.86	1.63	1.51
1	A	58	GLU	CG-CD	6.80	1.62	1.51
1	A	168	VAL	CB-CG2	5.88	1.65	1.52
1	C	68	GLU	CD-OE2	5.85	1.32	1.25
1	B	68	GLU	CG-CD	5.63	1.60	1.51
1	A	134	VAL	CB-CG1	5.57	1.64	1.52
1	B	23	GLU	CG-CD	5.51	1.60	1.51
1	B	216	VAL	CB-CG2	5.39	1.64	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	B	117	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	64	ASP	CB-CG-OD1	8.09	125.58	118.30
1	D	56	LEU	CB-CG-CD1	-8.00	97.40	111.00
1	A	26	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	A	139	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	C	117	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	B	139	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	122	MET	CG-SD-CE	6.13	110.01	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	64	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	26	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	167	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	D	139	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	117	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	127	PHE	CB-CG-CD1	5.42	124.60	120.80
1	A	139	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	64	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	167	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	127	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	A	103	ARG	NE-CZ-NH1	5.16	122.88	120.30

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	1720	0	1736	16	0
1	B	1754	0	1775	22	0
1	C	1757	0	1774	29	0
1	D	1749	0	1762	20	0
2	A	24	0	12	0	0
2	B	12	0	6	0	0
2	C	12	0	5	0	0
2	D	12	0	6	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
4	A	1	0	0	0	0
5	A	197	0	0	5	0
5	B	210	0	0	10	0
5	C	219	0	0	8	0
5	D	178	0	0	4	0
All	All	7860	0	7076	84	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 6.

All (84) 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:C:222:LEU:HD23	5:C:1977:HOH:O	1.62	0.99
1:D:153:ILE:HD13	1:D:187:THR:HG21	1.49	0.93
1:B:49[B]:GLU:HG2	5:B:1313:HOH:O	1.73	0.89
1:B:122:MET:SD	5:B:1975:HOH:O	2.32	0.87
1:C:153:ILE:HD11	1:C:189:VAL:HG21	1.64	0.77
1:C:26:ARG:HE	1:C:81:ASN:HD21	1.35	0.75
1:B:25:LEU:HG	1:B:122:MET:HE1	1.69	0.73
1:B:207:LEU:HD12	1:B:216:VAL:HG22	1.69	0.73
1:A:9:ASP:N	5:A:2014:HOH:O	2.21	0.72
1:C:192:VAL:HG22	5:C:1843:HOH:O	1.91	0.70
1:C:139:ARG:HD2	1:D:92:ASN:HD21	1.58	0.69
1:C:26:ARG:NE	1:C:81:ASN:HD21	1.90	0.69
1:A:185:GLU:OE1	5:A:1067:HOH:O	2.11	0.69
1:C:219:LEU:HD12	5:C:1977:HOH:O	1.92	0.68
1:B:215:ILE:HD12	5:B:1828:HOH:O	1.93	0.67
1:C:73:LYS:NZ	5:C:1839:HOH:O	2.30	0.64
1:B:49[B]:GLU:CD	5:B:1979:HOH:O	2.37	0.63
1:C:189:VAL:CG2	1:C:194:VAL:HG23	2.28	0.63
1:C:190:HIS:HB2	5:C:1834:HOH:O	2.02	0.60
1:C:189:VAL:HG22	1:C:194:VAL:CG2	2.31	0.60
1:C:157:PHE:CZ	1:C:198:LEU:HD21	2.38	0.59
1:A:58:GLU:HG2	5:A:1675:HOH:O	2.03	0.58
1:D:140:GLN:NE2	5:D:1888:HOH:O	2.27	0.58
1:A:194:VAL:O	1:A:198:LEU:HD13	2.03	0.58
1:B:95:TYR:CZ	1:B:97:THR:CG2	2.86	0.58
1:C:150:THR:HG22	1:C:197:VAL:HG21	1.87	0.56
1:B:24:LYS:HE3	5:B:1855:HOH:O	2.05	0.56
1:C:187:THR:OG1	1:C:189:VAL:HG13	2.06	0.56
1:A:209:LYS:HG2	1:A:214:ILE:HG12	1.88	0.55
1:D:168:VAL:HG21	1:D:173:GLU:OE1	2.06	0.55
1:C:189:VAL:CG2	1:C:194:VAL:CG2	2.84	0.55
1:C:13:ALA:N	5:C:1869:HOH:O	2.38	0.55
1:C:150:THR:HG22	1:C:197:VAL:CG2	2.39	0.53
1:A:206:ILE:HD13	1:A:225:LEU:HD12	1.90	0.52
1:A:153:ILE:HD11	1:A:189:VAL:HG11	1.91	0.52
1:C:139:ARG:HH11	1:D:92:ASN:HD22	1.56	0.52
1:D:209:LYS:NZ	3:D:602:PO4:O2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:NH2	1:A:57:VAL:O	2.42	0.52
1:D:150:THR:HG23	5:D:1401:HOH:O	2.08	0.51
1:B:68:GLU:CD	1:B:68:GLU:H	2.15	0.50
1:B:187:THR:OG1	1:B:189:VAL:HG13	2.11	0.50
1:C:73:LYS:NZ	5:C:1555:HOH:O	2.32	0.49
1:C:19:PHE:O	1:C:20:PHE:C	2.50	0.49
1:C:60:LYS:HB3	1:C:100:GLU:HG3	1.93	0.49
1:D:212:ASN:CB	5:D:1921:HOH:O	2.60	0.49
1:C:189:VAL:HG23	1:C:194:VAL:HG23	1.94	0.49
1:C:139:ARG:HH11	1:D:92:ASN:ND2	2.10	0.49
1:C:209:LYS:HG2	1:C:214:ILE:HG12	1.95	0.49
1:B:19:PHE:O	1:B:20:PHE:C	2.51	0.49
1:D:26:ARG:NH2	1:D:57:VAL:O	2.45	0.49
1:B:9:ASP:HA	5:B:1803:HOH:O	2.12	0.48
1:A:74:LEU:HD21	5:A:1827:HOH:O	2.14	0.48
1:C:151:ILE:HD13	1:C:154:LEU:HD12	1.94	0.48
1:D:23:GLU:O	1:D:26:ARG:HG3	2.14	0.48
1:A:200:SER:O	1:A:204:GLU:HG3	2.14	0.48
1:C:198:LEU:HD22	1:C:209:LYS:HB2	1.97	0.47
1:D:174:ILE:HG22	1:D:176:MET:HG2	1.96	0.47
1:C:206:ILE:HD13	1:C:225:LEU:HD11	1.96	0.47
1:B:174:ILE:HG22	1:B:176:MET:HG2	1.97	0.47
1:B:194:VAL:O	1:B:198:LEU:HD13	2.14	0.47
1:B:9:ASP:N	5:B:1803:HOH:O	2.48	0.46
1:C:95:TYR:CZ	1:C:97:THR:CG2	2.98	0.46
1:B:95:TYR:CZ	1:B:97:THR:HG21	2.51	0.46
1:D:209:LYS:C	1:D:209:LYS:HE2	2.36	0.46
1:A:188:GLY:C	5:A:1840:HOH:O	2.53	0.46
1:C:219:LEU:CD1	5:C:1977:HOH:O	2.57	0.46
1:D:161:CYS:HA	1:D:174:ILE:HD11	1.97	0.45
1:B:25:LEU:HG	1:B:122:MET:CE	2.45	0.45
1:B:24:LYS:CE	5:B:1855:HOH:O	2.65	0.44
1:A:158:TYR:OH	1:A:223:LYS:HE3	2.18	0.43
1:B:120:GLU:HG3	5:B:1812:HOH:O	2.17	0.43
1:D:66:ILE:HD13	1:D:72:GLU:HG3	2.01	0.43
1:D:223:LYS:NZ	1:D:227:GLU:OE1	2.52	0.42
1:A:31:MET:O	1:A:111:SER:HB2	2.18	0.42
1:A:46:PRO:HD3	1:A:95:TYR:CD2	2.54	0.42
1:A:206:ILE:HD13	1:A:225:LEU:CD1	2.50	0.41
1:D:23:GLU:HG3	5:D:1895:HOH:O	2.21	0.41
1:A:166:LYS:O	1:A:168:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ILE:CD1	1:D:176:MET:HE1	2.50	0.41
1:D:100:GLU:HB2	1:D:101:PRO:HD2	2.03	0.41
1:B:122:MET:HE2	1:B:122:MET:HB3	1.92	0.40
1:B:23:GLU:HG2	5:B:1455:HOH:O	2.22	0.40
1:D:19:PHE:O	1:D:20:PHE:C	2.60	0.40
1:B:25:LEU:CD2	1:B:122:MET:HE2	2.51	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	213/250 (85%)	207 (97%)	5 (2%)	1 (0%)	34	17
1	B	218/250 (87%)	214 (98%)	4 (2%)	0	100	100
1	C	219/250 (88%)	214 (98%)	4 (2%)	1 (0%)	34	17
1	D	220/250 (88%)	214 (97%)	5 (2%)	1 (0%)	34	17
All	All	870/1000 (87%)	849 (98%)	18 (2%)	3 (0%)	46	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	20	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%)	187 (99%)	2 (1%)	80	72
1	B	193/220 (88%)	189 (98%)	4 (2%)	61	45
1	C	193/220 (88%)	191 (99%)	2 (1%)	82	75
1	D	190/220 (86%)	188 (99%)	2 (1%)	80	72
All	All	765/880 (87%)	755 (99%)	10 (1%)	76	65

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	189	VAL
1	C	209	LYS
1	A	209	LYS
1	A	219	LEU
1	D	170	ASP
1	D	209	LYS
1	B	149	PRO
1	B	189	VAL
1	B	203	ARG
1	B	209	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	ASN
1	C	180	GLN
1	D	92	ASN
1	D	228	GLN
1	B	148	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	A	501	-	9,12,12	4.29	4 (44%)	13,16,16	2.05	6 (46%)
2	3C4	A	505	-	9,12,12	4.16	7 (77%)	13,16,16	3.39	6 (46%)
2	3C4	B	503	-	9,12,12	4.88	4 (44%)	13,16,16	2.38	6 (46%)
3	PO4	B	601	-	4,4,4	0.81	0	6,6,6	0.31	0
2	3C4	C	504	-	9,12,12	3.62	5 (55%)	13,16,16	2.39	5 (38%)
3	PO4	C	603	-	4,4,4	0.53	0	6,6,6	0.26	0
2	3C4	D	502	-	9,12,12	4.28	5 (55%)	13,16,16	2.33	5 (38%)
3	PO4	D	602	-	4,4,4	0.73	0	6,6,6	0.32	0

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	A	501	-	-	0/2/4/4	0/1/1/1
2	3C4	A	505	-	-	0/2/4/4	0/1/1/1
2	3C4	B	503	-	-	0/2/4/4	0/1/1/1
3	PO4	B	601	-	-	0/0/0/0	0/0/0/0
2	3C4	C	504	-	-	0/2/4/4	0/1/1/1
3	PO4	C	603	-	-	0/0/0/0	0/0/0/0
2	3C4	D	502	-	-	0/2/4/4	0/1/1/1
3	PO4	D	602	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	3C4	CE2-CD2	-7.42	1.25	1.38
2	A	505	3C4	CE2-CD2	-6.90	1.26	1.38
2	A	501	3C4	CE2-CD2	-5.86	1.28	1.38
2	D	502	3C4	CE2-CD2	-4.89	1.30	1.38
2	C	504	3C4	CE2-CD2	-4.71	1.30	1.38
2	C	504	3C4	CD1-CA	-3.28	1.33	1.39
2	A	505	3C4	CD1-CE1	-3.25	1.33	1.38
2	B	503	3C4	CD2-CA	-3.05	1.32	1.38
2	A	501	3C4	CD1-CA	-3.03	1.33	1.39
2	C	504	3C4	CD1-CE1	-2.79	1.33	1.38
2	D	502	3C4	CD1-CA	-2.79	1.34	1.39
2	A	505	3C4	CD2-CA	-2.68	1.33	1.38
2	A	505	3C4	CD1-CA	-2.48	1.34	1.39
2	A	505	3C4	CE2-CZ	2.73	1.44	1.39
2	A	505	3C4	OH-CZ	2.92	1.42	1.36
2	D	502	3C4	OH-CZ	3.47	1.43	1.36
2	A	501	3C4	CE2-CZ	3.78	1.46	1.39
2	C	504	3C4	CE2-CZ	4.68	1.48	1.39
2	B	503	3C4	CE2-CZ	5.01	1.48	1.39
2	D	502	3C4	CE2-CZ	5.14	1.49	1.39
2	C	504	3C4	CZ-CE1	7.14	1.46	1.39
2	A	505	3C4	CZ-CE1	8.13	1.47	1.39
2	D	502	3C4	CZ-CE1	9.61	1.48	1.39
2	A	501	3C4	CZ-CE1	10.26	1.49	1.39
2	B	503	3C4	CZ-CE1	10.98	1.50	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	505	3C4	CE2-CZ-CE1	-8.15	110.31	118.57
2	C	504	3C4	CE2-CZ-CE1	-5.85	112.64	118.57
2	B	503	3C4	CE2-CZ-CE1	-5.41	113.08	118.57
2	D	502	3C4	CE2-CZ-CE1	-5.04	113.46	118.57
2	A	505	3C4	CE1-CD1-CA	-4.92	117.18	120.36
2	A	501	3C4	CE2-CZ-CE1	-4.11	114.40	118.57
2	B	503	3C4	CD1-CE1-CZ	-3.72	119.15	121.22
2	D	502	3C4	CD1-CE1-CZ	-3.54	119.25	121.22
2	C	504	3C4	CD2-CE2-CZ	-2.10	118.34	120.49
2	A	501	3C4	CD2-CA-CD1	2.03	121.55	118.55
2	D	502	3C4	CD1-CE1-CL	2.19	121.87	118.50
2	B	503	3C4	CE2-CD2-CA	2.21	124.07	121.04
2	B	503	3C4	CD2-CA-CD1	2.33	121.99	118.55
2	D	502	3C4	OH-CZ-CE2	2.37	125.87	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	3C4	CD1-CE1-CL	2.39	122.19	118.50
2	B	503	3C4	OH-CZ-CE2	2.40	125.95	119.35
2	A	501	3C4	CE2-CD2-CA	2.45	124.40	121.04
2	A	505	3C4	CD2-CA-CD1	2.49	122.23	118.55
2	A	501	3C4	OH-CZ-CE2	2.52	126.28	119.35
2	A	505	3C4	CD2-CE2-CZ	2.59	123.15	120.49
2	A	505	3C4	OH-CZ-CE2	2.92	127.36	119.35
2	C	504	3C4	OH-CZ-CE2	2.95	127.46	119.35
2	A	501	3C4	C-CG-CA	2.97	118.62	112.73
2	B	503	3C4	CD1-CE1-CL	3.02	123.15	118.50
2	C	504	3C4	CD1-CE1-CZ	3.26	123.04	121.22
2	D	502	3C4	CE1-CD1-CA	3.48	122.61	120.36
2	C	504	3C4	CE2-CD2-CA	3.89	126.36	121.04
2	A	505	3C4	CD1-CE1-CZ	5.46	124.26	121.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	PO4	1	0

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	215/250 (86%)	0.67	19 (8%)	12 11	18, 25, 44, 52	0
1	B	218/250 (87%)	0.64	20 (9%)	11 10	18, 25, 33, 49	0
1	C	219/250 (87%)	0.68	20 (9%)	11 10	19, 27, 40, 47	0
1	D	220/250 (88%)	0.64	16 (7%)	18 16	18, 27, 42, 48	0
All	All	872/1000 (87%)	0.66	75 (8%)	13 11	18, 26, 42, 52	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	PRO	7.0
1	A	224	HIS	5.5
1	B	192	VAL	4.7
1	D	169	GLY	4.6
1	D	162	SER	4.4
1	B	190	HIS	4.4
1	B	84	ILE	4.1
1	D	170	ASP	4.0
1	C	212	ASN	3.7
1	C	203	ARG	3.6
1	C	148	ASN	3.6
1	C	190	HIS	3.6
1	C	224	HIS	3.5
1	B	191	HIS	3.5
1	A	166	LYS	3.5
1	C	84	ILE	3.5
1	B	43	VAL	3.4
1	A	157	PHE	3.4
1	A	207	LEU	3.4
1	A	214	ILE	3.4
1	C	163	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	198	LEU	3.3
1	B	83	LEU	3.3
1	D	163	SER	3.3
1	A	170	ASP	3.3
1	B	157	PHE	3.2
1	D	54	ILE	3.2
1	D	157	PHE	3.1
1	D	166	LYS	3.1
1	D	167	ARG	3.1
1	A	201	LEU	3.1
1	A	154	LEU	3.0
1	A	216	VAL	2.9
1	C	207	LEU	2.9
1	C	54	ILE	2.9
1	B	216	VAL	2.8
1	B	207	LEU	2.8
1	C	157	PHE	2.8
1	B	63	LEU	2.7
1	B	54	ILE	2.7
1	D	168	VAL	2.7
1	B	12	GLY	2.7
1	D	172	TYR	2.6
1	A	75	LEU	2.6
1	D	214	ILE	2.6
1	C	83	LEU	2.6
1	B	196	ARG	2.5
1	D	63	LEU	2.5
1	A	126	ILE	2.5
1	A	84	ILE	2.5
1	B	215	ILE	2.4
1	C	191	HIS	2.4
1	C	156	LEU	2.4
1	B	123	ILE	2.3
1	A	221	GLU	2.3
1	D	207	LEU	2.3
1	A	153	ILE	2.3
1	C	116	PHE	2.3
1	C	214	ILE	2.3
1	B	38	ALA	2.3
1	D	228	GLN	2.2
1	C	197	VAL	2.2
1	A	181	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	65	ILE	2.2
1	C	216	VAL	2.2
1	C	167	ARG	2.1
1	B	94	ILE	2.1
1	B	153	ILE	2.1
1	A	123	ILE	2.1
1	A	219	LEU	2.1
1	D	83	LEU	2.0
1	B	56	LEU	2.0
1	C	63	LEU	2.0
1	B	224	HIS	2.0
1	D	153	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	C	603	5/5	0.97	0.27	2.37	49,51,52,54	0
3	PO4	D	602	5/5	0.96	0.26	1.54	49,50,51,52	0
3	PO4	B	601	5/5	0.98	0.19	0.87	36,37,40,41	0
2	3C4	A	505	12/12	0.86	0.15	0.86	34,36,41,45	0
2	3C4	B	503	12/12	0.98	0.07	-1.73	14,16,19,19	0
2	3C4	C	504	12/12	0.99	0.06	-2.10	13,18,19,20	0
2	3C4	A	501	12/12	0.98	0.08	-2.14	14,16,19,19	0
2	3C4	D	502	12/12	0.98	0.08	-2.32	13,18,19,20	0
4	NA	A	701	1/1	0.96	0.08	-	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.