



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:09 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 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/ValidationPDFNotes.html>

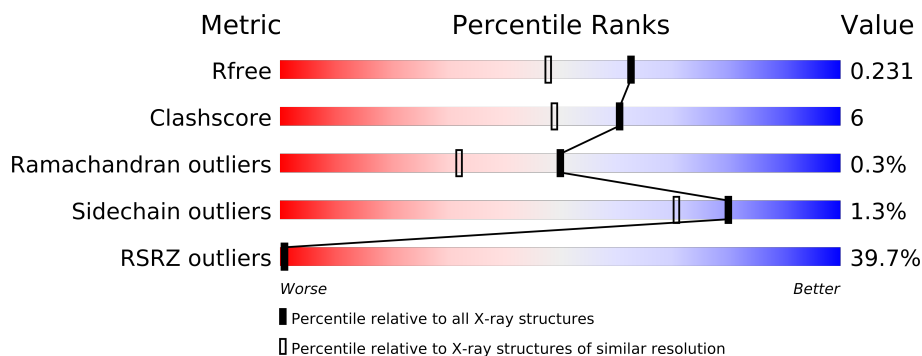
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1857 (1.86-1.82)
Clashscore	79885	2149 (1.86-1.82)
Ramachandran outliers	78287	2124 (1.86-1.82)
Sidechain outliers	78261	2125 (1.86-1.82)
RSRZ outliers	66119	1857 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	3C4	A	505	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7860 atoms, of which 0 are hydrogen and 0 are deuterium.

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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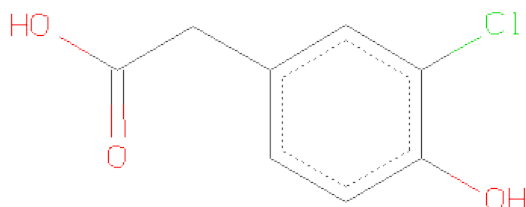
Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ASP	-	EXPRESSION TAG	UNP Q18R04
A	235	PRO	-	EXPRESSION TAG	UNP Q18R04
A	236	ASN	-	EXPRESSION TAG	UNP Q18R04
A	237	SER	-	EXPRESSION TAG	UNP Q18R04
A	238	SER	-	EXPRESSION TAG	UNP Q18R04
A	239	SER	-	EXPRESSION TAG	UNP Q18R04
A	240	VAL	-	EXPRESSION TAG	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)ACETICACID (three-letter code: 3C4) (formula: C₈H₇ClO₃).



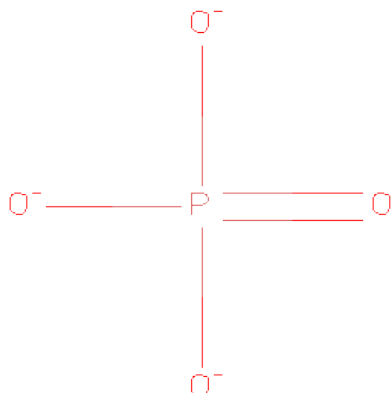
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Cl	O	0	0
			12	8	1	3		
2	A	1	Total	C	Cl	O	0	0
			12	8	1	3		
2	A	1	Total	C	Cl	O	0	0
			12	8	1	3		
2	D	1	Total	C	Cl	O	0	0
			12	8	1	3		

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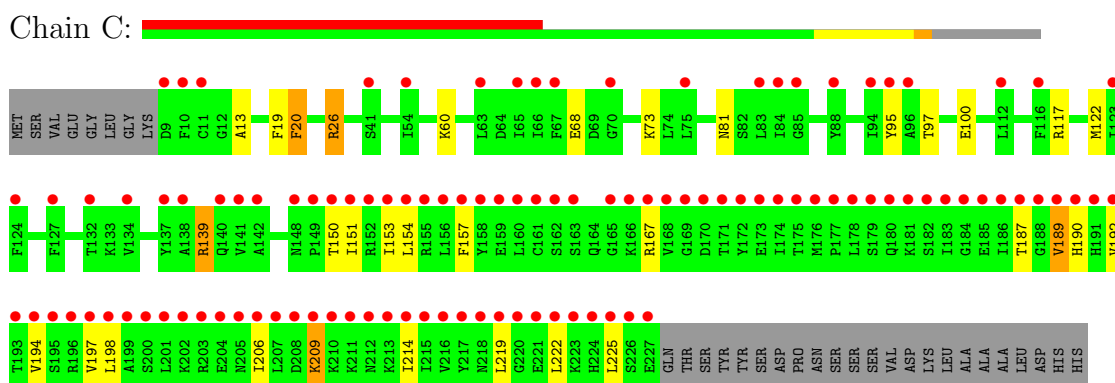
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	178	Total 178	O 178	0	0
5	B	210	Total 210	O 210	0	0

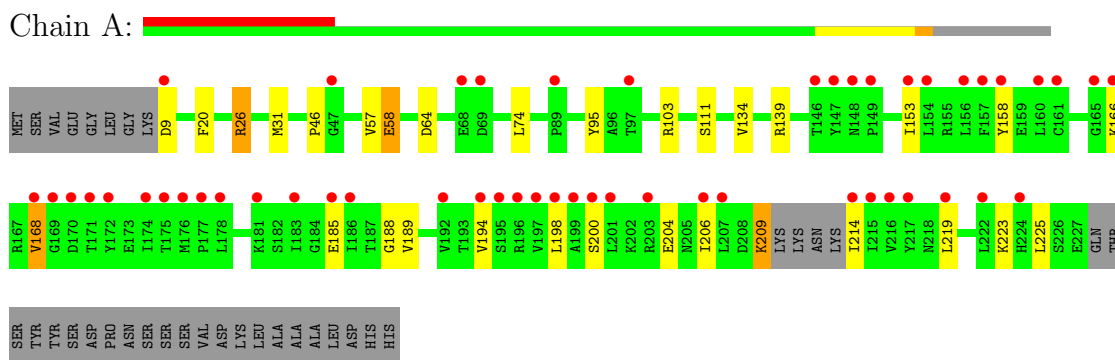
3 Residue-property plots

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.

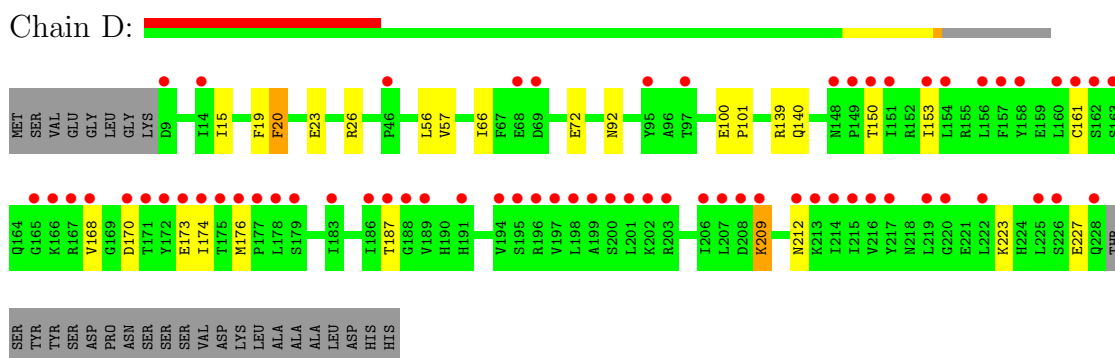
• Molecule 1: Cyclic nucleotide-binding protein



• Molecule 1: Cyclic nucleotide-binding protein

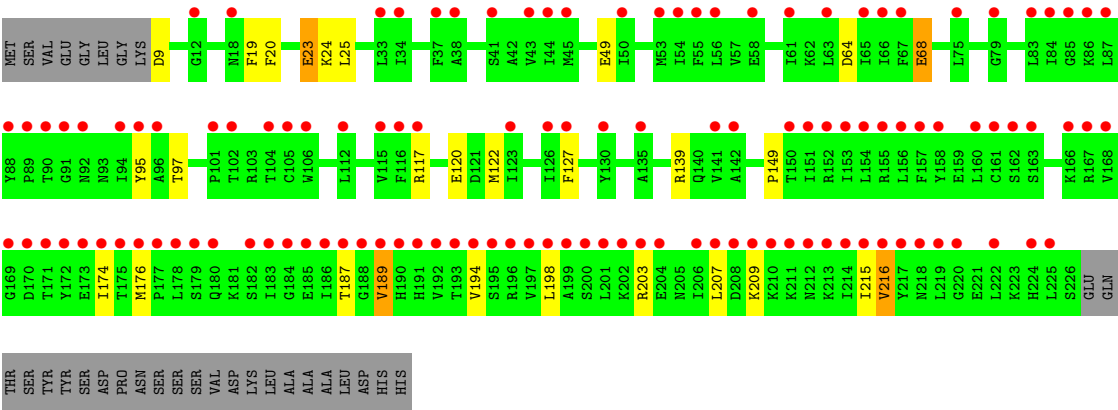


• Molecule 1: Cyclic nucleotide-binding protein



● Molecule 1: Cyclic nucleotide-binding protein

Chain B: 



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 0.188 , 0.231	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)	0.36 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 93327 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.86	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.

5 Model quality i

5.1 Standard geometry i

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	178	0	0	4	0
All	All	7860	0	7076	84	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (84) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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	213/250 (85%)	207 (97%)	5 (2%)	1 (0%)	38	19
1	B	218/250 (87%)	214 (98%)	4 (2%)	0	100	100
1	C	219/250 (88%)	214 (98%)	4 (2%)	1 (0%)	38	19
1	D	220/250 (88%)	214 (97%)	5 (2%)	1 (0%)	38	19
All	All	870/1000 (87%)	849 (98%)	18 (2%)	3 (0%)	50	32

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 ⓘ

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%)	84	77
1	B	193/220 (88%)	189 (98%)	4 (2%)	66	51
1	C	193/220 (88%)	191 (99%)	2 (1%)	85	80
1	D	190/220 (86%)	188 (99%)	2 (1%)	84	77
All	All	765/880 (87%)	755 (99%)	10 (1%)	80	71

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 chains 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	-	12,12,12	3.62	4 (33%)	16,16,16	2.05	7 (43%)
2	3C4	A	505	-	12,12,12	3.50	7 (58%)	16,16,16	3.64	9 (56%)
2	3C4	B	503	-	12,12,12	4.10	4 (33%)	16,16,16	2.58	8 (50%)
3	PO4	B	601	-	4,4,4	0.59	0	6,6,6	0.34	0
2	3C4	C	504	-	12,12,12	3.08	5 (41%)	16,16,16	2.63	6 (37%)
3	PO4	C	603	-	4,4,4	0.37	0	6,6,6	0.30	0
2	3C4	D	502	-	12,12,12	3.64	5 (41%)	16,16,16	2.34	5 (31%)
3	PO4	D	602	-	4,4,4	0.53	0	6,6,6	0.34	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	-	-	0/4/4/4	0/1/1/1
2	3C4	A	505	-	-	0/4/4/4	0/1/1/1
2	3C4	B	503	-	-	0/4/4/4	0/1/1/1
3	PO4	B	601	-	-	0/0/0/0	0/0/0/0
2	3C4	C	504	-	-	0/4/4/4	0/1/1/1
3	PO4	C	603	-	-	0/0/0/0	0/0/0/0
2	3C4	D	502	-	-	0/4/4/4	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	CZ-CE1	10.65	1.50	1.39
2	A	501	3C4	CZ-CE1	9.95	1.49	1.39
2	D	502	3C4	CZ-CE1	9.32	1.48	1.39
2	A	505	3C4	CZ-CE1	7.88	1.47	1.39
2	C	504	3C4	CZ-CE1	6.93	1.46	1.39
2	B	503	3C4	CE2-CD2	-6.92	1.25	1.38
2	A	505	3C4	CE2-CD2	-6.44	1.26	1.38
2	A	501	3C4	CE2-CD2	-5.47	1.28	1.38
2	D	502	3C4	CE2-CZ	5.00	1.49	1.39
2	B	503	3C4	CE2-CZ	4.86	1.48	1.39
2	D	502	3C4	CE2-CD2	-4.56	1.30	1.38
2	C	504	3C4	CE2-CZ	4.55	1.48	1.39
2	C	504	3C4	CE2-CD2	-4.39	1.30	1.38
2	A	501	3C4	CE2-CZ	3.67	1.46	1.39
2	D	502	3C4	OH-CZ	3.43	1.43	1.36
2	C	504	3C4	CD1-CA	-3.17	1.33	1.39
2	A	505	3C4	CD1-CE1	-3.08	1.33	1.38
2	A	501	3C4	CD1-CA	-2.93	1.33	1.39
2	A	505	3C4	OH-CZ	2.88	1.42	1.36
2	B	503	3C4	CD2-CA	-2.83	1.32	1.38
2	D	502	3C4	CD1-CA	-2.70	1.34	1.39
2	A	505	3C4	CE2-CZ	2.65	1.44	1.39
2	C	504	3C4	CD1-CE1	-2.65	1.33	1.38
2	A	505	3C4	CD2-CA	-2.48	1.33	1.38
2	A	505	3C4	CD1-CA	-2.40	1.34	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	505	3C4	CE2-CZ-CE1	-9.83	110.31	118.80
2	C	504	3C4	CE2-CZ-CE1	-7.13	112.64	118.80
2	B	503	3C4	CE2-CZ-CE1	-6.62	113.08	118.80
2	D	502	3C4	CE2-CZ-CE1	-6.18	113.46	118.80
2	A	505	3C4	CD1-CE1-CZ	6.04	124.26	121.13
2	A	501	3C4	CE2-CZ-CE1	-5.09	114.40	118.80
2	A	505	3C4	CE1-CD1-CA	-4.78	117.18	120.33
2	A	505	3C4	O2-C-CG	-3.95	113.47	123.19
2	B	503	3C4	CD1-CE1-CZ	-3.81	119.15	121.13
2	C	504	3C4	CD1-CE1-CZ	3.68	123.04	121.13
2	D	502	3C4	CD1-CE1-CZ	-3.62	119.25	121.13
2	C	504	3C4	CE2-CD2-CA	3.60	126.36	121.05
2	B	503	3C4	O2-C-CG	-3.46	114.69	123.19
2	D	502	3C4	CE1-CD1-CA	3.46	122.61	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	504	3C4	O1-C-CG	3.11	121.60	113.80
2	C	504	3C4	O2-C-CG	-3.08	115.62	123.19
2	A	505	3C4	O1-C-CG	2.98	121.28	113.80
2	C	504	3C4	OH-CZ-CE2	2.95	127.46	119.37
2	B	503	3C4	CD1-CE1-CL	2.92	123.15	118.55
2	A	505	3C4	OH-CZ-CE2	2.92	127.36	119.37
2	A	501	3C4	OH-CZ-CE2	2.52	126.28	119.37
2	A	505	3C4	CD2-CA-CD1	2.45	122.23	118.53
2	A	505	3C4	CD2-CE2-CZ	2.44	123.15	120.50
2	B	503	3C4	OH-CZ-CE2	2.40	125.95	119.37
2	D	502	3C4	OH-CZ-CE2	2.37	125.87	119.37
2	B	503	3C4	O1-C-CG	2.34	119.66	113.80
2	A	501	3C4	CD1-CE1-CL	2.31	122.19	118.55
2	B	503	3C4	CD2-CA-CD1	2.29	121.99	118.53
2	A	501	3C4	CE2-CD2-CA	2.27	124.40	121.05
2	A	501	3C4	CA-CG-C	2.19	118.62	113.58
2	A	501	3C4	O2-C-CG	-2.14	117.93	123.19
2	A	505	3C4	CG-CA-CD2	-2.13	117.66	120.88
2	D	502	3C4	CD1-CE1-CL	2.11	121.87	118.55
2	B	503	3C4	CE2-CD2-CA	2.05	124.07	121.05
2	A	501	3C4	CD2-CA-CD1	2.00	121.55	118.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	215/250 (86%)	1.37	52 (24%) 1 1	18, 25, 44, 52	0
1	B	218/250 (87%)	2.76	121 (55%) 0 0	18, 25, 33, 49	0
1	C	219/250 (87%)	4.04	109 (49%) 1 1	19, 27, 40, 47	0
1	D	220/250 (88%)	1.63	66 (30%) 1 1	18, 27, 42, 48	0
All	All	872/1000 (87%)	2.46	348 (39%) 1 1	18, 26, 42, 52	0

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	153	ILE	22.5
1	C	219	LEU	22.4
1	C	157	PHE	22.1
1	C	198	LEU	21.7
1	C	186	ILE	19.7
1	C	156	LEU	18.3
1	C	206	ILE	17.1
1	C	188	GLY	16.5
1	C	214	ILE	15.1
1	C	154	LEU	14.6
1	C	152	ARG	14.3
1	C	216	VAL	13.5
1	C	207	LEU	13.4
1	C	197	VAL	13.1
1	C	151	ILE	13.0
1	C	220	GLY	12.9
1	C	222	LEU	12.8
1	C	194	VAL	12.3
1	C	201	LEU	12.2
1	C	218	ASN	12.2
1	C	217	TYR	12.1

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Mol	Chain	Res	Type	RSRZ
1	C	160	LEU	11.9
1	B	207	LEU	11.8
1	C	187	THR	11.7
1	C	178	LEU	11.6
1	C	183	ILE	11.6
1	C	215	ILE	11.1
1	B	157	PHE	11.0
1	C	155	ARG	10.7
1	B	172	TYR	10.7
1	C	158	TYR	10.5
1	D	214	ILE	10.4
1	C	189	VAL	10.0
1	B	186	ILE	10.0
1	B	156	LEU	9.9
1	B	216	VAL	9.6
1	B	153	ILE	9.4
1	C	150	THR	9.4
1	B	187	THR	9.4
1	C	199	ALA	9.2
1	C	174	ILE	8.9
1	B	214	ILE	8.8
1	C	159	GLU	8.6
1	D	197	VAL	8.5
1	C	195	SER	8.5
1	C	172	TYR	8.4
1	B	215	ILE	8.4
1	D	198	LEU	8.3
1	C	193	THR	8.3
1	C	192	VAL	8.3
1	D	207	LEU	8.0
1	C	184	GLY	7.9
1	D	201	LEU	7.8
1	C	205	ASN	7.7
1	D	216	VAL	7.6
1	A	216	VAL	7.5
1	C	196	ARG	7.5
1	B	154	LEU	7.4
1	B	178	LEU	7.4
1	A	201	LEU	7.3
1	B	183	ILE	7.2
1	B	151	ILE	7.0
1	C	200	SER	7.0

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Mol	Chain	Res	Type	RSRZ
1	C	190	HIS	7.0
1	A	214	ILE	6.9
1	B	198	LEU	6.8
1	C	161	CYS	6.8
1	B	188	GLY	6.8
1	C	191	HIS	6.7
1	B	160	LEU	6.7
1	B	222	LEU	6.6
1	D	157	PHE	6.6
1	C	176	MET	6.5
1	A	197	VAL	6.5
1	B	174	ILE	6.4
1	B	206	ILE	6.4
1	B	84	ILE	6.4
1	D	153	ILE	6.4
1	A	154	LEU	6.4
1	D	154	LEU	6.4
1	C	170	ASP	6.3
1	C	179	SER	6.3
1	C	213	LYS	6.2
1	D	215	ILE	6.2
1	B	217	TYR	6.2
1	D	222	LEU	6.1
1	C	208	ASP	6.1
1	C	227	GLU	6.1
1	D	199	ALA	6.0
1	D	174	ILE	6.0
1	A	224	HIS	6.0
1	C	224	HIS	5.9
1	C	223	LYS	5.9
1	B	43	VAL	5.9
1	D	183	ILE	5.6
1	C	171	THR	5.6
1	D	170	ASP	5.6
1	C	221	GLU	5.5
1	A	157	PHE	5.5
1	C	162	SER	5.5
1	B	54	ILE	5.5
1	A	153	ILE	5.4
1	C	180	GLN	5.4
1	B	219	LEU	5.4
1	B	189	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	222	LEU	5.3
1	C	175	THR	5.3
1	D	166	LYS	5.3
1	B	152	ARG	5.3
1	C	212	ASN	5.3
1	A	206	ILE	5.3
1	D	206	ILE	5.2
1	D	161	CYS	5.1
1	A	177	PRO	5.1
1	A	170	ASP	5.0
1	A	198	LEU	5.0
1	B	199	ALA	5.0
1	C	182[A]	SER	4.9
1	C	209	LYS	4.9
1	C	203	ARG	4.9
1	C	225	LEU	4.9
1	C	185	GLU	4.9
1	C	226	SER	4.9
1	C	204	GLU	4.8
1	B	209	LYS	4.8
1	C	202	LYS	4.8
1	B	94	ILE	4.8
1	A	207	LEU	4.8
1	B	190	HIS	4.7
1	B	158	TYR	4.7
1	A	183	ILE	4.6
1	B	201	LEU	4.6
1	C	210	LYS	4.6
1	D	175	THR	4.6
1	D	212	ASN	4.5
1	B	194	VAL	4.5
1	D	172	TYR	4.5
1	C	163	SER	4.5
1	C	169	GLY	4.4
1	D	178	LEU	4.4
1	A	174	ILE	4.4
1	A	194	VAL	4.3
1	A	171	THR	4.3
1	C	148	ASN	4.3
1	C	84	ILE	4.3
1	B	208	ASP	4.2
1	D	156	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	171	THR	4.2
1	B	167	ARG	4.2
1	B	83	LEU	4.1
1	B	150	THR	4.1
1	B	67	PHE	4.1
1	B	65	ILE	4.1
1	D	225	LEU	4.1
1	B	192	VAL	4.0
1	A	147	TYR	4.0
1	B	44	ILE	4.0
1	D	209	LYS	4.0
1	D	194	VAL	4.0
1	B	12	GLY	3.9
1	C	65	ILE	3.8
1	C	85	GLY	3.8
1	B	162	SER	3.8
1	D	162	SER	3.8
1	C	116	PHE	3.8
1	D	186	ILE	3.7
1	D	163	SER	3.7
1	B	104	THR	3.7
1	B	161	CYS	3.7
1	A	215	ILE	3.7
1	B	170	ASP	3.6
1	B	200	SER	3.6
1	D	46	PRO	3.6
1	B	191	HIS	3.6
1	A	178	LEU	3.6
1	A	219	LEU	3.6
1	B	115	VAL	3.5
1	B	63	LEU	3.5
1	B	197	VAL	3.5
1	B	184	GLY	3.5
1	B	177	PRO	3.5
1	D	171	THR	3.5
1	C	166	LYS	3.4
1	C	54	ILE	3.4
1	D	151	ILE	3.4
1	B	101	PRO	3.4
1	D	203	ARG	3.4
1	B	85	GLY	3.3
1	C	173	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	213	LYS	3.3
1	B	126	ILE	3.3
1	D	177	PRO	3.3
1	C	167	ARG	3.3
1	B	96	ALA	3.3
1	D	213	LYS	3.2
1	A	186	ILE	3.2
1	B	75	LEU	3.2
1	D	226	SER	3.2
1	C	165	GLY	3.2
1	A	161	CYS	3.2
1	B	33	LEU	3.2
1	B	179	SER	3.2
1	A	172	TYR	3.1
1	C	177	PRO	3.1
1	A	156	LEU	3.1
1	D	228	GLN	3.1
1	D	173	GLU	3.1
1	B	66	ILE	3.1
1	B	168	VAL	3.1
1	A	166	LYS	3.1
1	C	94	ILE	3.0
1	B	88	TYR	3.0
1	D	168	VAL	3.0
1	A	148	ASN	3.0
1	A	160	LEU	3.0
1	B	185	GLU	3.0
1	A	217	TYR	3.0
1	D	217	TYR	3.0
1	C	168	VAL	2.9
1	D	167	ARG	2.9
1	B	61	ILE	2.9
1	B	210	LYS	2.9
1	B	182[A]	SER	2.9
1	B	55	PHE	2.9
1	C	127	PHE	2.9
1	B	38	ALA	2.9
1	B	37	PHE	2.9
1	B	56	LEU	2.9
1	B	123	ILE	2.9
1	B	196	ARG	2.9
1	C	142	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	41	SER	2.8
1	C	63	LEU	2.8
1	A	97	THR	2.8
1	D	160	LEU	2.8
1	B	141	VAL	2.8
1	B	112	LEU	2.8
1	D	95	TYR	2.8
1	C	149	PRO	2.8
1	A	195	SER	2.7
1	D	208	ASP	2.7
1	D	195	SER	2.7
1	B	202	LYS	2.7
1	C	66	ILE	2.7
1	D	176	MET	2.7
1	B	203	ARG	2.7
1	A	199	ALA	2.7
1	B	169	GLY	2.6
1	B	180	GLN	2.6
1	B	176	MET	2.6
1	C	112	LEU	2.6
1	B	50	ILE	2.6
1	B	116	PHE	2.6
1	A	69	ASP	2.6
1	B	130	TYR	2.6
1	B	87	LEU	2.6
1	C	134	VAL	2.6
1	B	195	SER	2.6
1	B	127	PHE	2.6
1	D	149	PRO	2.6
1	C	95	TYR	2.6
1	B	193	THR	2.6
1	B	95	TYR	2.6
1	B	173	GLU	2.6
1	A	9	ASP	2.6
1	D	200	SER	2.5
1	D	165	GLY	2.5
1	B	220	GLY	2.5
1	C	211	LYS	2.5
1	B	86	LYS	2.5
1	B	204	GLU	2.5
1	C	132	THR	2.5
1	B	166	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	176	MET	2.5
1	C	123	ILE	2.5
1	D	14	ILE	2.5
1	D	68	GLU	2.5
1	C	67	PHE	2.5
1	D	150	THR	2.5
1	B	175	THR	2.5
1	C	88	TYR	2.5
1	B	155	ARG	2.4
1	D	148	ASN	2.4
1	D	219	LEU	2.4
1	D	189	VAL	2.4
1	A	181	LYS	2.4
1	B	106	TRP	2.4
1	C	9	ASP	2.4
1	D	188	GLY	2.4
1	B	117	ARG	2.4
1	A	146	THR	2.4
1	D	97	THR	2.4
1	B	224	HIS	2.3
1	C	137	TYR	2.3
1	A	47	GLY	2.3
1	B	163	SER	2.3
1	B	105	CYS	2.3
1	C	41	SER	2.3
1	C	70	GLY	2.3
1	A	149	PRO	2.3
1	C	10	PHE	2.3
1	C	124	PHE	2.3
1	C	141	VAL	2.3
1	A	185	GLU	2.3
1	C	140	GLN	2.3
1	A	196	ARG	2.2
1	D	179	SER	2.2
1	C	181	LYS	2.2
1	B	53	MET	2.2
1	B	92	ASN	2.2
1	D	196	ARG	2.2
1	A	192	VAL	2.2
1	D	158	TYR	2.2
1	B	89	PRO	2.2
1	B	58	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	135	ALA	2.2
1	A	203	ARG	2.2
1	A	168	VAL	2.2
1	D	187	THR	2.2
1	C	83	LEU	2.2
1	A	200	SER	2.1
1	D	9	ASP	2.1
1	D	69	ASP	2.1
1	B	142	ALA	2.1
1	B	90	THR	2.1
1	A	158	TYR	2.1
1	B	212	ASN	2.1
1	C	138	ALA	2.1
1	D	191	HIS	2.1
1	B	79	GLY	2.1
1	C	75	LEU	2.1
1	A	165	GLY	2.1
1	B	102	THR	2.1
1	A	89	PRO	2.1
1	B	34	ILE	2.1
1	A	169	GLY	2.1
1	D	220	GLY	2.0
1	B	225	LEU	2.0
1	C	96	ALA	2.0
1	A	175	THR	2.0
1	B	18	ASN	2.0
1	D	202	LYS	2.0
1	B	91	GLY	2.0
1	B	211	LYS	2.0
1	A	68	GLU	2.0
1	C	11	CYS	2.0
1	B	218	ASN	2.0
1	B	45	MET	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	3C4	A	505	12/12	0.17	0.84	34,36,41,45	0
3	PO4	D	602	5/5	0.32	0.57	49,50,51,52	0
2	3C4	D	502	12/12	0.11	-0.61	13,18,19,20	0
2	3C4	A	501	12/12	0.11	-0.72	14,16,19,19	0
3	PO4	C	603	5/5	0.35	-0.95	49,51,52,54	0
3	PO4	B	601	5/5	0.27	-1.04	36,37,40,41	0
2	3C4	B	503	12/12	0.11	-1.50	14,16,19,19	0
4	NA	A	701	1/1	0.12	-2.07	32,32,32,32	0
2	3C4	C	504	12/12	0.10	-2.13	13,18,19,20	0

6.5 Other polymers

There are no such residues in this entry.