



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:59 PM GMT

PDB ID : 1W4A
Title : P4 PROTEIN FROM PHI12 IN COMPLEX WITH AMPCPP AND MN
Authors : Mancini, E.J.; Kainov, D.E.; Grimes, J.M.; Tuma, R.; Bamford, D.H.; Stuart, D.I.
Deposited on : 2004-07-22
Resolution : 2.40 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

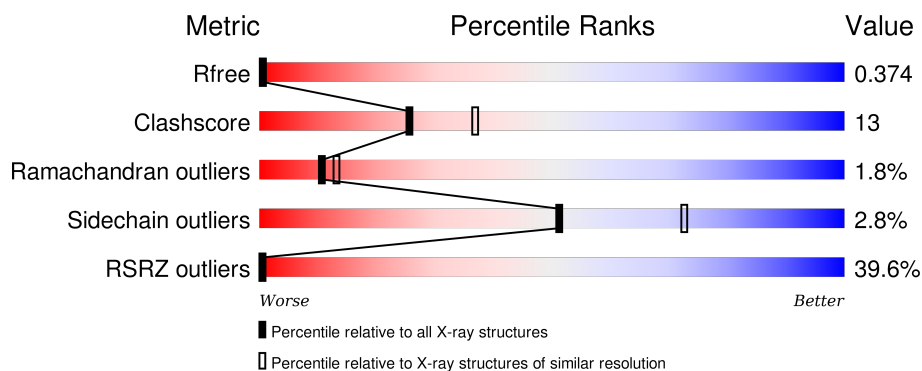
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	331	<div> <div>49%</div> <div>68%</div> <div>21%</div> <div>• 8%</div> </div>
1	B	331	<div> <div>33%</div> <div>70%</div> <div>20%</div> <div>• 8%</div> </div>
1	C	331	<div> <div>27%</div> <div>68%</div> <div>22%</div> <div>• 8%</div> </div>

2 Entry composition [i](#)

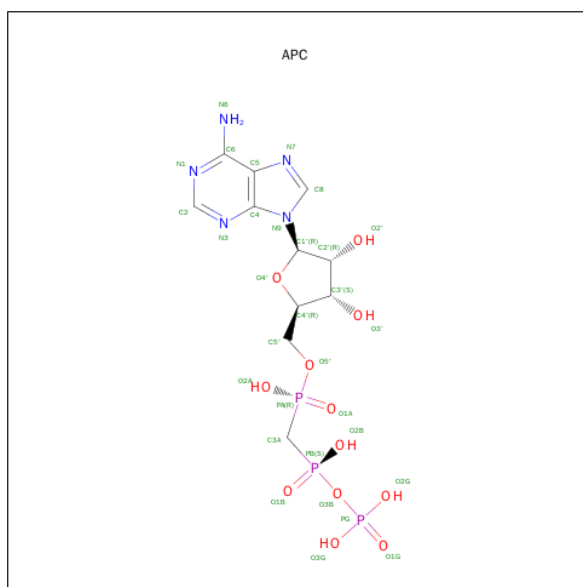
There are 4 unique types of molecules in this entry. The entry contains 7562 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NTPASE P4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	1
			2290	1434	400	449	7			
1	B	305	Total	C	N	O	S	0	0	1
			2290	1434	400	449	7			
1	C	305	Total	C	N	O	S	0	0	1
			2290	1434	400	449	7			

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mn 1	0	0
3	A	1	Total 1	Mn 1	0	0
3	C	1	Total 1	Mn 1	0	0

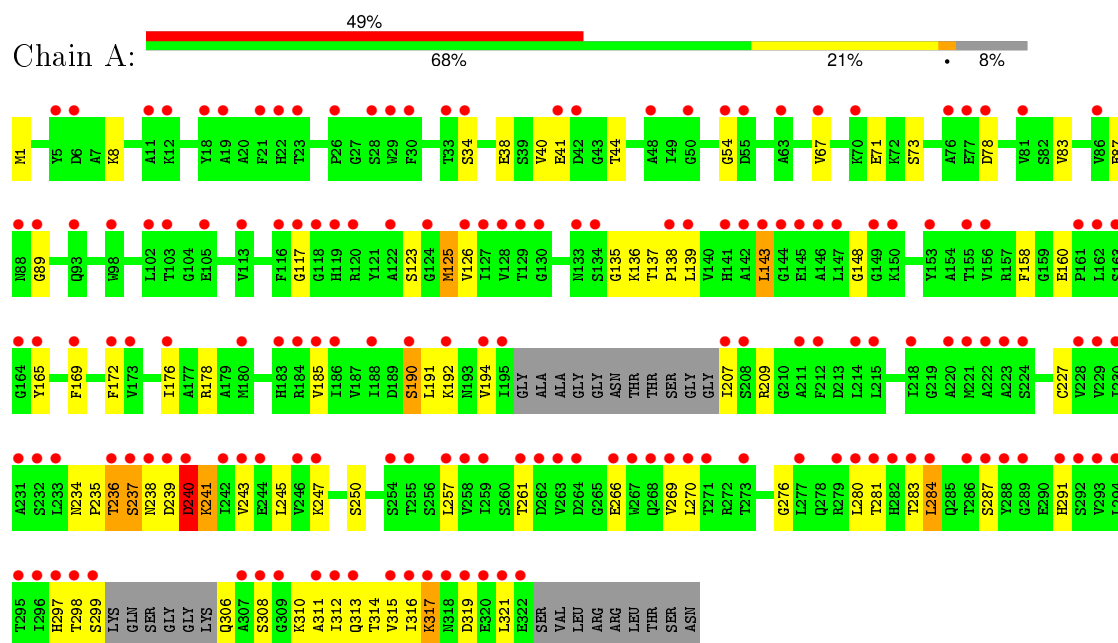
- Molecule 4 is water.

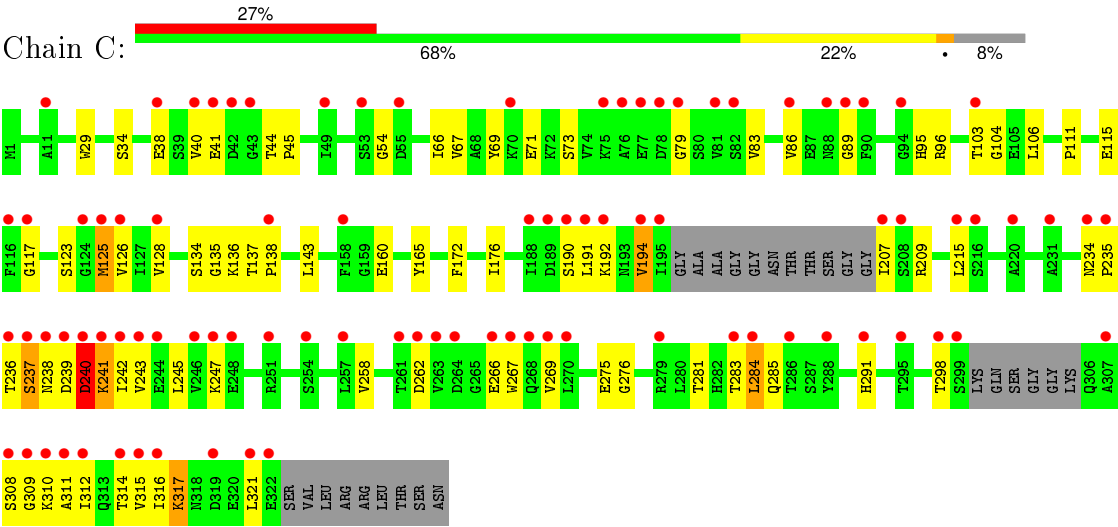
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	200	Total 200	O 200	0	0
4	B	193	Total 193	O 193	0	0
4	C	203	Total 203	O 203	0	0

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: NTPASE P4





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	105.60 Å 129.70 Å 159.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.34 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.40) 99.6 (29.34-2.41)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.73 (at 2.42 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.189 0.346 , 0.374	Depositor DCC
R_{free} test set	2131 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 42463 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	7562	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: APC, MN

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	0.43	0/2326	0.69	0/3148
1	B	0.42	0/2326	0.69	1/3148 (0.0%)
1	C	0.43	0/2326	0.68	0/3148
All	All	0.43	0/6978	0.68	1/9444 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	ASP	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2290	0	2270	64	7
1	B	2290	0	2271	52	3
1	C	2290	0	2270	53	8
2	A	31	0	13	5	0
2	B	31	0	13	8	0
2	C	31	0	13	5	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	200	0	0	7	3
4	B	193	0	0	7	2
4	C	203	0	0	5	1
All	All	7562	0	6850	173	13

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 13.

All (173) 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:B:240:ASP:HA	1:B:243:VAL:HG12	1.45	0.97
1:C:240:ASP:HA	1:C:243:VAL:HG12	1.48	0.95
1:A:240:ASP:HA	1:A:243:VAL:HG12	1.49	0.93
1:A:117:GLY:HA2	1:A:298:THR:HG23	1.64	0.79
1:B:312:ILE:O	1:B:316:ILE:HD13	1.83	0.78
1:C:117:GLY:HA2	1:C:298:THR:HG23	1.66	0.78
1:A:34:SER:O	1:A:38:GLU:HG2	1.87	0.75
1:C:312:ILE:O	1:C:316:ILE:HD13	1.87	0.74
1:A:317:LYS:HA	1:A:317:LYS:HZ3	1.52	0.74
1:C:311:ALA:O	1:C:315:VAL:HG23	1.87	0.73
1:C:104:GLY:HA3	4:C:2083:HOH:O	1.87	0.73
1:B:117:GLY:HA2	1:B:298:THR:HG23	1.70	0.73
1:A:317:LYS:HA	1:A:317:LYS:NZ	2.04	0.73
1:C:54:GLY:HA3	1:C:209:ARG:HD3	1.70	0.73
1:C:317:LYS:HA	1:C:317:LYS:NZ	2.04	0.72
1:C:190:SER:OG	1:C:192:LYS:HE2	1.91	0.70
1:B:136:LYS:N	2:B:700:APC:O2B	2.25	0.69
2:A:700:APC:H5'2	2:A:700:APC:PB	2.33	0.69
1:C:172:PHE:CZ	1:C:176:ILE:HD11	2.28	0.69
2:C:700:APC:PB	2:C:700:APC:H5'2	2.33	0.69
1:B:216:SER:HB3	4:B:2144:HOH:O	1.93	0.68
1:B:317:LYS:NZ	1:B:317:LYS:HA	2.10	0.67
1:A:312:ILE:O	1:A:316:ILE:HD13	1.94	0.67
1:C:240:ASP:HA	1:C:243:VAL:CG1	2.24	0.67
1:C:309:GLY:H	1:C:312:ILE:HD12	1.60	0.66
1:C:136:LYS:N	2:C:700:APC:O2B	2.24	0.66
1:C:317:LYS:HA	1:C:317:LYS:HZ3	1.61	0.65
1:B:34:SER:O	1:B:38:GLU:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:NH1	1:A:178:ARG:HB2	2.11	0.65
1:A:240:ASP:HA	1:A:243:VAL:CG1	2.25	0.64
2:B:700:APC:PB	2:B:700:APC:H5'2	2.37	0.64
1:A:311:ALA:O	1:A:315:VAL:HG23	1.98	0.64
1:B:135:GLY:HA3	2:B:700:APC:H4'	1.80	0.63
1:A:190:SER:OG	1:A:192:LYS:HE2	1.99	0.63
1:A:308:SER:HB2	4:A:2195:HOH:O	1.97	0.63
1:C:34:SER:O	1:C:38:GLU:HG2	1.98	0.63
1:B:73:SER:OG	1:B:83:VAL:HG22	1.98	0.63
1:B:172:PHE:CZ	1:B:176:ILE:HD11	2.33	0.62
1:B:240:ASP:HA	1:B:243:VAL:CG1	2.24	0.62
1:C:237:SER:O	1:C:239:ASP:N	2.32	0.62
1:A:270:LEU:HD23	1:A:313:GLN:HE21	1.63	0.62
1:C:314:THR:HA	1:C:317:LYS:HG3	1.82	0.61
1:C:136:LYS:HD2	1:C:234:ASN:OD1	1.99	0.61
1:B:317:LYS:HZ3	1:B:317:LYS:HA	1.66	0.61
1:A:191:LEU:O	1:A:194:VAL:HG22	2.01	0.61
1:B:311:ALA:O	1:B:315:VAL:HG23	2.00	0.60
1:B:136:LYS:HD2	1:B:234:ASN:OD1	2.01	0.60
1:A:237:SER:O	1:A:239:ASP:N	2.35	0.60
1:C:135:GLY:HA3	2:C:700:APC:H4'	1.84	0.59
1:B:298:THR:HG22	1:B:299:SER:N	2.16	0.59
1:A:207:ILE:HD12	1:A:245:LEU:HD21	1.86	0.58
1:B:237:SER:O	1:B:239:ASP:N	2.37	0.58
1:A:54:GLY:HA3	1:A:209:ARG:HD3	1.86	0.57
1:C:308:SER:HB2	4:C:2189:HOH:O	2.03	0.57
1:A:250:SER:HB3	1:A:257:LEU:HD13	1.87	0.56
1:C:137:THR:HB	1:C:138:PRO:HD3	1.86	0.56
1:B:95:HIS:HD2	1:B:96:ARG:O	1.87	0.56
1:B:115:GLU:HG2	4:B:2080:HOH:O	2.04	0.56
1:B:309:GLY:H	1:B:312:ILE:HD12	1.69	0.56
1:A:136:LYS:N	2:A:700:APC:O2B	2.30	0.56
1:A:136:LYS:HD2	1:A:234:ASN:OD1	2.06	0.55
1:A:250:SER:HB3	1:A:257:LEU:CD1	2.37	0.55
1:C:73:SER:OG	1:C:83:VAL:HG22	2.06	0.55
1:C:29:TRP:HZ2	1:C:103:THR:HG22	1.71	0.55
1:B:40:VAL:CG1	1:B:44:THR:HB	2.38	0.54
1:A:139:LEU:C	1:A:139:LEU:HD13	2.29	0.54
1:A:280:LEU:HD22	1:A:306:GLN:HG2	1.90	0.53
1:A:73:SER:OG	1:A:83:VAL:HG22	2.08	0.53
1:C:40:VAL:CG1	1:C:44:THR:HB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:MET:HG3	1:C:126:VAL:N	2.23	0.53
1:B:190:SER:OG	1:B:192:LYS:HE2	2.07	0.53
1:A:172:PHE:CZ	1:A:176:ILE:HD11	2.43	0.53
1:A:314:THR:HA	1:A:317:LYS:HG3	1.89	0.53
1:A:313:GLN:O	1:A:317:LYS:HG2	2.09	0.53
1:C:41:GLU:HB2	1:C:44:THR:OG1	2.08	0.53
1:A:269:VAL:O	1:A:281:THR:HA	2.10	0.52
4:A:2015:HOH:O	1:B:291:HIS:HD2	1.92	0.52
1:B:314:THR:HA	1:B:317:LYS:HG3	1.91	0.52
1:C:207:ILE:HD12	1:C:245:LEU:HD21	1.92	0.52
1:A:1:MET:HA	4:B:2129:HOH:O	2.09	0.52
1:B:207:ILE:N	4:B:2140:HOH:O	2.42	0.51
1:C:269:VAL:O	1:C:281:THR:HA	2.11	0.51
1:C:283:THR:HG22	1:C:284:LEU:N	2.26	0.50
1:B:126:VAL:HG22	1:B:256:SER:HB2	1.93	0.50
1:A:8:LYS:HG3	4:A:2011:HOH:O	2.12	0.49
1:C:247:LYS:NZ	1:C:321:LEU:HD11	2.27	0.49
4:B:2017:HOH:O	1:C:291:HIS:HD2	1.94	0.49
1:A:276:GLY:O	2:B:700:APC:H8	2.12	0.49
1:C:79:GLY:HA2	4:C:2066:HOH:O	2.13	0.49
1:A:41:GLU:HB2	1:A:44:THR:OG1	2.13	0.49
1:C:67:VAL:HA	1:C:89:GLY:HA2	1.93	0.49
1:B:247:LYS:NZ	1:B:321:LEU:HD11	2.27	0.49
1:C:160:GLU:HB2	1:C:165:TYR:CE1	2.48	0.49
1:C:239:ASP:HB3	1:C:242:ILE:HG22	1.95	0.49
1:A:139:LEU:HD13	1:A:139:LEU:O	2.13	0.48
1:B:207:ILE:HD12	1:B:245:LEU:HD21	1.94	0.48
1:A:291:HIS:HE1	4:A:2181:HOH:O	1.96	0.47
1:B:158:PHE:O	1:B:190:SER:HB3	2.15	0.47
1:A:40:VAL:CG1	1:A:44:THR:HB	2.44	0.47
1:B:269:VAL:O	1:B:281:THR:HA	2.14	0.47
1:C:239:ASP:O	1:C:241:LYS:N	2.48	0.47
1:B:239:ASP:O	1:B:241:LYS:N	2.48	0.46
1:A:87:GLU:HG3	4:A:2073:HOH:O	2.15	0.46
1:C:115:GLU:HG2	4:C:2090:HOH:O	2.15	0.46
1:C:194:VAL:HG23	1:C:215:LEU:HD21	1.98	0.46
1:B:54:GLY:HA3	1:B:209:ARG:HD3	1.98	0.46
1:A:178:ARG:HB2	1:A:178:ARG:HH11	1.78	0.46
1:C:160:GLU:HB2	1:C:165:TYR:CD1	2.51	0.46
1:A:207:ILE:CD1	1:A:245:LEU:HD21	2.46	0.46
1:B:239:ASP:O	1:B:242:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:SER:OG	1:A:297:HIS:HE1	1.99	0.46
1:A:239:ASP:O	1:A:241:LYS:N	2.49	0.45
1:A:283:THR:HG22	1:A:284:LEU:N	2.30	0.45
1:A:135:GLY:HA3	2:A:700:APC:H4'	1.97	0.45
1:C:239:ASP:O	1:C:242:ILE:HG22	2.15	0.45
1:A:1:MET:HE1	4:A:2068:HOH:O	2.16	0.45
1:B:207:ILE:CG2	1:B:211:ALA:HB3	2.46	0.45
1:B:287:SER:OG	1:B:297:HIS:HE1	2.00	0.45
1:A:192:LYS:HD3	1:A:234:ASN:HB2	1.99	0.45
1:A:160:GLU:HB2	1:A:165:TYR:CD1	2.52	0.45
1:B:239:ASP:HB3	1:B:242:ILE:HG22	1.98	0.45
1:B:160:GLU:HB2	1:B:165:TYR:CE1	2.52	0.45
1:C:135:GLY:CA	2:C:700:APC:H4'	2.47	0.44
1:A:137:THR:HB	1:A:138:PRO:HD3	1.98	0.44
1:A:125:MET:HG3	1:A:126:VAL:N	2.31	0.44
1:B:283:THR:HG22	1:B:284:LEU:N	2.31	0.44
1:C:234:ASN:HA	1:C:235:PRO:HD3	1.77	0.44
1:A:160:GLU:HB2	1:A:165:TYR:CE1	2.52	0.44
1:A:235:PRO:O	1:A:236:THR:C	2.56	0.44
1:B:194:VAL:HG23	1:B:215:LEU:HD21	2.00	0.44
1:C:54:GLY:HA3	1:C:209:ARG:CD	2.45	0.44
1:A:1:MET:HB2	1:A:78:ASP:OD1	2.18	0.43
1:B:160:GLU:HB2	1:B:165:TYR:CD1	2.53	0.43
1:B:192:LYS:HD3	1:B:234:ASN:HB2	2.01	0.43
1:B:191:LEU:O	1:B:194:VAL:HG22	2.18	0.43
1:A:169:PHE:O	1:A:172:PHE:HB3	2.18	0.43
1:C:314:THR:HA	1:C:317:LYS:CG	2.47	0.43
1:B:292:SER:OG	2:B:700:APC:N7	2.44	0.43
1:A:137:THR:HB	2:A:700:APC:H3A2	2.01	0.42
1:C:66:ILE:O	1:C:86:VAL:HG11	2.18	0.42
1:A:178:ARG:CB	1:A:178:ARG:HH11	2.32	0.42
1:B:1:MET:HA	4:C:2126:HOH:O	2.18	0.42
1:A:298:THR:HG22	1:A:299:SER:N	2.34	0.42
1:A:148:GLY:HA2	1:A:185:VAL:HG21	2.02	0.42
1:C:191:LEU:O	1:C:194:VAL:HG22	2.19	0.42
1:C:45:PRO:HD3	1:C:69:TYR:CE2	2.55	0.42
2:B:700:APC:O1B	2:B:700:APC:H5'2	2.20	0.42
1:B:41:GLU:HB2	1:B:44:THR:OG1	2.20	0.42
1:C:95:HIS:HD2	1:C:96:ARG:O	2.03	0.42
1:C:192:LYS:HD3	1:C:234:ASN:HB2	2.02	0.41
1:A:310:LYS:HD3	2:B:700:APC:O3'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LYS:NZ	1:A:321:LEU:HD11	2.35	0.41
1:A:8:LYS:HD2	4:A:2006:HOH:O	2.20	0.41
1:A:67:VAL:HA	1:A:89:GLY:HA2	2.02	0.41
1:C:111:PRO:HD2	1:C:123:SER:OG	2.20	0.41
1:B:45:PRO:HD3	1:B:69:TYR:CE2	2.56	0.41
1:B:313:GLN:O	1:B:317:LYS:HG2	2.21	0.41
1:A:235:PRO:O	1:A:237:SER:N	2.54	0.41
1:A:123:SER:HB2	1:A:227:CYS:O	2.21	0.41
1:C:310:LYS:HD2	1:C:310:LYS:HA	1.87	0.41
1:A:38:GLU:HG2	1:A:38:GLU:H	1.74	0.41
1:C:103:THR:HB	1:C:106:LEU:O	2.21	0.41
1:C:128:VAL:HG22	1:C:258:VAL:HB	2.03	0.41
1:B:136:LYS:HB2	2:B:700:APC:O2B	2.21	0.41
1:B:172:PHE:CE1	1:B:176:ILE:HD11	2.56	0.40
1:B:32:HIS:HE1	4:B:2074:HOH:O	2.04	0.40
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.88	0.40
1:B:178:ARG:HB2	1:B:178:ARG:NH1	2.36	0.40
1:A:158:PHE:O	1:A:190:SER:HB3	2.21	0.40
1:B:310:LYS:NZ	4:B:2187:HOH:O	2.53	0.40
1:B:276:GLY:O	2:C:700:APC:H8	2.20	0.40
1:A:234:ASN:OD1	2:A:700:APC:O1G	2.40	0.40
1:C:134:SER:HB3	1:C:267:TRP:CZ2	2.56	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:GLN:OE1	4:A:2164:HOH:O[2_665]	1.53	0.67
1:B:266:GLU:OE2	1:B:266:GLU:OE2[2_665]	1.70	0.50
1:A:266:GLU:OE1	1:C:266:GLU:OE1[2_665]	1.73	0.47
1:B:266:GLU:OE1	1:B:266:GLU:OE1[2_665]	1.93	0.27
4:A:2028:HOH:O	4:B:2041:HOH:O[8_555]	1.98	0.22
1:B:262:ASP:OD1	4:B:2190:HOH:O[2_665]	1.98	0.22
1:A:266:GLU:OE1	1:C:266:GLU:OE2[2_665]	1.99	0.21
1:A:165:TYR:OH	1:C:275:GLU:OE2[3_655]	2.04	0.16
1:A:319:ASP:OD2	1:C:262:ASP:OD1[2_665]	2.06	0.14
1:A:266:GLU:OE1	1:C:266:GLU:CD[2_665]	2.08	0.12
1:A:266:GLU:OE2	1:C:266:GLU:OE2[2_665]	2.14	0.06
1:C:276:GLY:N	4:A:2199:HOH:O[3_655]	2.17	0.03
1:A:261:THR:CB	4:C:2158:HOH:O[2_665]	2.18	0.02

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	299/331 (90%)	285 (95%)	8 (3%)	6 (2%)	9	11
1	B	299/331 (90%)	282 (94%)	12 (4%)	5 (2%)	11	14
1	C	299/331 (90%)	284 (95%)	10 (3%)	5 (2%)	11	14
All	All	897/993 (90%)	851 (95%)	30 (3%)	16 (2%)	11	13

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	THR
1	A	238	ASN
1	B	238	ASN
1	C	236	THR
1	C	238	ASN
1	A	237	SER
1	A	240	ASP
1	B	236	THR
1	B	237	SER
1	B	240	ASP
1	C	237	SER
1	C	240	ASP
1	B	190	SER
1	C	71	GLU
1	A	190	SER
1	A	71	GLU

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	247/265 (93%)	241 (98%)	6 (2%)	57	76
1	B	247/265 (93%)	239 (97%)	8 (3%)	46	68
1	C	247/265 (93%)	240 (97%)	7 (3%)	51	72
All	All	741/795 (93%)	720 (97%)	21 (3%)	51	72

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

Mol	Chain	Res	Type
1	A	125	MET
1	A	143	LEU
1	A	240	ASP
1	A	241	LYS
1	A	284	LEU
1	A	317	LYS
1	B	125	MET
1	B	143	LEU
1	B	215	LEU
1	B	240	ASP
1	B	241	LYS
1	B	270	LEU
1	B	284	LEU
1	B	317	LYS
1	C	125	MET
1	C	143	LEU
1	C	194	VAL
1	C	240	ASP
1	C	241	LYS
1	C	284	LEU
1	C	317	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	62	ASN
1	A	95	HIS
1	A	182	GLN
1	A	291	HIS
1	A	297	HIS

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Mol	Chain	Res	Type
1	A	318	ASN
1	B	32	HIS
1	B	95	HIS
1	B	119	HIS
1	B	182	GLN
1	B	268	GLN
1	B	291	HIS
1	B	297	HIS
1	B	318	ASN
1	C	95	HIS
1	C	182	GLN
1	C	268	GLN
1	C	291	HIS
1	C	297	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	APC	A	700	3	25,33,33	1.85	7 (28%)	30,52,52	2.91	6 (20%)
2	APC	B	700	-	25,33,33	1.85	7 (28%)	30,52,52	2.97	6 (20%)
2	APC	C	700	3	25,33,33	1.85	7 (28%)	30,52,52	2.77	6 (20%)

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	APC	A	700	3	-	0/15/38/38	0/3/3/3
2	APC	B	700	-	-	0/15/38/38	0/3/3/3
2	APC	C	700	3	-	0/15/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	APC	PB-O2B	-3.30	1.48	1.56
2	A	700	APC	PB-O2B	-3.30	1.48	1.56
2	C	700	APC	PB-O2B	-3.29	1.48	1.56
2	C	700	APC	PA-O2A	-3.29	1.48	1.56
2	B	700	APC	PA-O2A	-3.26	1.48	1.56
2	A	700	APC	PA-O2A	-3.25	1.48	1.56
2	A	700	APC	O4'-C1'	2.04	1.43	1.41
2	C	700	APC	O4'-C1'	2.05	1.43	1.41
2	B	700	APC	O4'-C1'	2.07	1.43	1.41
2	C	700	APC	PB-O3B	2.60	1.61	1.58
2	B	700	APC	PB-O3B	2.76	1.61	1.58
2	A	700	APC	PB-O3B	2.81	1.61	1.58
2	B	700	APC	PG-O1G	3.08	1.61	1.51
2	C	700	APC	PG-O1G	3.09	1.61	1.51
2	A	700	APC	PG-O1G	3.10	1.61	1.51
2	B	700	APC	C2-N1	3.49	1.40	1.33
2	A	700	APC	C2-N1	3.52	1.40	1.33
2	C	700	APC	C2-N1	3.60	1.40	1.33
2	A	700	APC	PA-O5'	3.82	1.61	1.57
2	B	700	APC	PA-O5'	3.88	1.61	1.57
2	C	700	APC	PA-O5'	3.94	1.61	1.57

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	APC	N3-C2-N1	-11.67	119.95	128.89
2	A	700	APC	N3-C2-N1	-11.46	120.12	128.89
2	C	700	APC	N3-C2-N1	-11.43	120.15	128.89
2	B	700	APC	C4'-O4'-C1'	-8.90	99.94	109.72
2	A	700	APC	C4'-O4'-C1'	-8.65	100.21	109.72
2	C	700	APC	C4'-O4'-C1'	-7.13	101.88	109.72
2	C	700	APC	PG-O3B-PB	-3.39	121.31	132.67
2	A	700	APC	PG-O3B-PB	-3.19	121.96	132.67
2	B	700	APC	PG-O3B-PB	-3.02	122.53	132.67
2	C	700	APC	C4-C5-N7	-2.26	107.40	109.48
2	B	700	APC	C4-C5-N7	-2.20	107.46	109.48
2	A	700	APC	C4-C5-N7	-2.12	107.53	109.48
2	B	700	APC	O2A-PA-O1A	2.42	117.73	110.12
2	A	700	APC	O2A-PA-O1A	2.43	117.76	110.12
2	A	700	APC	O2B-PB-O1B	2.44	117.81	110.12
2	C	700	APC	O2A-PA-O1A	2.46	117.86	110.12
2	B	700	APC	O2B-PB-O1B	2.50	117.98	110.12
2	C	700	APC	O2B-PB-O1B	2.53	118.08	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	APC	5	0
2	B	700	APC	8	0
2	C	700	APC	5	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	305/331 (92%)	2.31	162 (53%)  	8, 22, 67, 121	0
1	B	305/331 (92%)	1.90	109 (35%)  	9, 22, 68, 120	0
1	C	305/331 (92%)	1.64	91 (29%)  	9, 23, 68, 121	0
All	All	915/993 (92%)	1.95	362 (39%)  	8, 22, 68, 121	0

All (362) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	ASP	8.4
1	C	240	ASP	8.3
1	B	240	ASP	8.1
1	A	238	ASN	7.3
1	A	243	VAL	6.8
1	B	238	ASN	6.7
1	A	236	THR	6.5
1	A	89	GLY	6.4
1	C	236	THR	6.4
1	A	299	SER	6.3
1	B	236	THR	6.1
1	C	238	ASN	6.0
1	C	207	ILE	6.0
1	C	243	VAL	5.8
1	A	298	THR	5.7
1	A	242	ILE	5.7
1	B	207	ILE	5.6
1	A	312	ILE	5.5
1	B	315	VAL	5.5
1	A	315	VAL	5.4
1	B	316	ILE	5.4
1	C	239	ASP	5.4
1	A	316	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	316	ILE	5.2
1	A	239	ASP	5.1
1	B	77	GLU	5.1
1	C	315	VAL	4.9
1	C	241	LYS	4.9
1	A	295	THR	4.9
1	A	207	ILE	4.8
1	C	312	ILE	4.8
1	A	309	GLY	4.7
1	A	237	SER	4.6
1	B	299	SER	4.5
1	B	318	ASN	4.5
1	B	239	ASP	4.5
1	B	289	GLY	4.4
1	A	195	ILE	4.4
1	B	208	SER	4.4
1	C	89	GLY	4.3
1	B	241	LYS	4.3
1	B	312	ILE	4.3
1	A	307	ALA	4.2
1	A	244	GLU	4.2
1	A	289	GLY	4.2
1	A	259	ILE	4.2
1	B	89	GLY	4.2
1	A	208	SER	4.1
1	C	77	GLU	4.1
1	A	34	SER	4.1
1	A	117	GLY	4.1
1	C	299	SER	4.1
1	A	257	LEU	4.1
1	A	190	SER	4.0
1	A	139	LEU	4.0
1	A	318	ASN	4.0
1	A	292	SER	4.0
1	B	7	ALA	3.9
1	B	133	ASN	3.9
1	A	149	GLY	3.9
1	B	244	GLU	3.9
1	A	76	ALA	3.9
1	A	67	VAL	3.9
1	A	319	ASP	3.9
1	B	321	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	310	LYS	3.8
1	B	117	GLY	3.8
1	A	293	VAL	3.8
1	C	41	GLU	3.8
1	C	79	GLY	3.8
1	A	63	ALA	3.6
1	B	264	ASP	3.6
1	C	234	ASN	3.6
1	B	118	GLY	3.6
1	B	195	ILE	3.6
1	B	134	SER	3.5
1	B	298	THR	3.5
1	C	235	PRO	3.5
1	A	41	GLU	3.5
1	C	262	ASP	3.5
1	A	118	GLY	3.5
1	A	23	THR	3.5
1	B	267	TRP	3.5
1	A	246	VAL	3.5
1	A	262	ASP	3.5
1	A	284	LEU	3.5
1	A	142	ALA	3.4
1	B	290	GLU	3.4
1	A	88	ASN	3.4
1	A	263	VAL	3.4
1	B	309	GLY	3.4
1	A	282	HIS	3.4
1	B	233	LEU	3.4
1	C	321	LEU	3.4
1	B	55	ASP	3.4
1	C	76	ALA	3.4
1	A	133	ASN	3.3
1	C	247	LYS	3.3
1	C	298	THR	3.3
1	A	283	THR	3.3
1	B	308	SER	3.3
1	A	311	ALA	3.3
1	A	291	HIS	3.3
1	C	319	ASP	3.3
1	A	11	ALA	3.3
1	B	188	ILE	3.3
1	A	297	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	288	TYR	3.2
1	C	78	ASP	3.2
1	B	237	SER	3.2
1	A	296	ILE	3.2
1	C	208	SER	3.2
1	B	235	PRO	3.2
1	C	314	THR	3.2
1	C	279	ARG	3.2
1	A	270	LEU	3.2
1	B	266	GLU	3.2
1	B	88	ASN	3.2
1	B	246	VAL	3.2
1	A	54	GLY	3.2
1	B	190	SER	3.2
1	A	81	VAL	3.2
1	A	254	SER	3.2
1	A	143	LEU	3.1
1	A	231	ALA	3.1
1	A	321	LEU	3.1
1	A	273	THR	3.1
1	B	81	VAL	3.1
1	B	229	VAL	3.1
1	B	1	MET	3.1
1	B	313	GLN	3.1
1	A	223	ALA	3.1
1	B	295	THR	3.1
1	A	29	TRP	3.1
1	A	192	LYS	3.1
1	C	215	LEU	3.1
1	A	281	THR	3.1
1	A	286	THR	3.1
1	B	67	VAL	3.1
1	B	291	HIS	3.0
1	C	266	GLU	3.0
1	B	263	VAL	3.0
1	A	233	LEU	3.0
1	A	271	THR	3.0
1	A	156	VAL	3.0
1	A	280	LEU	3.0
1	A	308	SER	3.0
1	A	155	THR	3.0
1	B	243	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	143	LEU	3.0
1	C	261	THR	3.0
1	A	264	ASP	3.0
1	B	212	PHE	2.9
1	A	230	ILE	2.9
1	B	220	ALA	2.9
1	B	76	ALA	2.9
1	B	307	ALA	2.9
1	A	180	MET	2.9
1	B	78	ASP	2.9
1	A	261	THR	2.9
1	A	176	ILE	2.9
1	A	77	GLU	2.9
1	C	81	VAL	2.9
1	C	90	PHE	2.9
1	A	86	VAL	2.8
1	A	267	TRP	2.8
1	A	212	PHE	2.8
1	A	247	LYS	2.8
1	A	138	PRO	2.8
1	A	266	GLU	2.8
1	C	195	ILE	2.8
1	B	292	SER	2.8
1	A	228	VAL	2.8
1	C	117	GLY	2.8
1	A	268	GLN	2.8
1	C	190	SER	2.8
1	A	165	TYR	2.8
1	B	68	ALA	2.8
1	C	311	ALA	2.8
1	A	102	LEU	2.8
1	A	146	ALA	2.8
1	C	55	ASP	2.8
1	B	234	ASN	2.8
1	C	283	THR	2.7
1	A	119	HIS	2.7
1	A	322	GLU	2.7
1	C	322	GLU	2.7
1	A	78	ASP	2.7
1	A	126	VAL	2.7
1	A	128	VAL	2.7
1	B	269	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	48	ALA	2.7
1	A	211	ALA	2.7
1	B	311	ALA	2.7
1	A	294	LEU	2.7
1	C	291	HIS	2.7
1	A	22	HIS	2.7
1	A	229	VAL	2.7
1	C	126	VAL	2.7
1	C	269	VAL	2.7
1	A	188	ILE	2.6
1	B	242	ILE	2.6
1	B	283	THR	2.6
1	B	126	VAL	2.6
1	B	231	ALA	2.6
1	B	257	LEU	2.6
1	C	257	LEU	2.6
1	A	19	ALA	2.6
1	B	194	VAL	2.6
1	B	279	ARG	2.6
1	A	173	VAL	2.6
1	A	288	TYR	2.6
1	A	26	PRO	2.6
1	A	161	PRO	2.6
1	A	162	LEU	2.6
1	A	116	PHE	2.6
1	A	269	VAL	2.6
1	A	134	SER	2.6
1	B	314	THR	2.6
1	A	21	PHE	2.6
1	A	127	ILE	2.6
1	C	188	ILE	2.6
1	B	41	GLU	2.6
1	B	247	LYS	2.5
1	B	293	VAL	2.5
1	C	70	LYS	2.5
1	A	129	THR	2.5
1	C	103	THR	2.5
1	A	313	GLN	2.5
1	C	268	GLN	2.5
1	B	75	LYS	2.5
1	B	129	THR	2.5
1	A	185	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	82	SER	2.5
1	C	88	ASN	2.5
1	C	263	VAL	2.5
1	A	214	LEU	2.5
1	C	251	ARG	2.5
1	C	82	SER	2.5
1	B	109	CYS	2.5
1	B	43	GLY	2.5
1	C	307	ALA	2.5
1	B	187	VAL	2.5
1	C	191	LEU	2.5
1	A	258	VAL	2.5
1	A	70	LYS	2.5
1	A	153	TYR	2.5
1	A	130	GLY	2.4
1	A	287	SER	2.4
1	B	146	ALA	2.4
1	A	194	VAL	2.4
1	C	194	VAL	2.4
1	B	132	GLY	2.4
1	C	267	TRP	2.4
1	C	237	SER	2.4
1	A	169	PHE	2.4
1	C	192	LYS	2.4
1	B	102	LEU	2.4
1	C	308	SER	2.4
1	C	158	PHE	2.4
1	A	98	TRP	2.4
1	B	141	HIS	2.4
1	B	228	VAL	2.4
1	A	255	THR	2.4
1	A	224	SER	2.4
1	A	30	PHE	2.4
1	B	70	LYS	2.4
1	A	42	ASP	2.4
1	B	249	ALA	2.4
1	C	11	ALA	2.4
1	A	50	GLY	2.3
1	C	295	THR	2.3
1	B	72	LYS	2.3
1	B	154	ALA	2.3
1	A	279	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	94	GLY	2.3
1	C	284	LEU	2.3
1	A	183	HIS	2.3
1	C	220	ALA	2.3
1	C	53	SER	2.3
1	C	246	VAL	2.3
1	C	286	THR	2.3
1	A	186	ILE	2.3
1	A	220	ALA	2.3
1	A	150	LYS	2.3
1	A	120	ARG	2.3
1	A	124	GLY	2.3
1	A	144	GLY	2.3
1	C	124	GLY	2.3
1	A	105	GLU	2.3
1	B	265	GLY	2.3
1	C	43	GLY	2.3
1	B	86	VAL	2.3
1	B	111	PRO	2.3
1	A	221	MET	2.2
1	B	192	LYS	2.2
1	C	128	VAL	2.2
1	B	142	ALA	2.2
1	B	268	GLN	2.2
1	A	55	ASP	2.2
1	B	124	GLY	2.2
1	A	215	LEU	2.2
1	B	5	TYR	2.2
1	C	264	ASP	2.2
1	A	113	VAL	2.2
1	A	222	ALA	2.2
1	B	125	MET	2.2
1	A	164	GLY	2.2
1	B	158	PHE	2.2
1	A	277	LEU	2.2
1	C	49	ILE	2.2
1	C	242	ILE	2.2
1	B	30	PHE	2.2
1	B	191	LEU	2.2
1	C	42	ASP	2.2
1	A	5	TYR	2.2
1	A	12	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	189	ASP	2.2
1	C	309	GLY	2.1
1	A	93	GLN	2.1
1	A	317	LYS	2.1
1	A	33	THR	2.1
1	A	103	THR	2.1
1	A	232	SER	2.1
1	A	184	ARG	2.1
1	B	259	ILE	2.1
1	B	140	VAL	2.1
1	C	231	ALA	2.1
1	C	288	TYR	2.1
1	B	2	ILE	2.1
1	A	145	GLU	2.1
1	A	320	GLU	2.1
1	B	278	GLN	2.1
1	A	141	HIS	2.1
1	B	254	SER	2.1
1	B	80	SER	2.1
1	C	254	SER	2.1
1	A	18	TYR	2.1
1	A	147	LEU	2.1
1	B	172	PHE	2.1
1	B	284	LEU	2.1
1	B	44	THR	2.1
1	A	28	SER	2.1
1	A	163	SER	2.1
1	A	6	ASP	2.1
1	B	248	GLU	2.1
1	C	244	GLU	2.1
1	C	248	GLU	2.1
1	A	172	PHE	2.1
1	C	116	PHE	2.1
1	C	270	LEU	2.1
1	A	122	ALA	2.0
1	C	38	GLU	2.0
1	B	251	ARG	2.0
1	C	75	LYS	2.0
1	C	40	VAL	2.0
1	C	86	VAL	2.0
1	C	138	PRO	2.0
1	C	125	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	218	ILE	2.0
1	C	216	SER	2.0
1	B	33	THR	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 carbohydrates 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. 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
2	APC	C	700	31/31	0.74	0.32	0.80	16,36,57,65	0
2	APC	B	700	31/31	0.66	0.35	0.70	21,47,64,78	0
2	APC	A	700	31/31	0.75	0.31	0.08	23,43,60,71	0
3	MN	C	701	1/1	0.86	0.10	-3.13	35,35,35,35	0
3	MN	B	701	1/1	0.74	0.15	-	37,37,37,37	0
3	MN	A	701	1/1	0.46	0.17	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.