Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:06 PM GMT

PDB ID	:	4BHW
Title	:	Structural basis for autoinhibition of the acetyltransferase activity of p300
Authors	:	Delvecchio, M.; Gaucher, J.; Aguilar-Gurrieri, C.; Ortega, E.; Panne, D.
Deposited on	:	2013-04-08
Resolution	:	2.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

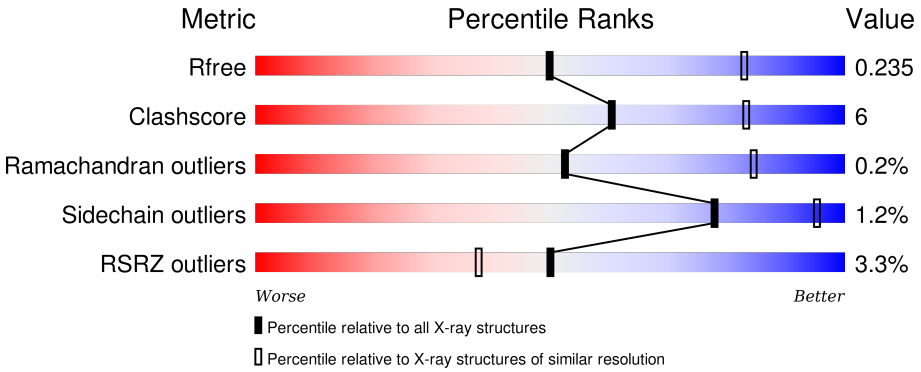
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	578	3% 83% 14%
1	B	578	4% 81% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9394 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 HISTONE ACETYLTRANSFERASE P300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4579	2921	777	848	33			
1	B	563	Total	C	N	O	S	0	0	0
			4598	2933	784	848	33			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1033	GLY	-	EXPRESSION TAG	UNP Q09472
A	1034	ALA	-	EXPRESSION TAG	UNP Q09472
A	1035	MET	-	EXPRESSION TAG	UNP Q09472
A	1036	ALA	-	EXPRESSION TAG	UNP Q09472
A	1037	GLY	-	EXPRESSION TAG	UNP Q09472
A	1038	LYS	-	EXPRESSION TAG	UNP Q09472
A	1039	ALA	-	EXPRESSION TAG	UNP Q09472
A	1040	VAL	-	EXPRESSION TAG	UNP Q09472
A	1041	PRO	-	EXPRESSION TAG	UNP Q09472
A	1042	MET	-	EXPRESSION TAG	UNP Q09472
A	1467	PHE	TYR	ENGINEERED MUTATION	UNP Q09472
A	1520	SER	-	LINKER	UNP Q09472
A	1521	GLY	-	LINKER	UNP Q09472
A	1522	GLY	-	LINKER	UNP Q09472
A	1523	SER	-	LINKER	UNP Q09472
A	1524	GLY	-	LINKER	UNP Q09472
B	1033	GLY	-	EXPRESSION TAG	UNP Q09472
B	1034	ALA	-	EXPRESSION TAG	UNP Q09472
B	1035	MET	-	EXPRESSION TAG	UNP Q09472
B	1036	ALA	-	EXPRESSION TAG	UNP Q09472
B	1037	GLY	-	EXPRESSION TAG	UNP Q09472
B	1038	LYS	-	EXPRESSION TAG	UNP Q09472
B	1039	ALA	-	EXPRESSION TAG	UNP Q09472
B	1040	VAL	-	EXPRESSION TAG	UNP Q09472
B	1041	PRO	-	EXPRESSION TAG	UNP Q09472

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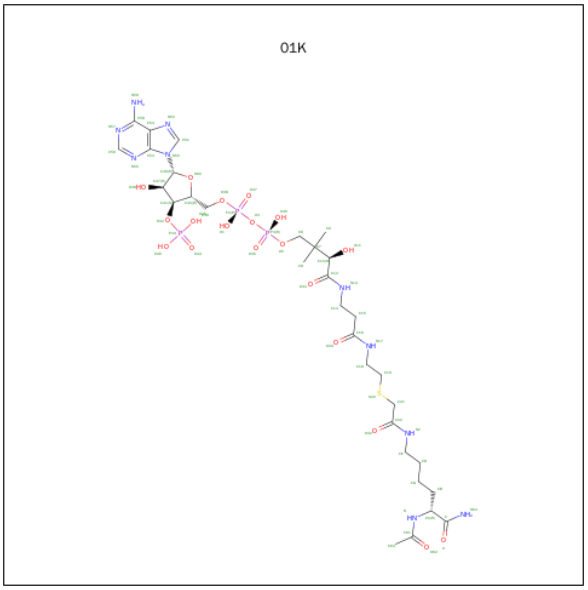
Chain	Residue	Modelled	Actual	Comment	Reference
B	1042	MET	-	EXPRESSION TAG	UNP Q09472
B	1467	PHE	TYR	ENGINEERED MUTATION	UNP Q09472
B	1520	SER	-	LINKER	UNP Q09472
B	1521	GLY	-	LINKER	UNP Q09472
B	1522	GLY	-	LINKER	UNP Q09472
B	1523	SER	-	LINKER	UNP Q09472
B	1524	GLY	-	LINKER	UNP Q09472

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Zn 3 3	0	0
2	A	4	Total Zn 4 4	0	0

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-3-(PHOSPHONOOXY)TETRAHYDROFURAN-2-YL]METHYL (3R,20R)-20-CARBAMOYL-3-HYDROXY-2,2-DIMETHYL-4,8,14,22-TETRAOXO-12-THIA-5,9,15,21-TETRAAZATRICOS-1-YL DIHYDROGEN DIPHOSPHATE (three-letter code: 01K) (formula: $C_{31}H_{53}N_{10}O_{19}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 64 31 10 19 3 1	0	0
3	B	1	Total C N O P S 64 31 10 19 3 1	0	0

- Molecule 4 is water.

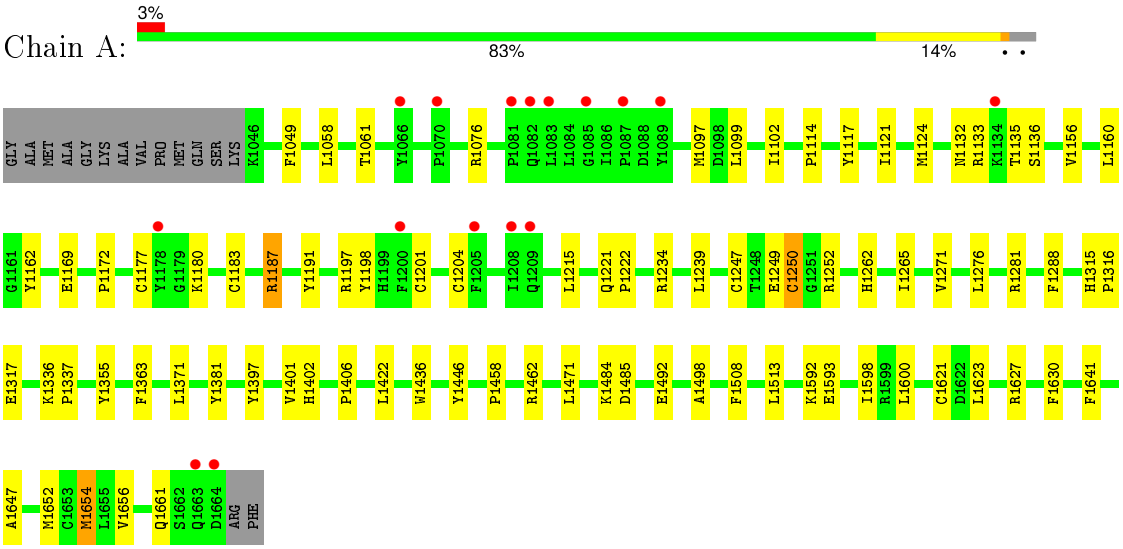
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	55	Total O 55 55	0	0
4	B	27	Total O 27 27	0	0

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.

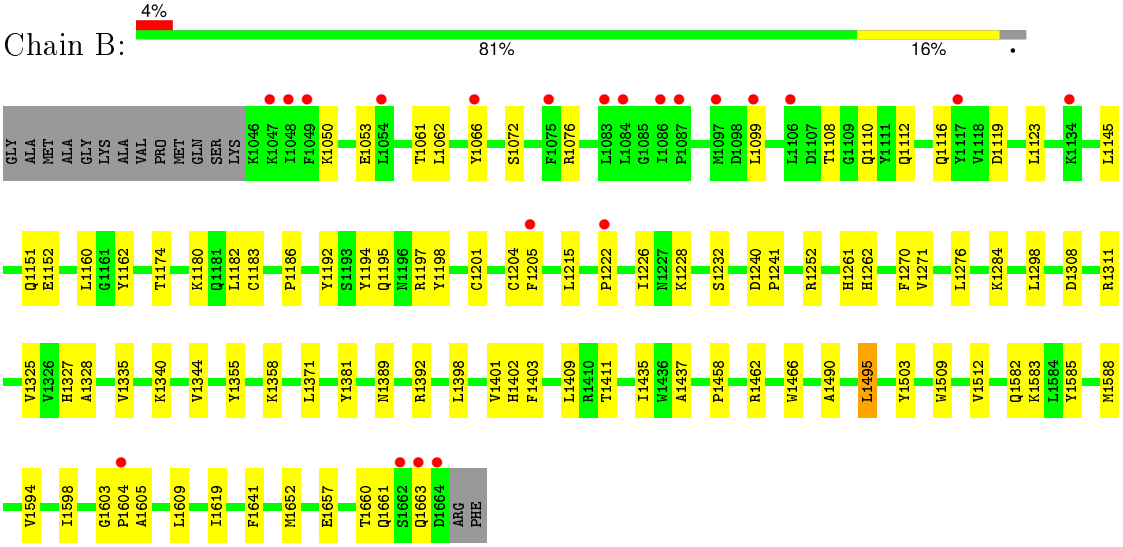
- Molecule 1: HISTONE ACETYLTRANSFERASE P300

Chain A:



- Molecule 1: HISTONE ACETYLTRANSFERASE P300

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.05Å 92.89Å 123.31Å 90.00° 98.43° 90.00°	Depositor
Resolution (Å)	46.62 – 2.80 46.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.62-2.80) 97.8 (46.62-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.208 , 0.244 0.189 , 0.235	Depositor DCC
R_{free} test set	2092 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 41387 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9394	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, 01K

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	0.45	0/4704	0.60	0/6367
1	B	0.39	0/4723	0.57	2/6389 (0.0%)
All	All	0.42	0/9427	0.59	2/12756 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1495	LEU	CA-CB-CG	6.21	129.59	115.30
1	B	1398	LEU	CA-CB-CG	5.89	128.85	115.30

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	4579	0	4441	52	0
1	B	4598	0	4482	50	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
3	A	64	0	48	2	0
3	B	64	0	48	0	0
4	A	55	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	0	0	0
All	All	9394	0	9019	103	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 (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:LEU:HD11	1:A:1647:ALA:HB1	1.60	0.83
1:A:1172:PRO:HG2	1:A:1187:ARG:HG3	1.69	0.74
1:A:1363:PHE:HE2	1:A:1654:MET:HE1	1.53	0.73
1:B:1174:THR:HG22	1:B:1186:PRO:HA	1.71	0.73
1:B:1660:THR:HG22	1:B:1663:GLN:HE21	1.53	0.72
1:A:1250:CYS:SG	1:A:1252:ARG:NH1	2.63	0.69
1:B:1112:GLN:H	1:B:1116:GLN:HE22	1.41	0.66
1:A:1371:LEU:HD11	1:A:1647:ALA:CB	2.26	0.64
4:A:2039:HOH:O	1:B:1151:GLN:OE1	2.15	0.64
1:A:1363:PHE:CE2	1:A:1654:MET:HE1	2.35	0.62
1:B:1605:ALA:HB1	1:B:1609:LEU:HD21	1.83	0.61
1:B:1180:LYS:HB2	1:B:1183:CYS:HB2	1.81	0.61
1:A:1317:GLU:HB2	1:A:1406:PRO:HB3	1.83	0.60
1:A:1262:HIS:HB2	1:A:1652:MET:HE2	1.84	0.59
1:B:1401:VAL:HG11	1:B:1641:PHE:HB3	1.85	0.58
1:B:1328:ALA:HB3	1:B:1619:ILE:H	1.67	0.58
1:B:1355:TYR:HB3	1:B:1381:TYR:CE2	2.38	0.58
1:A:1265:ILE:HG12	1:A:1288:PHE:HD2	1.68	0.57
1:B:1050:LYS:HB2	1:B:1053:GLU:HG3	1.87	0.57
1:A:1446:TYR:O	1:A:1627:ARG:HD2	2.05	0.57
1:A:1355:TYR:HB3	1:A:1381:TYR:CE2	2.39	0.57
1:A:1221:GLN:N	1:A:1222:PRO:HD2	2.22	0.54
1:A:1471:LEU:HD21	1:A:1598:ILE:HD13	1.89	0.54
1:A:1371:LEU:CD1	1:A:1647:ALA:HB1	2.34	0.53
1:A:1247:CYS:SG	1:A:1250:CYS:HB2	2.48	0.53
1:B:1509:TRP:HA	1:B:1512:VAL:HG12	1.88	0.53
1:A:1180:LYS:HB3	1:A:1183:CYS:HB2	1.91	0.53
1:B:1215:LEU:HD12	1:B:1226:ILE:HG13	1.91	0.53
1:A:1436:TRP:CH2	1:A:1508:PHE:HB2	2.43	0.52
1:B:1112:GLN:H	1:B:1116:GLN:NE2	2.08	0.52
1:A:1172:PRO:HD3	1:A:1239:LEU:HD23	1.92	0.52
1:B:1585:TYR:HA	1:B:1588:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:VAL:HG12	1:A:1276:LEU:HG	1.93	0.51
1:A:1133:ARG:C	1:A:1135:THR:H	2.14	0.51
1:B:1162:TYR:CE2	1:B:1252:ARG:HB3	2.45	0.51
1:B:1197:ARG:NH1	1:B:1198:TYR:OH	2.43	0.51
1:A:1498:ALA:HB1	1:A:1513:LEU:HD13	1.93	0.51
1:A:1401:VAL:HG11	1:A:1641:PHE:HB3	1.91	0.51
3:A:700:01K:O32	3:A:700:01K:H19A	2.07	0.50
1:B:1160:LEU:O	1:B:1252:ARG:NH1	2.46	0.49
1:B:1061:THR:HG22	1:B:1152:GLU:HB3	1.93	0.49
1:B:1298:LEU:HD23	1:B:1325:VAL:HG21	1.95	0.49
1:B:1458:PRO:HB3	1:B:1462:ARG:HD2	1.94	0.49
1:B:1197:ARG:HD2	1:B:1198:TYR:CZ	2.49	0.48
1:B:1308:ASP:OD1	1:B:1311:ARG:NH2	2.46	0.48
1:B:1582:GLN:HG3	1:B:1583:LYS:N	2.28	0.48
1:A:1249:GLU:OE2	1:A:1281:ARG:NH2	2.46	0.48
1:B:1194:TYR:CD2	1:B:1195:GLN:HG3	2.49	0.48
1:B:1205:PHE:CZ	1:B:1228:LYS:HG3	2.49	0.47
1:A:1623:LEU:HB2	1:A:1661:GLN:HE22	1.79	0.47
1:A:1355:TYR:HB3	1:A:1381:TYR:CD2	2.50	0.47
1:B:1490:ALA:HB1	1:B:1495:LEU:HG	1.95	0.47
1:A:1458:PRO:HB3	1:A:1462:ARG:HD2	1.96	0.46
1:B:1409:LEU:HD23	1:B:1409:LEU:HA	1.64	0.46
1:A:1177:CYS:HB3	1:A:1183:CYS:HB3	1.65	0.46
1:B:1119:ASP:O	1:B:1123:LEU:N	2.43	0.46
1:A:1371:LEU:CD1	1:A:1647:ALA:CB	2.93	0.45
1:A:1132:ASN:HB3	1:A:1136:SER:OG	2.16	0.45
1:A:1262:HIS:HB2	1:A:1652:MET:CE	2.45	0.45
1:B:1271:VAL:HG12	1:B:1276:LEU:HG	1.98	0.45
1:A:1397:TYR:OH	3:A:700:01K:N64	2.49	0.45
1:A:1114:PRO:HG2	1:A:1162:TYR:CE2	2.52	0.45
1:A:1513:LEU:HA	1:A:1513:LEU:HD23	1.74	0.44
1:B:1108:THR:OG1	1:B:1110:GLN:NE2	2.48	0.44
1:A:1484:LYS:HE2	1:A:1492:GLU:OE2	2.18	0.44
1:A:1160:LEU:O	1:A:1252:ARG:NH2	2.50	0.44
1:A:1485:ASP:HB2	1:A:1592:LYS:O	2.17	0.44
1:B:1261:HIS:CG	1:B:1270:PHE:HB2	2.53	0.44
1:A:1191:TYR:CE1	1:A:1234:ARG:HB2	2.52	0.43
1:A:1162:TYR:CE1	1:A:1252:ARG:HB3	2.53	0.43
1:B:1145:LEU:HD23	1:B:1145:LEU:HA	1.86	0.43
1:B:1603:GLY:HA3	1:B:1604:PRO:HD3	1.85	0.43
1:A:1058:LEU:HD13	1:A:1117:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1422:LEU:HD22	1:A:1600:LEU:HD21	2.01	0.43
1:B:1192:TYR:HA	1:B:1232:SER:O	2.18	0.43
1:A:1593:GLU:H	1:A:1593:GLU:CD	2.22	0.43
1:A:1169:GLU:OE2	1:A:1239:LEU:HD13	2.19	0.43
1:A:1315:HIS:ND1	1:A:1316:PRO:HD2	2.34	0.43
1:A:1061:THR:CG2	1:A:1156:VAL:HG21	2.49	0.43
1:B:1437:ALA:O	1:B:1594:VAL:HG13	2.19	0.43
1:B:1072:SER:O	1:B:1076:ARG:HG3	2.19	0.43
1:B:1411:THR:HG23	1:B:1466:TRP:HE1	1.84	0.42
1:B:1182:LEU:HD23	1:B:1182:LEU:HA	1.95	0.42
1:B:1355:TYR:HB3	1:B:1381:TYR:CD2	2.53	0.42
1:B:1657:GLU:O	1:B:1661:GLN:HG3	2.19	0.42
1:A:1097:MET:HB3	1:A:1124:MET:HB2	2.02	0.42
1:B:1262:HIS:HB2	1:B:1652:MET:CE	2.50	0.42
1:B:1062:LEU:HD11	1:B:1099:LEU:HD22	2.02	0.41
1:A:1336:LYS:HB3	1:A:1337:PRO:HD2	2.02	0.41
1:B:1389:ASN:HA	1:B:1392:ARG:HD2	2.00	0.41
1:B:1371:LEU:HD21	1:B:1403:PHE:HB2	2.01	0.41
1:A:1076:ARG:HA	1:A:1099:LEU:HB2	2.03	0.41
1:B:1327:HIS:O	1:B:1358:LYS:HA	2.21	0.41
1:B:1284:LYS:HD2	1:B:1284:LYS:N	2.36	0.41
1:B:1435:ILE:HD12	1:B:1598:ILE:HD11	2.03	0.41
1:A:1630:PHE:CE1	1:A:1654:MET:HG3	2.56	0.41
1:B:1340:LYS:O	1:B:1344:VAL:HB	2.21	0.41
1:A:1102:ILE:HD13	1:A:1121:ILE:HD13	2.03	0.40
1:B:1240:ASP:HA	1:B:1241:PRO:HD3	1.97	0.40
1:A:1114:PRO:HG2	1:A:1162:TYR:HE2	1.87	0.40
1:B:1335:VAL:HA	1:B:1503:TYR:CE2	2.57	0.40
1:A:1198:TYR:HB3	1:A:1215:LEU:HD11	2.03	0.40
1:A:1652:MET:O	1:A:1656:VAL:HG23	2.21	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	561/578 (97%)	530 (94%)	30 (5%)	1 (0%)	52 84
1	B	561/578 (97%)	536 (96%)	24 (4%)	1 (0%)	52 84
All	All	1122/1156 (97%)	1066 (95%)	54 (5%)	2 (0%)	52 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1621	CYS
1	B	1222	PRO

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	507/522 (97%)	499 (98%)	8 (2%)	70 93
1	B	511/522 (98%)	507 (99%)	4 (1%)	86 97
All	All	1018/1044 (98%)	1006 (99%)	12 (1%)	78 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1049	PHE
1	A	1187	ARG
1	A	1197	ARG
1	A	1201	CYS
1	A	1204	CYS
1	A	1250	CYS
1	A	1402	HIS
1	A	1654	MET
1	B	1066	TYR
1	B	1201	CYS
1	B	1204	CYS

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Mol	Chain	Res	Type
1	B	1402	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1415	HIS
1	B	1116	GLN
1	B	1663	GLN

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, 7 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	01K	A	700	-	56,66,66	1.88	10 (17%)	69,95,95	1.84	13 (18%)
3	01K	B	700	-	56,66,66	1.88	11 (19%)	69,95,95	2.16	16 (23%)

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
3	01K	A	700	-	-	0/64/84/84	0/3/3/3
3	01K	B	700	-	-	0/64/84/84	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	01K	O48-C47	-3.07	1.35	1.43
3	A	700	01K	O48-C47	-2.74	1.36	1.43
3	A	700	01K	O11-C10	-2.25	1.37	1.42
3	A	700	01K	C21-S20	-2.18	1.76	1.81
3	B	700	01K	O11-C10	-2.16	1.37	1.42
3	A	700	01K	O60-C40	-2.10	1.40	1.45
3	B	700	01K	C21-S20	-2.04	1.77	1.81
3	B	700	01K	C41-C40	2.22	1.59	1.52
3	A	700	01K	C61-N	2.40	1.43	1.34
3	B	700	01K	C61-N	2.41	1.43	1.34
3	B	700	01K	O60-C49	2.55	1.44	1.41
3	B	700	01K	C58-N59	3.10	1.44	1.34
3	A	700	01K	C58-N59	3.33	1.45	1.34
3	B	700	01K	C12-N13	4.27	1.42	1.33
3	A	700	01K	C12-N13	5.08	1.44	1.33
3	A	700	01K	C22-NZ	5.19	1.45	1.33
3	B	700	01K	C16-N17	5.71	1.47	1.33
3	B	700	01K	C22-NZ	5.82	1.47	1.33
3	A	700	01K	C16-N17	5.92	1.47	1.33
3	B	700	01K	C-N64	6.20	1.45	1.32
3	A	700	01K	C-N64	6.30	1.45	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	700	01K	N55-C56-N57	-10.73	120.68	128.89
3	A	700	01K	N55-C56-N57	-9.05	121.97	128.89
3	B	700	01K	C18-N17-C16	-4.83	113.29	122.79
3	B	700	01K	P4-O3-P2	-4.77	119.35	132.73
3	A	700	01K	P4-O3-P2	-4.33	120.56	132.73
3	B	700	01K	C18-C19-S20	-3.68	100.60	114.25
3	B	700	01K	O62-C61-N	-3.30	115.13	121.86
3	A	700	01K	CG-CB-CA	-3.19	104.09	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	700	01K	O11-C10-C12	-3.05	103.39	110.38
3	B	700	01K	O5-C6-C7	-3.02	105.69	110.55
3	B	700	01K	CG-CB-CA	-2.55	106.05	113.91
3	B	700	01K	O33-C16-N17	-2.53	117.92	122.94
3	A	700	01K	C47-C49-N50	-2.50	110.48	114.29
3	B	700	01K	C54-C53-N52	-2.46	107.22	109.48
3	A	700	01K	C54-C53-N52	-2.45	107.22	109.48
3	B	700	01K	C47-C49-N50	-2.39	110.64	114.29
3	A	700	01K	O62-C61-N	-2.19	117.39	121.86
3	A	700	01K	O62-C61-C63	-2.14	118.14	122.06
3	A	700	01K	C18-C19-S20	-2.11	106.44	114.25
3	B	700	01K	O42-C41-C47	2.06	119.52	111.51
3	A	700	01K	C8-C7-C6	2.06	111.17	108.50
3	B	700	01K	CA-N-C61	2.14	128.68	121.37
3	B	700	01K	C15-C16-N17	2.20	120.29	116.46
3	A	700	01K	O3-P4-O5	2.24	108.89	102.94
3	B	700	01K	C8-C7-C6	2.31	111.50	108.50
3	B	700	01K	O3-P2-O38	2.33	109.11	102.94
3	A	700	01K	O60-C49-N50	2.39	113.10	108.10
3	A	700	01K	C63-C61-N	4.36	124.46	116.11
3	B	700	01K	C63-C61-N	5.06	125.79	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	01K	2	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, 95^{th} 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	563/578 (97%)	-0.04	16 (2%) 56 44	32, 62, 150, 186	0
1	B	563/578 (97%)	0.01	21 (3%) 45 33	45, 81, 153, 188	0
All	All	1126/1156 (97%)	-0.01	37 (3%) 50 38	32, 74, 152, 188	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1664	ASP	7.2
1	B	1604	PRO	6.5
1	A	1664	ASP	5.5
1	B	1663	GLN	5.0
1	A	1087	PRO	4.9
1	B	1087	PRO	4.6
1	A	1663	GLN	4.0
1	A	1083	LEU	3.6
1	B	1134	LYS	3.6
1	B	1086	ILE	3.5
1	B	1099	LEU	3.4
1	B	1097	MET	3.2
1	A	1081	PRO	3.0
1	B	1083	LEU	2.9
1	B	1222	PRO	2.8
1	B	1084	LEU	2.8
1	A	1085	GLY	2.7
1	A	1134	LYS	2.7
1	B	1049	PHE	2.7
1	B	1117	TYR	2.6
1	B	1106	LEU	2.5
1	B	1047	LYS	2.5
1	A	1089	TYR	2.4
1	A	1082	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1205	PHE	2.3
1	B	1054	LEU	2.3
1	A	1208	ILE	2.2
1	B	1075	PHE	2.2
1	B	1662	SER	2.2
1	A	1178	TYR	2.2
1	A	1066	TYR	2.2
1	B	1048	ILE	2.1
1	A	1209	GLN	2.1
1	A	1200	PHE	2.1
1	B	1066	TYR	2.1
1	A	1070	PRO	2.0
1	A	1205	PHE	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, 95^{th} 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	01K	A	700	64/64	0.98	0.19	0.64	34,45,64,72	0
3	01K	B	700	64/64	0.97	0.17	0.18	40,54,68,80	0
2	ZN	A	2	1/1	0.99	0.12	-0.17	74,74,74,74	0
2	ZN	B	1	1/1	0.99	0.13	-0.40	70,70,70,70	0
2	ZN	B	2	1/1	0.98	0.08	-0.60	105,105,105,105	0
2	ZN	A	3	1/1	0.96	0.11	-0.88	131,131,131,131	0
2	ZN	B	3	1/1	0.96	0.10	-0.98	123,123,123,123	0
2	ZN	A	1	1/1	1.00	0.11	-1.28	59,59,59,59	0
2	ZN	A	4	1/1	0.98	0.14	-	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.