Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:05 PM GMT

PDB ID	:	4BGD
Title	:	Crystal structure of Brr2 in complex with the Jab1/MPN domain of Prp8
Authors	:	Nguyen, T.H.D.; Li, J.; Nagai, K.
Deposited on	:	2013-03-25
Resolution	:	3.10 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:

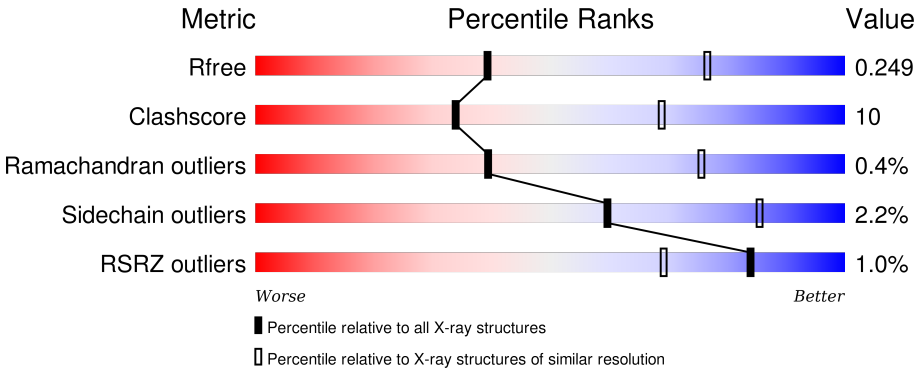
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	1722	% 74% 24% ··
2	C	248	% 87% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15738 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.

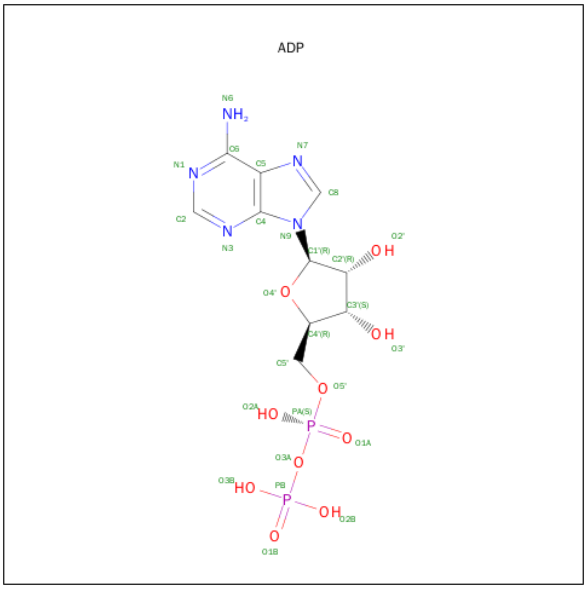
- Molecule 1 is a protein called PRE-MRNA-SPLICING HELICASE BRR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1707	13679	8761	2279	2584	55	0	1	0

- Molecule 2 is a protein called PRE-MRNA-SPLICING FACTOR 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	248	1989	1284	322	377	6	0	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

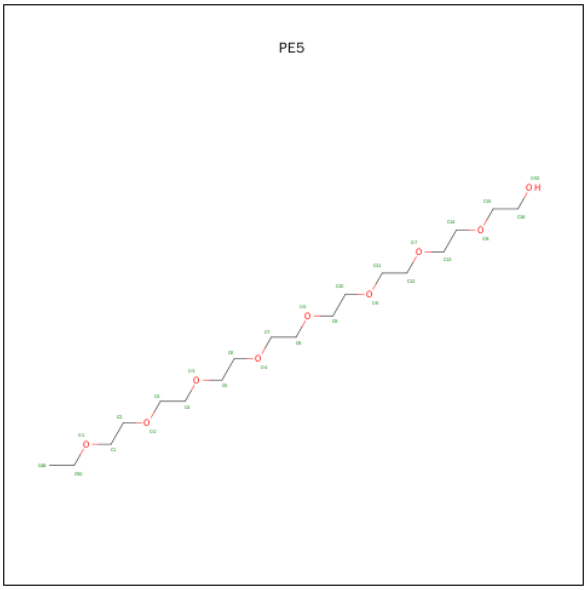


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: $C_{18}H_{38}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 27 18 9	0	0

- Molecule 6 is water.

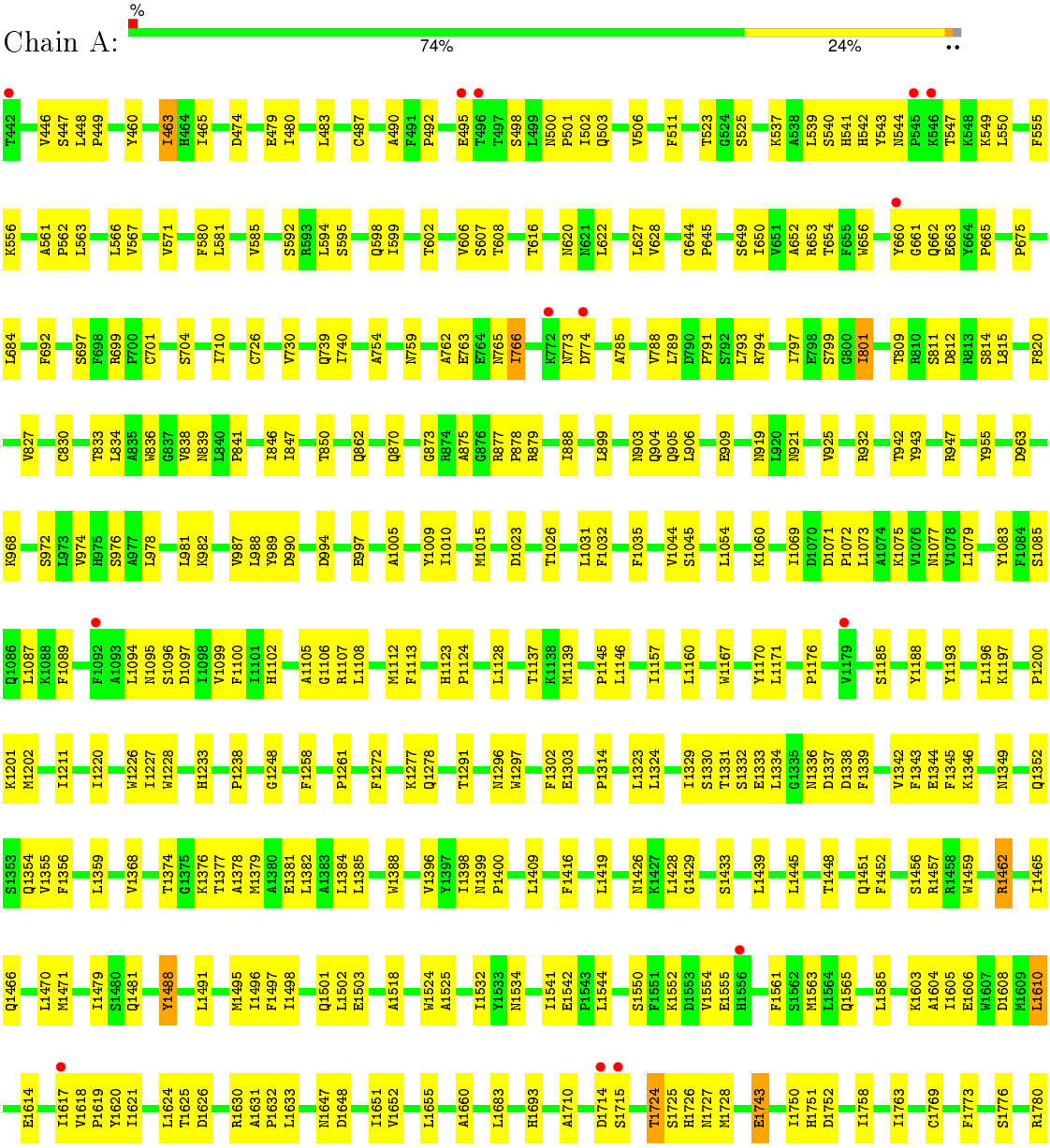
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	14	Total O 14 14	0	0
6	C	1	Total O 1 1	0	0

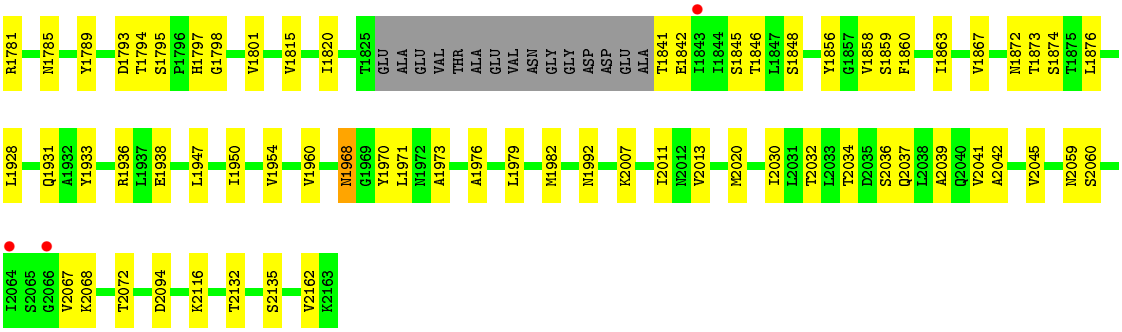
3 Residue-property plots (i)

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.

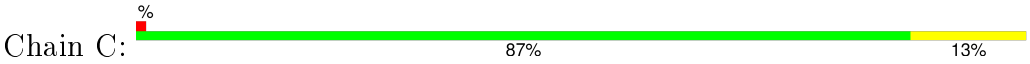
- Molecule 1: PRE-MRNA-SPLICING HELICASE BRR2

Chain A:





- Molecule 2: PRE-MRNA-SPLICING FACTOR 8



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.64Å 178.64Å 180.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.37 – 3.10 92.20 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (92.37-3.10) 99.4 (92.20-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.214 , 0.270 0.192 , 0.249	Depositor DCC
R_{free} test set	3204 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	101.4	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 83.0	EDS
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 63429 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15738	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: PE5, MG, ADP

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	0.52	0/13978	0.74	1/18952 (0.0%)
2	C	0.55	0/2038	0.73	0/2764
All	All	0.53	0/16016	0.73	1/21716 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1462	ARG	NE-CZ-NH1	5.84	123.22	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	13679	0	13683	297	0
2	C	1989	0	1951	21	0
3	A	27	0	12	1	0
4	A	1	0	0	0	0
5	A	27	0	38	3	0
6	A	14	0	0	3	0
6	C	1	0	0	0	0
All	All	15738	0	15684	317	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 10.

All (317) 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:1518:ALA:HB2	1:A:1534:ASN:HD22	1.31	0.94
1:A:1185:SER:OG	1:A:1188:TYR:HD2	1.55	0.87
1:A:1409:LEU:HD22	1:A:1426:ASN:HB2	1.55	0.86
1:A:567:VAL:HG13	1:A:606:VAL:HG12	1.62	0.80
1:A:1439:LEU:HA	1:A:1445:LEU:HD11	1.64	0.80
1:A:556:LYS:NZ	1:A:602:THR:O	2.14	0.79
1:A:523:THR:HG22	1:A:873:GLY:HA2	1.64	0.79
1:A:699:ARG:NH2	1:A:875:ALA:O	2.17	0.77
1:A:580:PHE:CE1	1:A:581:LEU:HG	2.19	0.77
1:A:495:GLU:HG2	1:A:879:ARG:HG2	1.66	0.77
1:A:1005:ALA:HB2	1:A:1015:MET:HG3	1.67	0.76
1:A:789:LEU:HD23	1:A:794:ARG:HA	1.66	0.75
1:A:1781:ARG:HG3	1:A:1789:TYR:OH	1.88	0.73
1:A:903:ASN:O	1:A:905:GLN:HG3	1.88	0.73
1:A:2034:THR:OG1	1:A:2037:GLN:HG3	1.90	0.72
1:A:616:THR:HG23	1:A:653:ARG:HH11	1.52	0.72
1:A:1743:GLU:OE2	1:A:1781:ARG:HD2	1.90	0.72
1:A:1023[B]:ASP:OD2	6:A:3003:HOH:O	2.08	0.72
1:A:1185:SER:HG	1:A:1188:TYR:HD2	0.76	0.71
1:A:1023[B]:ASP:OD2	6:A:3002:HOH:O	2.08	0.71
2:C:2225:VAL:HG11	2:C:2242:PRO:HG3	1.71	0.70
1:A:523:THR:HG22	1:A:873:GLY:CA	2.21	0.69
1:A:1758:ILE:HG22	1:A:1846:THR:HG23	1.74	0.68
1:A:1863:ILE:O	1:A:1867:VAL:HG23	1.93	0.67
1:A:830:CYS:SG	1:A:834:LEU:HD22	2.35	0.67
1:A:1793:ASP:HB3	1:A:1798:GLY:HA3	1.76	0.67
1:A:1858:VAL:HG21	1:A:1960:VAL:HG21	1.75	0.67
1:A:1226:TRP:HD1	1:A:1233:HIS:CE1	2.13	0.66
1:A:921:ASN:O	1:A:925:VAL:HG23	1.94	0.66
1:A:1876:LEU:HD11	1:A:1982:MET:CE	2.26	0.66
1:A:1624:LEU:CD1	1:A:1630:ARG:HD2	2.26	0.66
1:A:1045:SER:O	1:A:1075:LYS:HE2	1.96	0.66
1:A:1518:ALA:HB2	1:A:1534:ASN:ND2	2.09	0.66
1:A:1409:LEU:CD2	1:A:1426:ASN:HB2	2.26	0.65
1:A:1631:ALA:HB3	1:A:1632:PRO:HD3	1.78	0.65
1:A:2011:ILE:HD12	1:A:2030:ILE:HD11	1.77	0.65
1:A:740:ILE:HD11	1:A:846:ILE:CD1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1429:GLY:HA2	1:A:1451:GLN:HG2	1.78	0.64
1:A:663:GLU:O	1:A:663:GLU:HG3	1.98	0.64
1:A:1872:ASN:OD1	1:A:1873:THR:HG23	1.98	0.64
1:A:2020:MET:HG2	1:A:2045:VAL:CG1	2.28	0.63
1:A:1456:SER:HA	1:A:1465:ILE:HD13	1.79	0.63
1:A:988:LEU:HB2	1:A:997:GLU:HB3	1.81	0.62
1:A:981:LEU:HB3	1:A:987:VAL:HG22	1.81	0.62
1:A:1625:THR:OG1	1:A:1648:ASP:CG	2.37	0.62
1:A:487:CYS:O	1:A:490:ALA:N	2.33	0.62
1:A:1585:LEU:HD21	1:A:1683:LEU:HD23	1.82	0.62
1:A:1554:VAL:HG21	1:A:1563:MET:CE	2.30	0.62
1:A:1226:TRP:CD1	1:A:1233:HIS:CE1	2.88	0.61
1:A:1355:VAL:HG12	1:A:1359:LEU:HG	1.82	0.61
1:A:765:ASN:OD1	1:A:766:ILE:N	2.34	0.61
1:A:1973:ALA:O	1:A:1976:ALA:HB3	2.01	0.60
1:A:809:THR:HB	1:A:812:ASP:HB2	1.82	0.60
1:A:1758:ILE:HG22	1:A:1846:THR:CG2	2.30	0.60
1:A:537:LYS:HE2	1:A:541:HIS:HE1	1.66	0.60
1:A:740:ILE:HD11	1:A:846:ILE:HD11	1.83	0.60
1:A:1054:LEU:HD13	1:A:1094:LEU:HD11	1.84	0.60
1:A:1171:LEU:HD23	1:A:1196:LEU:HD22	1.82	0.59
2:C:2183:TYR:CE2	2:C:2289:ILE:HG21	2.37	0.59
1:A:1452:PHE:HD2	1:A:1491:LEU:HD11	1.67	0.59
1:A:1524:TRP:HB2	1:A:1780:ARG:HD2	1.85	0.59
1:A:785:ALA:O	1:A:789:LEU:HD22	2.02	0.58
1:A:1561:PHE:HE1	1:A:1565:GLN:HE21	1.50	0.58
1:A:543:TYR:HB3	1:A:550:LEU:CD1	2.34	0.58
1:A:1324:LEU:N	1:A:1354:GLN:HE22	2.01	0.58
1:A:556:LYS:HG3	1:A:627:LEU:HB2	1.84	0.58
1:A:1633:LEU:HD21	1:A:1655:LEU:HD13	1.85	0.58
1:A:789:LEU:HB3	1:A:794:ARG:HB2	1.86	0.58
1:A:1604:ALA:O	1:A:1605:ILE:HD13	2.04	0.57
1:A:1334:LEU:CD1	1:A:1339:PHE:HB2	2.33	0.57
1:A:1330:SER:H	1:A:1333:GLU:HG3	1.67	0.57
1:A:1220:ILE:HD11	1:A:1272:PHE:HE2	1.70	0.57
1:A:1776:SER:O	1:A:1780:ARG:NH1	2.38	0.57
1:A:2034:THR:OG1	1:A:2037:GLN:CG	2.53	0.56
1:A:834:LEU:HD12	1:A:838:VAL:HG21	1.87	0.56
1:A:660:TYR:HE1	1:A:1605:ILE:HD11	1.69	0.56
1:A:542:HIS:CD2	1:A:555:PHE:HB3	2.40	0.56
1:A:544:ASN:HB2	1:A:547:THR:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1750:ILE:HD11	1:A:1773:PHE:HZ	1.71	0.56
1:A:1079:LEU:HD21	1:A:1094:LEU:HD21	1.88	0.56
1:A:1336:ASN:OD1	1:A:1337:ASP:N	2.39	0.56
1:A:1378:ALA:HA	1:A:1381:GLU:OE1	2.05	0.56
1:A:1763:ILE:HG21	1:A:1769:CYS:SG	2.46	0.56
2:C:2354:GLY:O	2:C:2355:ASN:HB2	2.05	0.56
1:A:1625:THR:HG21	1:A:1647:ASN:HB2	1.87	0.55
1:A:1334:LEU:CD1	1:A:1339:PHE:CB	2.84	0.55
2:C:2388:ARG:HD2	2:C:2391:HIS:CD2	2.41	0.55
1:A:1751:HIS:CD2	1:A:1860:PHE:CE2	2.94	0.55
1:A:1329:ILE:HG21	1:A:1356:PHE:CD2	2.41	0.55
1:A:1197:LYS:HB3	1:A:1227:ILE:HD12	1.89	0.55
1:A:628:VAL:O	1:A:665:PRO:HB3	2.07	0.55
1:A:1795:SER:O	1:A:1798:GLY:N	2.39	0.55
1:A:1343:PHE:O	1:A:1344:GLU:HG2	2.06	0.55
1:A:1083:TYR:CE2	1:A:1102:HIS:HB2	2.42	0.55
1:A:692:PHE:HA	5:A:3166:PE5:H61	1.89	0.55
1:A:1291:THR:HG23	1:A:1303:GLU:HB3	1.89	0.55
1:A:1044:VAL:O	1:A:1072:PRO:HB3	2.07	0.55
1:A:1781:ARG:CG	1:A:1789:TYR:OH	2.54	0.55
1:A:1928:LEU:O	1:A:1931:GLN:N	2.40	0.55
1:A:1396:VAL:HG12	1:A:1398:ILE:CD1	2.37	0.54
1:A:644:GLY:N	1:A:645:PRO:CD	2.71	0.54
1:A:523:THR:O	1:A:699:ARG:NH1	2.41	0.54
1:A:539:LEU:HD23	1:A:581:LEU:HD13	1.90	0.54
1:A:1933:TYR:HB2	1:A:1947:LEU:HD21	1.88	0.53
1:A:1462:ARG:HH11	1:A:1462:ARG:HG3	1.73	0.53
1:A:650:ILE:O	1:A:654:THR:HG23	2.08	0.53
1:A:847:ILE:HD12	1:A:888:ILE:HG13	1.91	0.53
1:A:1876:LEU:HD11	1:A:1982:MET:HE1	1.89	0.53
1:A:543:TYR:HB3	1:A:550:LEU:HD12	1.88	0.53
1:A:660:TYR:CE1	1:A:1605:ILE:HD11	2.44	0.53
1:A:762:ALA:HB2	1:A:766:ILE:HD12	1.90	0.53
1:A:2059:ASN:O	1:A:2059:ASN:OD1	2.27	0.53
1:A:1374:THR:O	1:A:1374:THR:HG22	2.07	0.53
1:A:547:THR:HG22	1:A:549:LYS:N	2.23	0.53
1:A:789:LEU:CD1	1:A:815:LEU:HD22	2.39	0.53
1:A:547:THR:HG22	1:A:549:LYS:H	1.73	0.52
1:A:1624:LEU:HD13	1:A:1630:ARG:HD2	1.90	0.52
1:A:2007:LYS:HB3	1:A:2030:ILE:HD13	1.91	0.52
1:A:2020:MET:HG2	1:A:2045:VAL:HG13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:LEU:HD12	1:A:997:GLU:HG2	1.91	0.52
1:A:1054:LEU:HB3	1:A:1069:ILE:HD11	1.91	0.52
1:A:2135:SER:HA	1:A:2162:VAL:HB	1.90	0.52
1:A:1502:LEU:O	1:A:1503:GLU:C	2.47	0.52
1:A:762:ALA:HA	1:A:766:ILE:HB	1.91	0.52
1:A:739:GLN:NE2	1:A:820:PHE:O	2.42	0.52
1:A:1428:LEU:CD2	1:A:2094:ASP:H	2.22	0.52
1:A:1248:GLY:HA3	2:C:2378:ILE:HG12	1.92	0.51
1:A:1399:ASN:O	1:A:1448:THR:HA	2.10	0.51
1:A:1429:GLY:CA	1:A:1451:GLN:HG2	2.39	0.51
1:A:1113:PHE:N	1:A:1128:LEU:HD13	2.25	0.51
1:A:1950:ILE:O	1:A:1954:VAL:HG13	2.11	0.51
1:A:1724:THR:HG23	1:A:1725:SER:N	2.25	0.51
1:A:1089:PHE:CD1	1:A:1094:LEU:HD22	2.46	0.51
1:A:1541:ILE:HD12	1:A:1542:GLU:N	2.26	0.51
1:A:1336:ASN:OD1	1:A:1338:ASP:N	2.43	0.51
1:A:1544:LEU:CD1	1:A:1710:ALA:HB3	2.40	0.51
1:A:1452:PHE:CD2	1:A:1491:LEU:HD11	2.46	0.51
1:A:479:GLU:HA	1:A:498:SER:CB	2.40	0.51
1:A:523:THR:CG2	1:A:873:GLY:CA	2.88	0.51
1:A:789:LEU:HD21	1:A:797:ILE:HG13	1.92	0.51
1:A:1743:GLU:HB3	1:A:1789:TYR:OH	2.10	0.51
1:A:1399:ASN:OD1	1:A:1400:PRO:HD2	2.10	0.51
1:A:561:ALA:HB1	1:A:566:LEU:HD22	1.93	0.51
2:C:2290:ASP:C	2:C:2290:ASP:OD1	2.50	0.51
1:A:1137:THR:OG1	1:A:1139:MET:HG2	2.10	0.51
1:A:1856:TYR:OH	1:A:2116:LYS:NZ	2.41	0.51
2:C:2320:ASP:OD1	2:C:2321:ILE:N	2.44	0.51
1:A:1376:LYS:HE2	6:A:3012:HOH:O	2.11	0.50
1:A:1620:TYR:HD1	1:A:1651:ILE:HD11	1.77	0.50
1:A:1727:ASN:OD1	1:A:1728:MET:N	2.45	0.50
1:A:1876:LEU:HD11	1:A:1982:MET:HE3	1.93	0.50
1:A:1462:ARG:HH11	1:A:1462:ARG:CG	2.25	0.50
1:A:1625:THR:OG1	1:A:1648:ASP:OD2	2.29	0.50
1:A:2036:SER:O	1:A:2039:ALA:HB3	2.11	0.50
2:C:2251:GLU:OE1	2:C:2251:GLU:N	2.45	0.50
1:A:850:THR:OG1	1:A:862:GLN:NE2	2.44	0.50
1:A:1752:ASP:OD1	1:A:1860:PHE:N	2.44	0.49
1:A:1550:SER:HB2	1:A:1726:HIS:HA	1.93	0.49
1:A:906:LEU:HD23	1:A:906:LEU:O	2.12	0.49
2:C:2189:LEU:HD11	2:C:2347:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:VAL:HG13	1:A:585:VAL:HG12	1.93	0.49
1:A:480:ILE:HG23	1:A:483:LEU:HD12	1.93	0.49
1:A:1331:THR:O	1:A:1334:LEU:HG	2.13	0.49
1:A:500:ASN:HB2	1:A:501:PRO:CD	2.43	0.49
1:A:1794:THR:O	1:A:1794:THR:HG22	2.13	0.49
1:A:1614:GLU:O	1:A:1617:ILE:HG12	2.13	0.48
1:A:1462:ARG:HD3	1:A:1465:ILE:HD12	1.95	0.48
1:A:1976:ALA:O	1:A:1979:LEU:HB3	2.14	0.48
1:A:1858:VAL:HG21	1:A:1960:VAL:CG2	2.43	0.48
1:A:1009:TYR:O	1:A:1107:ARG:NH1	2.46	0.48
2:C:2238:ILE:HG22	2:C:2239:SER:O	2.13	0.48
1:A:1201:LYS:HG3	1:A:1202:MET:N	2.29	0.48
1:A:963:ASP:OD1	1:A:968:LYS:N	2.41	0.48
1:A:982:LYS:HD3	1:A:989:TYR:HB3	1.96	0.48
1:A:449:PRO:HG2	1:A:465:ILE:HG23	1.96	0.48
1:A:1479:ILE:HG22	1:A:1488:TYR:HB3	1.95	0.48
1:A:1323:LEU:HD12	1:A:1323:LEU:O	2.13	0.48
1:A:1146:LEU:HB2	1:A:1157:ILE:HG22	1.96	0.48
1:A:1085:SER:HB2	1:A:1087:LEU:HD13	1.96	0.47
1:A:1160:LEU:HD22	1:A:1170:TYR:CZ	2.49	0.47
1:A:446:VAL:O	1:A:448:LEU:HD12	2.14	0.47
1:A:793:LEU:HD23	1:A:797:ILE:HG13	1.96	0.47
1:A:616:THR:CG2	1:A:653:ARG:HH11	2.23	0.47
1:A:1343:PHE:O	1:A:1345:PHE:CD2	2.67	0.47
1:A:1368:VAL:HG11	1:A:1379:MET:SD	2.54	0.47
1:A:1331:THR:HG23	1:A:1346:LYS:O	2.15	0.47
1:A:1459:TRP:CD1	1:A:1498:ILE:HD11	2.49	0.47
1:A:1238:PRO:HD2	1:A:1296:ASN:ND2	2.30	0.47
1:A:495:GLU:HG3	1:A:879:ARG:HE	1.80	0.47
1:A:701:CYS:HB2	1:A:878:PRO:HA	1.97	0.47
1:A:1176:PRO:HA	1:A:1193:TYR:CD2	2.49	0.46
1:A:942:THR:HG22	1:A:943:TYR:N	2.30	0.46
1:A:793:LEU:HD23	1:A:797:ILE:CG1	2.45	0.46
1:A:1856:TYR:HB2	1:A:1858:VAL:HG23	1.96	0.46
1:A:1724:THR:CG2	1:A:1725:SER:N	2.78	0.46
2:C:2270:ALA:O	2:C:2274:VAL:HG23	2.15	0.46
1:A:759:ASN:O	1:A:763:GLU:HG3	2.14	0.46
1:A:838:VAL:HG12	1:A:839:ASN:N	2.31	0.46
1:A:1648:ASP:O	1:A:1651:ILE:HG22	2.15	0.46
1:A:754:ALA:O	1:A:801:ILE:HD11	2.15	0.46
1:A:1035:PHE:HA	1:A:1112:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:ALA:O	1:A:656:TRP:HB3	2.16	0.46
1:A:1060:LYS:O	2:C:2395:PHE:CD1	2.68	0.46
1:A:1648:ASP:O	1:A:1652:VAL:HG23	2.16	0.46
2:C:2204:ALA:CB	2:C:2238:ILE:HD11	2.46	0.46
1:A:1633:LEU:HD21	1:A:1655:LEU:CD1	2.45	0.45
1:A:932:ARG:HB2	1:A:974:VAL:HG11	1.98	0.45
1:A:841:PRO:HB2	1:A:877:ARG:HG2	1.98	0.45
1:A:1334:LEU:CD1	1:A:1339:PHE:HB3	2.47	0.45
1:A:1343:PHE:O	1:A:1345:PHE:N	2.49	0.45
1:A:675:PRO:HD3	1:A:904:GLN:O	2.16	0.45
1:A:1071:ASP:OD2	1:A:1073:LEU:HB2	2.16	0.45
1:A:1388:TRP:HZ3	1:A:1419:LEU:HD12	1.82	0.45
1:A:903:ASN:O	1:A:905:GLN:CG	2.61	0.45
1:A:1079:LEU:HA	1:A:1079:LEU:HD23	1.82	0.45
1:A:726:CYS:O	1:A:730:VAL:HG23	2.17	0.45
1:A:598:GLN:CG	1:A:599:ILE:N	2.80	0.44
1:A:1428:LEU:HD23	1:A:2094:ASP:H	1.83	0.44
1:A:1200:PRO:HG2	1:A:1297:TRP:CD1	2.52	0.44
1:A:540:SER:HA	1:A:543:TYR:CE2	2.53	0.44
1:A:773:ASN:OD1	1:A:774:ASP:N	2.51	0.44
1:A:1377:THR:OG1	3:A:3164:ADP:O2A	2.25	0.44
1:A:1146:LEU:CD1	1:A:1160:LEU:HD12	2.47	0.44
1:A:1382:LEU:O	1:A:1385:LEU:N	2.50	0.44
1:A:1032:PHE:HB3	1:A:1077:ASN:ND2	2.33	0.44
1:A:1714:ASP:HB3	1:A:1715:SER:H	1.63	0.44
2:C:2351:ILE:HB	2:C:2352:PRO:HD2	1.98	0.44
1:A:562:PRO:C	1:A:563:LEU:HD12	2.38	0.44
1:A:1105:ALA:O	1:A:1106:GLY:C	2.54	0.44
1:A:1496:ILE:HD11	1:A:1525:ALA:HA	2.00	0.44
1:A:607:SER:OG	1:A:608:THR:O	2.35	0.44
1:A:1060:LYS:O	2:C:2395:PHE:CE1	2.70	0.44
1:A:990:ASP:O	1:A:994:ASP:N	2.45	0.44
1:A:1277:LYS:HG2	1:A:1278:GLN:N	2.33	0.44
1:A:1031:LEU:HD22	1:A:1128:LEU:HD21	1.99	0.44
1:A:1938:GLU:CD	1:A:1938:GLU:H	2.20	0.44
1:A:495:GLU:HG2	1:A:879:ARG:CG	2.44	0.43
1:A:2037:GLN:O	1:A:2041:VAL:HG23	2.18	0.43
2:C:2189:LEU:HD13	2:C:2224:VAL:HG23	2.00	0.43
2:C:2278:SER:O	2:C:2282:ALA:HB2	2.18	0.43
1:A:1010:ILE:HD12	1:A:1108:LEU:HD23	2.00	0.43
1:A:500:ASN:HB2	1:A:501:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:ASP:O	1:A:1100:PHE:HB3	2.19	0.43
1:A:1123:HIS:N	1:A:1124:PRO:HD2	2.33	0.43
2:C:2368:GLN:O	2:C:2368:GLN:CG	2.66	0.43
1:A:1603:LYS:HA	1:A:1608:ASP:OD2	2.18	0.43
1:A:1095:ASN:O	1:A:1099:VAL:HG23	2.18	0.43
1:A:1626:ASP:C	1:A:1626:ASP:OD1	2.57	0.43
1:A:1342:VAL:HG11	1:A:1416:PHE:CE1	2.54	0.43
1:A:463:ILE:HD11	1:A:899:LEU:HD21	2.01	0.43
1:A:836:TRP:CH2	1:A:870:GLN:HG3	2.54	0.43
2:C:2152:TRP:CZ2	2:C:2391:HIS:CD2	3.07	0.43
1:A:1197:LYS:CB	1:A:1227:ILE:HD12	2.49	0.43
1:A:1620:TYR:CD1	1:A:1651:ILE:HD11	2.54	0.43
1:A:1524:TRP:HB2	1:A:1780:ARG:CD	2.49	0.43
2:C:2388:ARG:O	2:C:2389:PRO:C	2.57	0.43
1:A:594:LEU:HD22	1:A:1258:PHE:CE1	2.53	0.43
1:A:1552:LYS:HG3	1:A:1726:HIS:HE2	1.83	0.42
1:A:909:GLU:HG3	1:A:947:ARG:HH21	1.84	0.42
1:A:649:SER:HG	1:A:919:ASN:CG	2.22	0.42
1:A:1094:LEU:O	1:A:1097:ASP:HB2	2.19	0.42
1:A:1201:LYS:HA	1:A:1302:PHE:CE2	2.54	0.42
2:C:2392:PHE:CD1	2:C:2392:PHE:N	2.87	0.42
1:A:947:ARG:HG3	1:A:955:TYR:HE2	1.84	0.42
1:A:1815:VAL:HG12	1:A:1820:ILE:HG13	2.02	0.42
1:A:788:VAL:HG11	1:A:811:SER:HB3	2.02	0.42
1:A:1554:VAL:HG21	1:A:1563:MET:HE3	2.02	0.42
1:A:511:PHE:O	1:A:537:LYS:HD3	2.19	0.42
1:A:1501:GLN:HB3	1:A:1502:LEU:HD13	2.01	0.42
1:A:1544:LEU:HD11	1:A:1710:ALA:HB3	2.01	0.42
1:A:1471:MET:SD	1:A:1495:MET:HG3	2.59	0.42
1:A:1532:ILE:O	1:A:1532:ILE:HG22	2.19	0.42
1:A:1314:PRO:HG3	1:A:1785:ASN:ND2	2.34	0.42
1:A:1797:HIS:O	1:A:1801:VAL:HG23	2.19	0.42
1:A:1349:ASN:HB2	1:A:1352:GLN:OE1	2.19	0.42
1:A:500:ASN:OD1	1:A:503:GLN:HG3	2.19	0.42
1:A:1968:ASN:O	1:A:1970:TYR:CD1	2.73	0.42
1:A:1145:PRO:CG	1:A:1167:TRP:CZ2	3.03	0.42
1:A:1228:TRP:CE2	1:A:1261:PRO:HG3	2.55	0.42
1:A:1462:ARG:HD3	1:A:1465:ILE:CD1	2.50	0.42
1:A:801:ILE:HG21	1:A:801:ILE:HD13	1.84	0.42
1:A:740:ILE:HG23	1:A:827:VAL:HG22	2.02	0.41
1:A:1026:THR:CG2	1:A:1124:PRO:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:GLY:O	1:A:662:GLN:HG2	2.20	0.41
1:A:1859:SER:O	1:A:1863:ILE:HG12	2.20	0.41
1:A:1334:LEU:HD11	1:A:1339:PHE:CB	2.49	0.41
1:A:909:GLU:HG2	1:A:955:TYR:OH	2.20	0.41
1:A:474:ASP:OD1	1:A:474:ASP:N	2.53	0.41
1:A:1618:VAL:N	1:A:1619:PRO:CD	2.83	0.41
1:A:2067:VAL:HG12	1:A:2068:LYS:N	2.35	0.41
1:A:479:GLU:N	1:A:479:GLU:OE1	2.53	0.41
1:A:1459:TRP:CG	1:A:1498:ILE:HD11	2.56	0.41
1:A:788:VAL:HG11	1:A:811:SER:CB	2.51	0.41
1:A:1145:PRO:HG2	1:A:1167:TRP:CZ2	2.55	0.41
1:A:502:ILE:HD12	1:A:525:SER:HB2	2.03	0.41
1:A:1617:ILE:O	1:A:1621:ILE:HG23	2.19	0.41
1:A:460:TYR:HB3	1:A:710:ILE:HD13	2.03	0.41
1:A:1610:LEU:O	1:A:1660:ALA:O	2.38	0.41
1:A:1971:LEU:HG	1:A:1971:LEU:O	2.20	0.41
1:A:1185:SER:OG	1:A:1188:TYR:CD2	2.46	0.41
1:A:580:PHE:CD1	1:A:580:PHE:C	2.94	0.41
1:A:1329:ILE:HG23	1:A:1333:GLU:HG3	2.03	0.41
1:A:1416:PHE:HD1	1:A:1416:PHE:N	2.18	0.41
1:A:1497:PHE:CD1	1:A:1497:PHE:C	2.94	0.41
1:A:2039:ALA:O	1:A:2042:ALA:HB3	2.21	0.41
1:A:1552:LYS:CG	1:A:1726:HIS:HE2	2.34	0.41
1:A:974:VAL:HG12	1:A:978:LEU:HD12	2.02	0.41
1:A:1343:PHE:N	1:A:1343:PHE:CD1	2.88	0.40
1:A:833:THR:O	1:A:834:LEU:C	2.58	0.40
1:A:947:ARG:HG3	1:A:955:TYR:CE2	2.56	0.40
1:A:2011:ILE:HG22	1:A:2013:VAL:HG23	2.03	0.40
1:A:1334:LEU:HD11	1:A:1339:PHE:HB2	2.03	0.40
1:A:1534:ASN:C	1:A:1534:ASN:OD1	2.60	0.40
1:A:1605:ILE:HG22	1:A:1606:GLU:N	2.37	0.40
5:A:3166:PE5:C16	5:A:3166:PE5:C13	2.99	0.40
5:A:3166:PE5:C13	5:A:3166:PE5:H161	2.52	0.40
1:A:1459:TRP:O	1:A:1466:GLN:NE2	2.46	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	1704/1722 (99%)	1587 (93%)	109 (6%)	8 (0%)	34 72
2	C	246/248 (99%)	236 (96%)	10 (4%)	0	100 100
All	All	1950/1970 (99%)	1823 (94%)	119 (6%)	8 (0%)	39 75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	766	ILE
1	A	1693	HIS
1	A	492	PRO
1	A	1936	ARG
1	A	1555	GLU
1	A	1968	ASN
1	A	622	LEU
1	A	791	PRO

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	1537/1546 (99%)	1501 (98%)	36 (2%)	58 84
2	C	220/220 (100%)	217 (99%)	3 (1%)	74 90
All	All	1757/1766 (100%)	1718 (98%)	39 (2%)	60 85

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	SER
1	A	463	ILE
1	A	506	VAL
1	A	592	SER
1	A	595	SER
1	A	620	ASN
1	A	684	LEU
1	A	697	SER
1	A	704	SER
1	A	799	SER
1	A	801	ILE
1	A	814	SER
1	A	972	SER
1	A	976	SER
1	A	1096	SER
1	A	1211	ILE
1	A	1332	SER
1	A	1384	LEU
1	A	1433	SER
1	A	1457	ARG
1	A	1470	LEU
1	A	1481	GLN
1	A	1488	TYR
1	A	1610	LEU
1	A	1724	THR
1	A	1743	GLU
1	A	1841	THR
1	A	1842	GLU
1	A	1845	SER
1	A	1848	SER
1	A	1874	SER
1	A	1992	ASN
1	A	2032	THR
1	A	2060	SER
1	A	2072	THR
1	A	2132	THR
2	C	2191	LYS
2	C	2334	SER
2	C	2385	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	HIS
1	A	542	HIS
1	A	637	HIS
1	A	676	ASN
1	A	862	GLN
1	A	894	ASN
1	A	1095	ASN
1	A	1143	ASN
1	A	1280	ASN
1	A	1354	GLN
1	A	1435	ASN
1	A	1443	HIS
1	A	1477	HIS
1	A	1513	ASN
1	A	1565	GLN
1	A	1579	ASN
1	A	1751	HIS
1	A	1968	ASN
1	A	2058	ASN
1	A	2059	ASN
1	A	2124	GLN
2	C	2391	HIS
2	C	2394	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 3 ligands modelled in this entry, 1 is 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	ADP	A	3164	4	22,29,29	1.19	2 (9%)	27,45,45	2.23	6 (22%)
5	PE5	A	3166	-	26,26,26	0.70	0	25,25,25	0.56	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
3	ADP	A	3164	4	-	0/12/32/32	0/3/3/3
5	PE5	A	3166	-	-	0/24/24/24	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3164	ADP	C5-C4	2.70	1.46	1.40
3	A	3164	ADP	O4'-C1'	3.56	1.45	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3164	ADP	N3-C2-N1	-8.36	122.50	128.89
3	A	3164	ADP	PA-O3A-PB	-3.83	119.83	132.67
3	A	3164	ADP	C4-C5-N7	-3.51	106.25	109.48
3	A	3164	ADP	C1'-N9-C4	-2.09	123.79	126.94
3	A	3164	ADP	O3'-C3'-C2'	-2.04	105.18	111.83
3	A	3164	ADP	O3B-PB-O2B	2.99	118.77	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3164	ADP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3166	PE5	3	0

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, 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	1707/1722 (99%)	-0.06	17 (0%) 84 69	76, 115, 192, 269	0
2	C	248/248 (100%)	-0.10	2 (0%) 87 75	77, 109, 173, 240	0
All	All	1955/1970 (99%)	-0.07	19 (0%) 84 69	76, 114, 190, 269	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	545	PRO	7.6
1	A	546	LYS	6.0
2	C	2324	VAL	4.8
1	A	496	THR	4.6
1	A	660	TYR	4.4
1	A	495	GLU	3.5
1	A	2066	GLY	3.4
1	A	1714	ASP	3.1
1	A	442	THR	3.0
1	A	772	LYS	2.7
1	A	1617	ILE	2.4
1	A	1092	PHE	2.4
1	A	2064	ILE	2.4
1	A	1715	SER	2.3
1	A	774	ASP	2.3
1	A	1843	ILE	2.3
1	A	1179	VAL	2.3
2	C	2395	PHE	2.3
1	A	1556	HIS	2.1

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 (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
5	PE5	A	3166	27/27	0.84	0.32	1.70	112,146,169,173	0
3	ADP	A	3164	27/27	0.96	0.18	-0.59	87,115,141,145	0
4	MG	A	3165	1/1	0.98	0.13	-	86,86,86,86	0

6.5 Other polymers (i)

There are no such residues in this entry.