Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TH1
Title : Beta-catenin in complex with a phosphorylated APC 20aa repeat fragment
Authors : Xing, Y.; Clements, W.K.; Le Trong, I.; Hinds, T.R.; Stenkamp, R.; Kimelman, D.; Xu, W.
Deposited on : 2004-05-31
Resolution : 2.50 Å(reported)

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

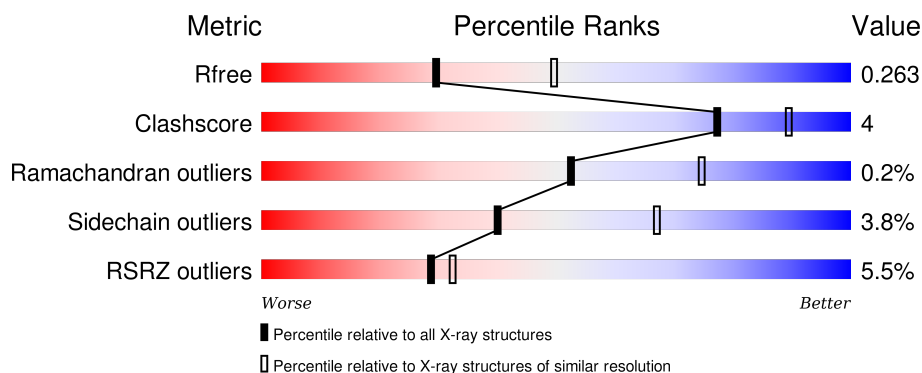|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.50 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	Percentile Ranks	Value
Rfree		0.263
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		3.8%
RSRZ outliers		5.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	532	2% · 88% · 8% · ·
1	B	532	6% · 86% · 10% · ·
2	C	179	8% · 27% · 69%
2	D	179	3% · 28% · 70%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8667 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 Beta-catenin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total 3912	C 2456	N 710	O 720	S 26	0	0	0
1	B	513	Total 3904	C 2452	N 709	O 717	S 26	0	0	0

- Molecule 2 is a protein called Adenomatous polyposis coli protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	56	Total 416	C 249	N 65	O 96	P 5	S 1	0	0	0
2	D	54	Total 389	C 232	N 61	O 90	P 5	S 1	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1487	TPO	THR	MODIFIED RESIDUE	UNP P25054
C	1504	SEP	SER	MODIFIED RESIDUE	UNP P25054
C	1505	SEP	SER	MODIFIED RESIDUE	UNP P25054
C	1507	SEP	SER	MODIFIED RESIDUE	UNP P25054
C	1510	SEP	SER	MODIFIED RESIDUE	UNP P25054
D	1487	TPO	THR	MODIFIED RESIDUE	UNP P25054
D	1504	SEP	SER	MODIFIED RESIDUE	UNP P25054
D	1505	SEP	SER	MODIFIED RESIDUE	UNP P25054
D	1507	SEP	SER	MODIFIED RESIDUE	UNP P25054
D	1510	SEP	SER	MODIFIED RESIDUE	UNP P25054

- Molecule 3 is water.

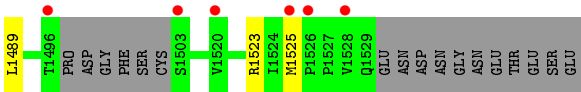| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	20	Total 20	O 20	0	0
3	C	2	Total 2	O 2	0	0
3	D	2	Total 2	O 2	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: Beta-catenin

- Molecule 1: Beta-catenin

- Molecule 2: Adenomatous polyposis coli protein

• Molecule 2: Adenomatous polyposis coli protein

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.16Å　　133.80Å　　82.17Å 90.00°　　110.85°　　90.00°	Depositor
Resolution (Å)	47.98　–　2.50 47.98　–　2.22	Depositor EDS
% Data completeness (in resolution range)	85.1 (47.98-2.50) 87.3 (47.98-2.22)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225　,　0.257 0.234　,　0.263	Depositor DCC
R_{free} test set	2814 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 30.7	EDS
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 84747 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8667	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.55	0/3966	0.72	0/5381
1	B	0.55	0/3958	0.72	1/5370 (0.0%)
2	C	0.64	0/366	0.78	0/495
2	D	0.60	0/340	0.85	0/462
All	All	0.55	0/8630	0.73	1/11708 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

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	B	624	ASP	CB-CG-OD1	7.40	124.96	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	624	ASP	Mainchain

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	3912	0	4050	29	0
1	B	3904	0	4046	35	0
2	C	416	0	358	2	0
2	D	389	0	318	7	0
3	A	22	0	0	0	0
3	B	20	0	0	1	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	8667	0	8772	65	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 4.

All (65) 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:483:ASN:HD22	1:A:486:ARG:HH21	1.22	0.87
1:B:364:GLN:H	1:B:364:GLN:HE21	1.26	0.84
1:B:205:THR:HG22	1:B:207:ASP:H	1.45	0.81
1:B:280:GLN:H	1:B:280:GLN:HE21	1.27	0.78
1:A:483:ASN:HD22	1:A:486:ARG:NH2	1.83	0.76
1:A:364:GLN:H	1:A:364:GLN:HE21	1.34	0.76
1:B:206:ASN:HD22	1:B:206:ASN:H	1.34	0.73
1:A:648:ASN:HD22	1:A:651:VAL:HG23	1.55	0.71
1:B:364:GLN:H	1:B:364:GLN:NE2	1.90	0.68
1:A:535:ARG:HH11	1:A:538:GLN:NE2	1.96	0.63
1:A:414:ILE:H	1:A:414:ILE:HD12	1.64	0.63
1:A:483:ASN:ND2	1:A:486:ARG:HH21	1.95	0.62
1:A:472:THR:HG22	1:A:516:ASN:HB3	1.83	0.61
1:A:612:ARG:HH11	1:A:648:ASN:HD21	1.49	0.60
1:B:206:ASN:HD22	1:B:206:ASN:N	1.99	0.60
1:A:364:GLN:H	1:A:364:GLN:NE2	1.99	0.60
1:B:470:HIS:CD2	2:D:1486:ASP:HB2	2.36	0.59
1:B:220:ASN:HD21	2:D:1513:GLU:HG2	1.66	0.59
1:B:280:GLN:NE2	1:B:280:GLN:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:40:HOH:O	2:D:1486:ASP:HB3	2.04	0.57
1:B:612:ARG:HE	2:D:1482:LEU:HD13	1.70	0.56
1:A:472:THR:HG23	1:A:482:GLN:HG3	1.88	0.56
1:A:153:ILE:HG23	1:A:194:MET:HG3	1.87	0.55
1:B:472:THR:HG23	1:B:482:GLN:HG3	1.89	0.55
1:A:654:TYR:O	1:A:658:VAL:HG23	2.11	0.50
1:A:535:ARG:HH11	1:A:538:GLN:HE21	1.59	0.49
2:C:1472:VAL:O	2:C:1476:VAL:HG23	2.12	0.49
1:A:507:ILE:O	1:A:511:VAL:HG23	2.13	0.49
1:B:206:ASN:ND2	1:B:206:ASN:H	2.07	0.49
1:B:612:ARG:NE	2:D:1482:LEU:HD13	2.29	0.47
1:B:355:PRO:O	1:B:359:GLU:HG2	2.14	0.47
1:B:220:ASN:HD21	2:D:1513:GLU:CG	2.28	0.47
1:B:472:THR:CG2	1:B:482:GLN:HG3	2.45	0.47
1:B:287:ASN:H	1:B:287:ASN:HD22	1.63	0.46
1:B:472:THR:HG22	1:B:516:ASN:HB3	1.97	0.46
1:B:654:TYR:O	1:B:658:VAL:HG23	2.16	0.46
1:B:218:LEU:HD22	1:B:231:ILE:HG12	1.98	0.46
1:B:171:ALA:O	1:B:175:VAL:HG23	2.16	0.45
1:A:483:ASN:ND2	1:A:486:ARG:NH2	2.56	0.45
1:A:491:LEU:HD13	1:A:527:LEU:HD13	1.99	0.45
1:B:461:THR:HG22	1:B:506:LEU:HD11	2.00	0.44
1:A:160:LEU:HD12	1:A:168:VAL:HG13	2.00	0.44
1:A:502:SER:HB2	1:A:506:LEU:HD23	1.98	0.44
1:A:461:THR:HG22	1:A:506:LEU:HD11	2.00	0.44
1:A:331:TYR:HD2	1:B:158:LYS:HZ2	1.66	0.44
1:A:171:ALA:O	1:A:175:VAL:HG23	2.17	0.43
1:A:476:GLN:HE22	1:B:310:GLU:HG2	1.83	0.43
1:A:393:THR:HG23	1:A:429:CYS:O	2.19	0.43
1:A:537:VAL:O	1:A:541:VAL:HG23	2.19	0.43
1:B:507:ILE:O	1:B:511:VAL:HG23	2.19	0.43
1:B:206:ASN:N	1:B:206:ASN:ND2	2.67	0.43
1:A:191:SER:HA	1:A:192:PRO:HD3	1.90	0.42
1:B:469:ARG:HH21	2:D:1486:ASP:HA	1.85	0.42
1:B:220:ASN:N	1:B:220:ASN:HD22	2.16	0.42
1:B:298:THR:HG21	1:B:340:THR:HA	2.01	0.42
2:C:1475:ALA:O	2:C:1479:VAL:HG23	2.20	0.42
1:B:305:ALA:O	1:B:312:LYS:HE2	2.19	0.41
1:B:544:HIS:O	1:B:548:GLN:HG2	2.21	0.41
1:A:658:VAL:O	1:A:662:MET:HG3	2.20	0.41
1:A:169:ASN:O	1:A:173:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ALA:O	1:B:153:ILE:HG12	2.20	0.41
1:A:169:ASN:HD22	1:A:169:ASN:N	2.18	0.40
1:B:202:MET:HB2	1:B:214:THR:HG21	2.02	0.40
1:B:490:GLY:O	1:B:494:VAL:HG23	2.22	0.40
1:B:515:ARG:HH11	1:B:572:GLY:HA2	1.87	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	510/532 (96%)	502 (98%)	8 (2%)	0	100	100
1	B	509/532 (96%)	503 (99%)	4 (1%)	2 (0%)	39	61
2	C	47/179 (26%)	45 (96%)	2 (4%)	0	100	100
2	D	46/179 (26%)	41 (89%)	5 (11%)	0	100	100
All	All	1112/1422 (78%)	1091 (98%)	19 (2%)	2 (0%)	52	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	181	LYS
1	B	182	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	424/441 (96%)	410 (97%)	14 (3%)	45	73
1	B	423/441 (96%)	405 (96%)	18 (4%)	35	61
2	C	35/155 (23%)	32 (91%)	3 (9%)	13	24
2	D	29/155 (19%)	29 (100%)	0	100	100
All	All	911/1192 (76%)	876 (96%)	35 (4%)	40	67

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	LEU
1	A	165	GLN
1	A	186	HIS
1	A	194	MET
1	A	364	GLN
1	A	407	GLN
1	A	429	CYS
1	A	449	ARG
1	A	452	LEU
1	A	453	ARG
1	A	527	LEU
1	A	559	GLN
1	A	580	LEU
1	A	626	GLU
1	B	160	LEU
1	B	206	ASN
1	B	212	ARG
1	B	252	LEU
1	B	280	GLN
1	B	287	ASN
1	B	309	GLN
1	B	321	PRO
1	B	354	LYS
1	B	364	GLN
1	B	373	PRO
1	B	437	MET
1	B	452	LEU
1	B	527	LEU
1	B	559	GLN
1	B	578	HIS
1	B	580	LEU

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Mol	Chain	Res	Type
1	B	661	ARG
2	C	1489	LEU
2	C	1523	ARG
2	C	1525	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	169	ASN
1	A	220	ASN
1	A	223	HIS
1	A	326	ASN
1	A	364	GLN
1	A	395	GLN
1	A	483	ASN
1	A	538	GLN
1	A	648	ASN
1	B	169	ASN
1	B	206	ASN
1	B	220	ASN
1	B	280	GLN
1	B	287	ASN
1	B	309	GLN
1	B	322	GLN
1	B	326	ASN
1	B	364	GLN
1	B	395	GLN
1	B	470	HIS
1	B	516	ASN
1	B	538	GLN
1	B	611	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	TPO	C	1487	2	8,10,11	1.49	1 (12%)	7,14,16	0.96	0
2	SEP	C	1504	2	8,9,10	1.10	0	8,12,14	3.06	3 (37%)
2	SEP	C	1505	2	8,9,10	1.25	0	8,12,14	3.28	3 (37%)
2	SEP	C	1507	2	8,9,10	1.03	0	8,12,14	4.14	3 (37%)
2	SEP	C	1510	2	8,9,10	1.20	0	8,12,14	3.09	3 (37%)
2	TPO	D	1487	2	8,10,11	1.72	4 (50%)	7,14,16	1.33	1 (14%)
2	SEP	D	1504	2	8,9,10	1.23	0	8,12,14	4.06	3 (37%)
2	SEP	D	1505	2	8,9,10	1.16	0	8,12,14	3.44	4 (50%)
2	SEP	D	1507	2	8,9,10	0.99	0	8,12,14	3.27	3 (37%)
2	SEP	D	1510	2	8,9,10	1.14	0	8,12,14	3.47	3 (37%)

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	TPO	C	1487	2	-	0/8/11/13	0/0/0/0
2	SEP	C	1504	2	-	0/6/8/10	0/0/0/0
2	SEP	C	1505	2	-	0/6/8/10	0/0/0/0
2	SEP	C	1507	2	-	0/6/8/10	0/0/0/0
2	SEP	C	1510	2	-	0/6/8/10	0/0/0/0
2	TPO	D	1487	2	-	0/8/11/13	0/0/0/0
2	SEP	D	1504	2	-	0/6/8/10	0/0/0/0
2	SEP	D	1505	2	-	0/6/8/10	0/0/0/0
2	SEP	D	1507	2	-	0/6/8/10	0/0/0/0
2	SEP	D	1510	2	-	0/6/8/10	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1487	TPO	P-O2P	2.10	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1487	TPO	P-O3P	2.13	1.62	1.54
2	D	1487	TPO	P-OG1	2.13	1.66	1.60
2	D	1487	TPO	P-O1P	2.33	1.58	1.51
2	C	1487	TPO	P-O1P	2.49	1.59	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1507	SEP	O2P-P-OG	-5.33	91.22	106.56
2	C	1510	SEP	O2P-P-OG	-5.32	91.25	106.56
2	C	1505	SEP	O2P-P-OG	-5.12	91.81	106.56
2	D	1510	SEP	O2P-P-OG	-5.02	92.11	106.56
2	D	1505	SEP	O2P-P-OG	-5.00	92.18	106.56
2	C	1504	SEP	O2P-P-OG	-4.97	92.25	106.56
2	D	1504	SEP	O2P-P-OG	-4.94	92.34	106.56
2	C	1507	SEP	O2P-P-OG	-4.75	92.89	106.56
2	D	1505	SEP	O-C-CA	-2.02	120.23	125.49
2	C	1504	SEP	OG-CB-CA	2.16	110.11	108.27
2	C	1510	SEP	OG-CB-CA	2.21	110.16	108.27
2	D	1487	TPO	C-CA-N	2.38	114.81	109.83
2	D	1507	SEP	OG-CB-CA	2.89	110.74	108.27
2	C	1505	SEP	OG-CB-CA	4.31	111.95	108.27
2	D	1510	SEP	OG-CB-CA	5.01	112.55	108.27
2	D	1505	SEP	OG-CB-CA	5.24	112.75	108.27
2	C	1505	SEP	OG-P-O1P	5.84	122.00	107.14
2	D	1505	SEP	OG-P-O1P	5.85	122.03	107.14
2	C	1507	SEP	OG-P-O1P	5.97	122.33	107.14
2	D	1504	SEP	OG-P-O1P	5.99	122.38	107.14
2	C	1510	SEP	OG-P-O1P	6.04	122.53	107.14
2	C	1504	SEP	OG-P-O1P	6.23	123.00	107.14
2	D	1510	SEP	OG-P-O1P	6.35	123.31	107.14
2	D	1507	SEP	OG-P-O1P	6.42	123.48	107.14
2	D	1504	SEP	OG-CB-CA	7.95	115.06	108.27
2	C	1507	SEP	OG-CB-CA	8.54	115.56	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	514/532 (96%)	-0.06	11 (2%)	67	71	19, 36, 80, 117	0
1	B	513/532 (96%)	0.17	32 (6%)	24	27	21, 43, 98, 120	0
2	C	51/179 (28%)	1.19	14 (27%)	1	0	32, 77, 96, 97	0
2	D	49/179 (27%)	0.81	5 (10%)	9	9	34, 82, 101, 103	0
All	All	1127/1422 (79%)	0.14	62 (5%)	29	32	19, 42, 97, 120	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	ALA	6.4
1	B	551	THR	6.3
1	B	552	SER	6.3
1	B	148	LEU	5.9
2	C	1484	ASP	5.7
2	C	1471	ALA	5.3
1	B	560	PHE	5.3
1	B	559	GLN	5.3
2	C	1479	VAL	4.9
1	A	551	THR	4.9
1	B	604	TYR	4.4
2	C	1468	LYS	3.9
1	B	147	GLU	3.8
1	B	550	ARG	3.8
1	B	606	PRO	3.8
1	B	542	ARG	3.8
2	D	1477	GLN	3.8
1	A	148	LEU	3.7
1	B	629	GLU	3.7
1	A	552	SER	3.5
1	B	549	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	1526	PRO	3.4
1	B	146	ALA	3.4
1	B	647	ARG	3.4
1	B	660	PHE	3.4
2	C	1472	VAL	3.4
1	A	147	GLU	3.2
2	C	1503	SER	3.1
2	D	1484	ASP	3.1
1	B	603	LEU	2.8
1	B	637	THR	2.8
1	B	600	VAL	2.7
1	A	158	LYS	2.7
1	B	642	GLU	2.7
1	B	548	GLN	2.7
1	A	163	GLU	2.7
1	A	145	ASP	2.6
1	B	545	GLN	2.6
1	B	595	THR	2.6
2	D	1479	VAL	2.5
1	B	664	GLU	2.5
1	A	559	GLN	2.5
2	C	1525	MET	2.4
1	A	208	VAL	2.4
1	B	643	LEU	2.3
1	B	174	MET	2.3
2	C	1528	VAL	2.3
1	B	432	TYR	2.3
1	B	662	MET	2.2
1	B	181	LYS	2.2
1	B	634	GLU	2.2
2	C	1470	ALA	2.2
1	B	659	LEU	2.2
2	C	1496	THR	2.1
1	B	633	ALA	2.1
2	C	1476	VAL	2.1
2	D	1471	ALA	2.1
1	A	645	HIS	2.1
2	C	1477	GLN	2.1
2	D	1525	MET	2.0
2	C	1520	VAL	2.0
1	B	476	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	SEP	C	1507	10/11	0.94	0.14	-	55,58,61,62	0
2	SEP	D	1505	10/11	0.83	0.13	-	67,75,85,86	0
2	SEP	C	1504	10/11	0.79	0.23	-	87,91,98,98	0
2	SEP	C	1510	10/11	0.87	0.16	-	64,70,79,80	0
2	SEP	D	1510	10/11	0.87	0.13	-	50,58,70,71	0
2	TPO	C	1487	11/12	0.93	0.12	-	43,49,61,61	0
2	SEP	C	1505	10/11	0.90	0.19	-	78,85,92,92	0
2	SEP	D	1507	10/11	0.97	0.17	-	39,43,45,48	0
2	TPO	D	1487	11/12	0.75	0.28	-	60,72,84,84	0
2	SEP	D	1504	10/11	0.68	0.22	-	77,82,88,89	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.