Full wwPDB X-ray Structure Validation Report (i)

Aug 14, 2016 – 10:49 PM EDT

PDB ID : 5F55
Title : Structure of RecJ complexed with DNA
Authors : Hua, Y.; Zhao, Y.; Cheng, K.
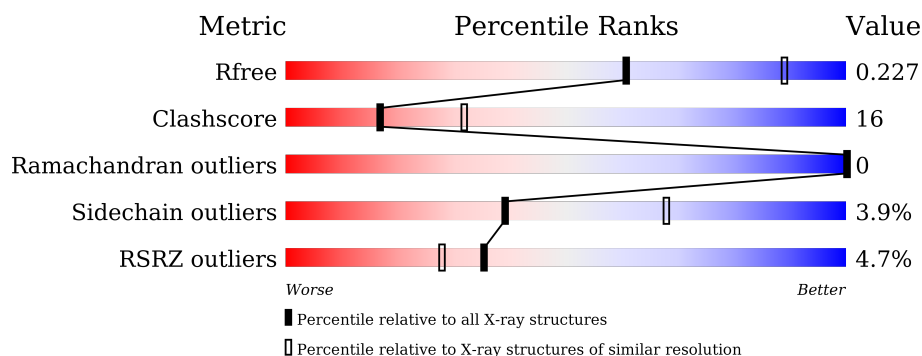Deposited on : 2015-12-04
Resolution : 2.60 Å(reported)

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 2.60 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		0.227
Clashscore		16
Ramachandran outliers		0
Sidechain outliers		3.9%
RSRZ outliers		4.7%

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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	705	4% 72% 27% •
2	C	14	36% 21% 79%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	801	-	-	X	-
3	SO4	A	803	-	-	X	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5696 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 Single-stranded-DNA-specific exonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total 5373	C 3391	N 984	O 986	S 12	0	2	0

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*TP*GP*TP*AP*CP*GP*CP*TP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total 286	C 137	N 55	O 81	P 13	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
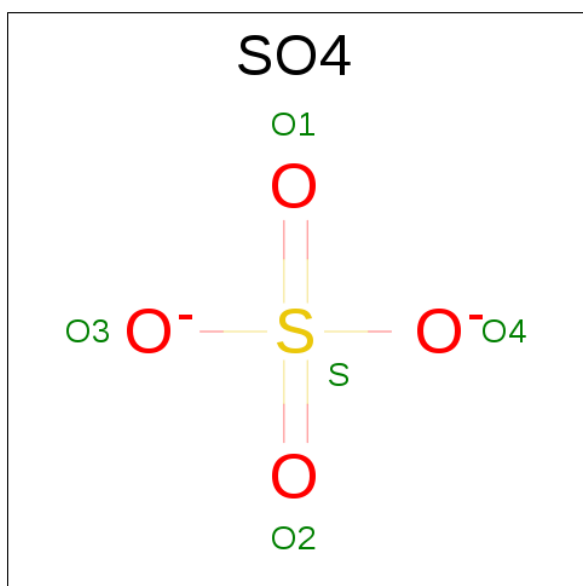
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mn 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: Single-stranded-DNA-specific exonuclease
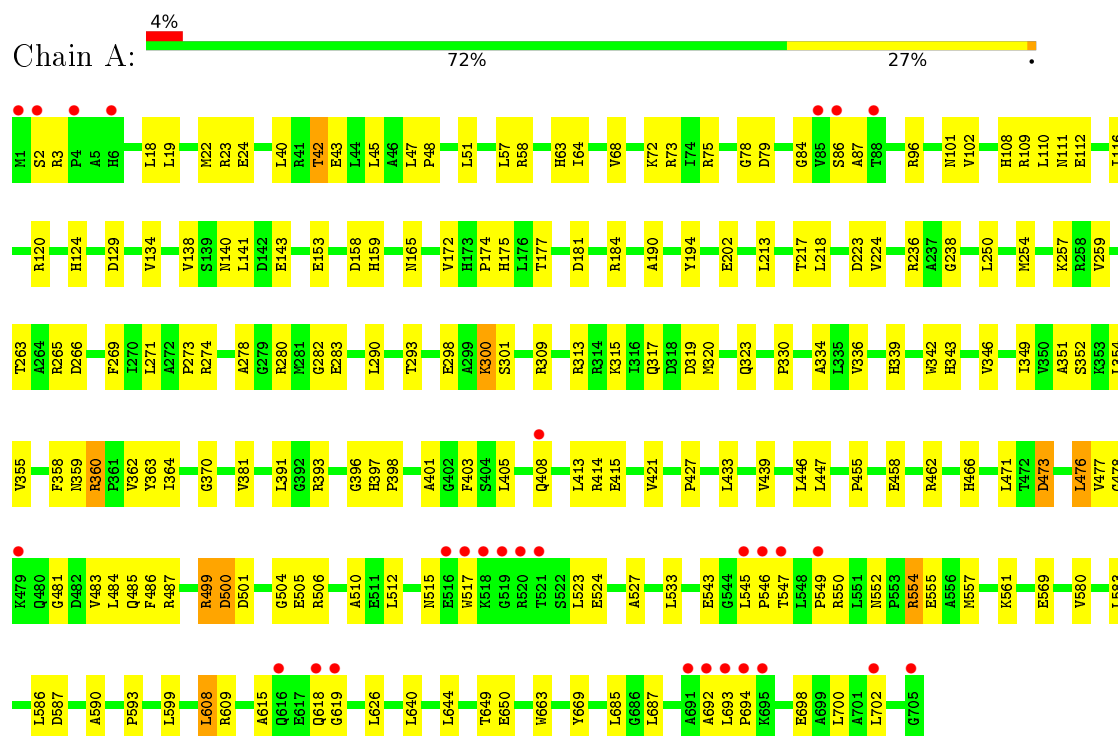
- Molecule 2: DNA (5'-D(*GP*AP*TP*GP*TP*AP*CP*GP*CP*TP*AP*GP*GP*C)-3')
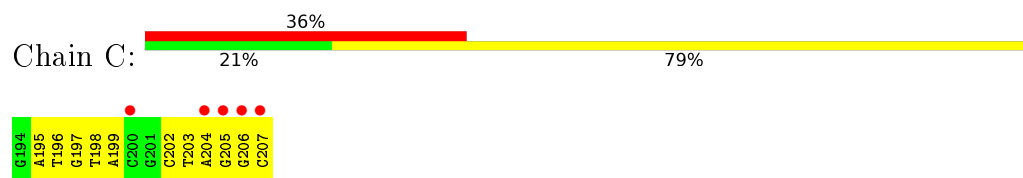
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.82Å 105.82Å 165.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.33 – 2.60 29.33 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.33-2.60) 99.7 (29.33-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.82 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.185 , 0.228 0.180 , 0.227	Depositor DCC
R_{free} test set	1641 reflections (4.90%)	DCC
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.2	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
Reported twinning fraction	0.030 for -h,-k,l	Depositor
Outliers	0 of 33594 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5696	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MN, SO4

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	0.30	0/5501	0.49	0/7511
2	C	0.25	0/321	0.59	0/495
All	All	0.30	0/5822	0.50	0/8006

There are no bond length outliers.

There are no bond angle outliers.

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	5373	0	5368	172	0
2	C	286	0	156	25	0
3	A	35	0	0	6	0
4	A	2	0	0	0	0
All	All	5696	0	5524	184	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 16.

All (184) 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)
2:C:202:DC:H2"	2:C:203:DT:H5"	1.25	1.19
1:A:358:PHE:HB3	1:A:360:ARG:HD3	1.24	1.16
1:A:554:ARG:HH22	1:A:561:LYS:NZ	1.53	1.06
1:A:517:TRP:CZ3	2:C:203:DT:C2	2.47	1.02
1:A:692:ALA:HB1	1:A:694:PRO:HD3	1.39	1.01
1:A:273:PRO:HG3	2:C:197:DG:H5'	1.44	0.99
1:A:517:TRP:CZ3	2:C:203:DT:O2	2.23	0.91
1:A:476:LEU:HD21	1:A:481:GLY:O	1.71	0.91
1:A:554:ARG:HH22	1:A:561:LYS:HZ2	1.20	0.89
1:A:358:PHE:HB3	1:A:360:ARG:CD	2.07	0.84
1:A:476:LEU:CD2	1:A:481:GLY:O	2.27	0.82
1:A:693:LEU:H	1:A:693:LEU:HD23	1.45	0.79
1:A:554:ARG:HH22	1:A:561:LYS:HZ1	1.30	0.78
1:A:111:ASN:HB2	1:A:112:GLU:OE1	1.84	0.78
1:A:523:LEU:HD13	1:A:524:GLU:N	1.99	0.78
1:A:317:GLN:HB2	1:A:346:VAL:HG11	1.64	0.77
1:A:140:ASN:HB3	1:A:143:GLU:HB2	1.66	0.77
2:C:202:DC:H2"	2:C:203:DT:C5'	2.12	0.76
1:A:112:GLU:N	1:A:112:GLU:OE1	2.16	0.75
1:A:546:PRO:O	1:A:547:THR:CG2	2.35	0.75
2:C:202:DC:C2'	2:C:203:DT:H5"	2.11	0.75
1:A:546:PRO:O	1:A:547:THR:HG23	1.88	0.74
2:C:195:DA:H2"	2:C:196:DT:O5'	1.88	0.74
1:A:692:ALA:HB1	1:A:694:PRO:CD	2.18	0.73
1:A:517:TRP:CE3	2:C:203:DT:N3	2.56	0.73
1:A:545:LEU:HD13	1:A:545:LEU:O	1.89	0.72
1:A:586:LEU:HD11	1:A:593:PRO:HD3	1.71	0.72
1:A:500:ASP:N	1:A:500:ASP:OD1	2.19	0.71
1:A:517:TRP:CH2	2:C:203:DT:C2	2.78	0.70
1:A:263:THR:OG1	1:A:266:ASP:OD1	2.04	0.70
1:A:2:SER:OG	1:A:360:ARG:NH2	2.26	0.68
1:A:320:MET:HE1	1:A:343:HIS:H	1.59	0.67
1:A:359:ASN:O	1:A:427:PRO:HB2	1.94	0.67
1:A:557:MET:HG3	1:A:561:LYS:HE3	1.76	0.67
2:C:198:DT:H2"	2:C:199:DA:H5'	1.76	0.67
1:A:517:TRP:CE3	2:C:203:DT:C2	2.83	0.66
1:A:547:THR:O	1:A:549:PRO:HD3	1.96	0.66
1:A:471:LEU:HD23	1:A:504:GLY:O	1.96	0.66
1:A:499:ARG:HH11	1:A:499:ARG:CG	2.10	0.65
1:A:545:LEU:C	1:A:545:LEU:HD13	2.17	0.64
2:C:206:DG:C5	2:C:207:DC:N4	2.66	0.64
1:A:505:GLU:O	1:A:506:ARG:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:GLN:HG2	1:A:618:GLN:O	1.96	0.64
1:A:554:ARG:NH2	1:A:561:LYS:NZ	2.37	0.62
1:A:471:LEU:H	1:A:471:LEU:HD23	1.63	0.62
1:A:108:HIS:CE1	1:A:110:LEU:HB2	2.35	0.62
1:A:433:LEU:HG	1:A:466:HIS:HB2	1.81	0.62
1:A:543:GLU:O	1:A:543:GLU:HG3	1.99	0.62
1:A:663:TRP:NE1	3:A:801:SO4:O4	2.32	0.62
1:A:58:ARG:NH1	1:A:202:GLU:OE2	2.32	0.62
1:A:138:VAL:HG23	1:A:158:ASP:OD2	2.01	0.61
1:A:484:LEU:HD23	1:A:485:GLN:N	2.16	0.61
1:A:415:GLU:HA	1:A:415:GLU:OE2	2.01	0.59
1:A:63[A]:HIS:NE2	1:A:153:GLU:OE1	2.36	0.59
1:A:158:ASP:OD1	1:A:159:HIS:N	2.34	0.58
1:A:554:ARG:NH2	1:A:561:LYS:HZ2	1.95	0.58
1:A:546:PRO:C	1:A:547:THR:HG23	2.23	0.58
1:A:499:ARG:HH11	1:A:499:ARG:HG3	1.67	0.58
1:A:78:GLY:HA2	1:A:134:VAL:HG23	1.87	0.57
1:A:57:LEU:HD12	1:A:172:VAL:HG11	1.85	0.57
1:A:487:ARG:HD3	3:A:807:SO4:O3	2.04	0.57
1:A:174:PRO:O	1:A:177:THR:OG1	2.15	0.56
2:C:196:DT:H2"	2:C:197:DG:O4'	2.05	0.56
1:A:692:ALA:CB	1:A:694:PRO:HD3	2.26	0.56
1:A:693:LEU:N	1:A:693:LEU:HD23	2.19	0.56
1:A:523:LEU:HD13	1:A:523:LEU:C	2.26	0.55
1:A:24:GLU:OE2	1:A:42:THR:HB	2.07	0.55
1:A:315:LYS:HE2	1:A:319:ASP:OD1	2.06	0.55
1:A:552:ASN:OD1	1:A:555:GLU:HG3	2.07	0.55
1:A:615:ALA:O	1:A:619:GLY:N	2.39	0.55
1:A:698:GLU:OE2	1:A:702:LEU:HD22	2.07	0.54
1:A:550:ARG:NH1	1:A:669:TYR:O	2.41	0.53
1:A:615:ALA:O	1:A:619:GLY:O	2.25	0.53
1:A:515:ASN:ND2	2:C:203:DT:O4	2.39	0.53
1:A:278:ALA:HB1	1:A:283:GLU:O	2.08	0.53
1:A:313:ARG:C	1:A:313:ARG:HD2	2.29	0.53
2:C:198:DT:C2	2:C:199:DA:C6	2.97	0.53
1:A:346:VAL:HG13	1:A:349:ILE:HD12	1.90	0.53
1:A:217:THR:OG1	1:A:238:GLY:HA3	2.09	0.53
1:A:273:PRO:CG	2:C:197:DG:H5'	2.27	0.53
1:A:477:VAL:HG21	1:A:485:GLN:NE2	2.25	0.52
1:A:358:PHE:O	1:A:359:ASN:HB2	2.10	0.51
1:A:692:ALA:CB	1:A:694:PRO:CD	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ARG:NE	3:A:803:SO4:O2	2.42	0.51
1:A:484:LEU:HD23	1:A:484:LEU:C	2.31	0.51
1:A:96:ARG:NH2	1:A:102:VAL:O	2.37	0.51
1:A:293:THR:OG1	1:A:298:GLU:OE1	2.19	0.51
1:A:484:LEU:HD22	1:A:486:PHE:HD2	1.74	0.50
2:C:207:DC:H6	2:C:207:DC:O5'	1.94	0.50
1:A:79:ASP:HB3	1:A:84:GLY:HA3	1.93	0.50
1:A:63[A]:HIS:NE2	1:A:153:GLU:CD	2.65	0.50
1:A:397:HIS:NE2	2:C:195:DA:OP2	2.40	0.50
1:A:381:VAL:HG23	1:A:397:HIS:O	2.12	0.49
1:A:265:ARG:NH2	3:A:803:SO4:O2	2.42	0.49
1:A:358:PHE:CB	1:A:360:ARG:HD3	2.17	0.49
1:A:334:ALA:HB2	1:A:421:VAL:HG21	1.95	0.49
1:A:319:ASP:O	1:A:323:GLN:HG3	2.13	0.48
1:A:250:LEU:O	1:A:254:MET:HG3	2.13	0.48
1:A:483:VAL:HG21	2:C:202:DC:H4'	1.95	0.48
1:A:499:ARG:NH1	1:A:499:ARG:CG	2.72	0.48
1:A:397:HIS:HE2	2:C:195:DA:P	2.36	0.48
1:A:194:TYR:CZ	1:A:213:LEU:HD13	2.49	0.48
1:A:608:LEU:HD13	1:A:685:LEU:HD11	1.95	0.48
1:A:473:ASP:OD1	1:A:473:ASP:N	2.48	0.47
1:A:702:LEU:HG	1:A:702:LEU:O	2.15	0.47
1:A:554:ARG:NH2	1:A:561:LYS:HZ1	2.05	0.47
1:A:609:ARG:HG2	1:A:687:LEU:HD11	1.96	0.47
1:A:257:LYS:HE3	1:A:274:ARG:NH2	2.30	0.47
1:A:580:VAL:CG1	1:A:583:LEU:HB2	2.45	0.47
1:A:693:LEU:N	1:A:694:PRO:CD	2.78	0.47
1:A:477:VAL:HG12	1:A:478:GLY:N	2.29	0.47
1:A:43:GLU:O	1:A:47:LEU:HB2	2.14	0.47
1:A:236:ARG:HG2	1:A:455:PRO:HD3	1.97	0.47
1:A:397:HIS:HB3	1:A:398:PRO:CD	2.45	0.47
1:A:506:ARG:HH11	1:A:506:ARG:HG2	1.79	0.47
1:A:108:HIS:HE1	1:A:110:LEU:HB2	1.76	0.46
1:A:510:ALA:HA	1:A:527:ALA:HA	1.96	0.46
1:A:87:ALA:HB2	1:A:190:ALA:HA	1.98	0.46
1:A:3:ARG:NH2	1:A:360:ARG:NH1	2.63	0.46
1:A:626:LEU:HB2	1:A:669:TYR:CZ	2.51	0.46
1:A:51:LEU:HD23	1:A:58:ARG:CZ	2.47	0.45
1:A:364:ILE:O	1:A:370:GLY:HA2	2.16	0.45
1:A:405:LEU:HD13	1:A:413:LEU:HD22	1.97	0.45
1:A:546:PRO:C	1:A:547:THR:CG2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:198:DT:N3	2:C:199:DA:N6	2.65	0.45
1:A:523:LEU:C	1:A:523:LEU:CD1	2.85	0.45
1:A:484:LEU:CD2	1:A:484:LEU:C	2.85	0.45
1:A:505:GLU:HG2	1:A:533:LEU:HD11	1.98	0.44
1:A:546:PRO:O	1:A:547:THR:HG22	2.14	0.44
1:A:446:LEU:HD23	1:A:512:LEU:HD11	1.98	0.44
1:A:587:ASP:OD1	1:A:590:ALA:N	2.50	0.44
1:A:72:LYS:HB3	1:A:129:ASP:HB2	2.00	0.44
1:A:300:LYS:HG3	1:A:301:SER:N	2.33	0.44
1:A:73:ARG:HG3	1:A:101:ASN:ND2	2.33	0.44
1:A:320:MET:HE1	1:A:343:HIS:N	2.31	0.43
1:A:47:LEU:HD12	1:A:48:PRO:HD2	2.00	0.43
1:A:108:HIS:NE2	1:A:282:GLY:O	2.52	0.43
1:A:476:LEU:HD11	1:A:499:ARG:O	2.19	0.43
1:A:265:ARG:HD3	2:C:198:DT:O4	2.18	0.43
1:A:649:THR:HG22	1:A:650:GLU:N	2.34	0.43
1:A:693:LEU:CD2	1:A:693:LEU:N	2.81	0.43
1:A:86:SER:OG	1:A:218:LEU:HD23	2.18	0.43
1:A:545:LEU:CD1	1:A:545:LEU:C	2.86	0.43
1:A:640:LEU:HD11	1:A:644:LEU:HD22	2.00	0.43
1:A:330:PRO:O	1:A:360:ARG:NH1	2.51	0.43
1:A:354:LEU:HD12	1:A:362:VAL:HG11	2.00	0.43
1:A:545:LEU:N	1:A:546:PRO:HD2	2.34	0.43
1:A:64:ILE:O	1:A:68:VAL:HG23	2.18	0.43
1:A:309:ARG:HD3	1:A:309:ARG:HA	1.64	0.43
1:A:47:LEU:HD11	1:A:184:ARG:HH21	1.82	0.43
1:A:693:LEU:H	1:A:693:LEU:CD2	2.24	0.43
1:A:462:ARG:NH2	3:A:803:SO4:O2	2.52	0.43
1:A:339:HIS:HB3	1:A:342:TRP:CG	2.54	0.42
1:A:336:VAL:HG22	1:A:363:TYR:HB2	2.00	0.42
1:A:439:VAL:HG23	3:A:801:SO4:O3	2.19	0.42
1:A:269:PHE:CD2	2:C:197:DG:H2"	2.54	0.42
1:A:181:ASP:HB3	1:A:184:ARG:HB3	2.01	0.42
1:A:336:VAL:HB	1:A:414:ARG:HG3	2.00	0.42
1:A:396:GLY:HA3	1:A:401:ALA:HA	2.01	0.42
1:A:397:HIS:HB3	1:A:398:PRO:HD2	2.02	0.42
1:A:370:GLY:HA3	1:A:403:PHE:CZ	2.54	0.42
1:A:476:LEU:HD12	1:A:501:ASP:HB3	2.01	0.42
1:A:580:VAL:HG12	1:A:583:LEU:HB2	2.02	0.42
1:A:2:SER:HG	1:A:360:ARG:NH2	2.18	0.42
1:A:116:ILE:O	1:A:393[A]:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD13	1:A:45:LEU:HD13	2.01	0.42
1:A:471:LEU:CD2	1:A:506:ARG:HG3	2.50	0.41
2:C:204:DA:H2"	2:C:205:DG:C8	2.55	0.41
1:A:18:LEU:O	1:A:22:MET:HG3	2.20	0.41
1:A:477:VAL:HG12	1:A:478:GLY:H	1.84	0.41
1:A:109:ARG:HD3	1:A:280:ARG:HA	2.02	0.41
1:A:391:LEU:HD21	1:A:413:LEU:HD13	2.01	0.41
1:A:351:ALA:O	1:A:355:VAL:HG23	2.20	0.41
1:A:257:LYS:HB2	1:A:259:VAL:HG23	2.03	0.41
1:A:290:LEU:O	1:A:293:THR:HG22	2.20	0.41
1:A:471:LEU:CD2	1:A:504:GLY:O	2.65	0.41
1:A:587:ASP:OD1	1:A:590:ALA:HB2	2.21	0.41
1:A:19:LEU:O	1:A:23:ARG:HG3	2.21	0.41
1:A:2:SER:O	1:A:3:ARG:HG3	2.21	0.41
1:A:75:ARG:NH1	1:A:124:HIS:ND1	2.65	0.41
1:A:640:LEU:O	1:A:640:LEU:HD12	2.21	0.41
1:A:138:VAL:CG2	1:A:158:ASP:HB3	2.51	0.40
1:A:224:VAL:HG13	1:A:458:GLU:HG3	2.03	0.40
2:C:206:DG:C6	2:C:207:DC:N4	2.90	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	705/705 (100%)	695 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	543/543 (100%)	522 (96%)	21 (4%)	39	68

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

Mol	Chain	Res	Type
1	A	42	THR
1	A	120	ARG
1	A	141	LEU
1	A	165	ASN
1	A	175	HIS
1	A	223	ASP
1	A	271	LEU
1	A	300	LYS
1	A	352	SER
1	A	360	ARG
1	A	408	GLN
1	A	447	LEU
1	A	473	ASP
1	A	476	LEU
1	A	499	ARG
1	A	500	ASP
1	A	554	ARG
1	A	569	GLU
1	A	599	LEU
1	A	608	LEU
1	A	700	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	SO4	A	801	-	4,4,4	0.30	0	6,6,6	0.09	0
3	SO4	A	802	-	4,4,4	0.28	0	6,6,6	0.12	0
3	SO4	A	803	-	4,4,4	0.29	0	6,6,6	0.14	0
3	SO4	A	804	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	A	805	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	A	806	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	A	807	-	4,4,4	0.26	0	6,6,6	0.05	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	SO4	A	801	-	-	0/0/0/0	0/0/0/0
3	SO4	A	802	-	-	0/0/0/0	0/0/0/0
3	SO4	A	803	-	-	0/0/0/0	0/0/0/0
3	SO4	A	804	-	-	0/0/0/0	0/0/0/0
3	SO4	A	805	-	-	0/0/0/0	0/0/0/0
3	SO4	A	806	-	-	0/0/0/0	0/0/0/0
3	SO4	A	807	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	SO4	2	0
3	A	803	SO4	3	0
3	A	807	SO4	1	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 (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	705/705 (100%)	-0.01	29 (4%)	41	33	39, 65, 107, 154	0
2	C	14/14 (100%)	1.52	5 (35%)	0	0	56, 87, 153, 169	0
All	All	719/719 (100%)	0.02	34 (4%)	35	28	39, 66, 108, 169	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	692	ALA	8.6
1	A	705	GLY	5.7
1	A	517	TRP	5.3
1	A	1	MET	5.2
2	C	207	DC	5.1
1	A	691	ALA	5.0
1	A	516	GLU	4.8
2	C	206	DG	4.7
1	A	702	LEU	4.4
2	C	205	DG	4.1
1	A	520	ARG	4.0
1	A	518	LYS	3.9
1	A	2	SER	3.8
1	A	618	GLN	3.6
2	C	204	DA	3.3
1	A	693	LEU	3.2
1	A	519	GLY	2.9
1	A	694	PRO	2.7
1	A	695	LYS	2.7
1	A	479	LYS	2.7
1	A	85	VAL	2.5
1	A	545	LEU	2.5
1	A	546	PRO	2.4
1	A	88	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	4	PRO	2.4
1	A	408	GLN	2.4
1	A	521	THR	2.3
2	C	200	DC	2.3
1	A	547	THR	2.3
1	A	6	HIS	2.2
1	A	616	GLN	2.2
1	A	549	PRO	2.2
1	A	86	SER	2.1
1	A	619	GLY	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(Å²)	Q<0.9
3	SO4	A	803	5/5	0.87	0.21	3.77	99,100,100,101	0
3	SO4	A	802	5/5	0.96	0.24	1.25	51,60,60,63	0
4	MN	A	809	1/1	0.97	0.20	-0.18	66,66,66,66	0
4	MN	A	808	1/1	0.97	0.20	-0.58	69,69,69,69	0
3	SO4	A	801	5/5	0.94	0.14	-2.34	84,84,84,85	0
3	SO4	A	804	5/5	0.93	0.47	-	105,106,106,106	0
3	SO4	A	805	5/5	0.70	0.36	-	106,106,106,107	0
3	SO4	A	807	5/5	0.92	0.13	-	128,128,128,129	0
3	SO4	A	806	5/5	0.94	0.41	-	112,112,112,112	0

6.5 Other polymers (i)

There are no such residues in this entry.