



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:43 pm BST

PDB ID : 5F56
Title : Structure of RecJ complexed with DNA and SSB-ct
Authors : Zhao, Y.; Hua, Y.; Cheng, K.
Deposited on : 2015-12-04
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

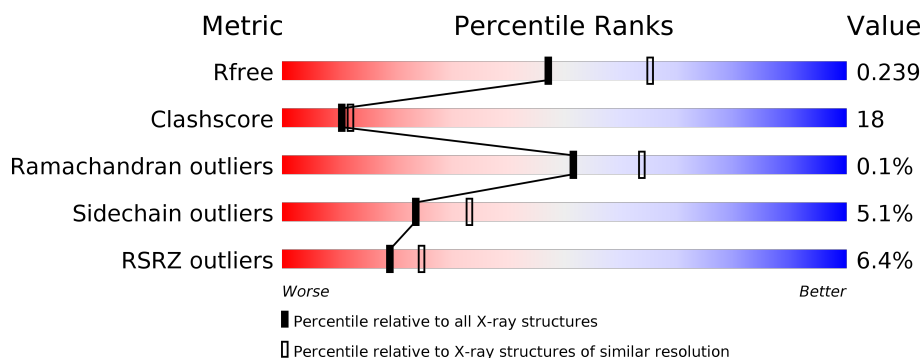
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	705	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div></div> </div> </div>
2	C	9	<div> <div>33%</div> <div> <div>22%</div> <div>78%</div> </div> </div>
3	B	5	<div> <div>20%</div> <div> <div></div> <div>100%</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5723 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	703	Total	C	N	O	S	0	0	0
			5342	3374	975	981	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			182	88	35	51	8			

- Molecule 3 is a protein called ALA-ASP-LEU-PRO-PHE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	5	Total	C	N	O	0	0	0
			40	27	5	8			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mn 2 2	0	0

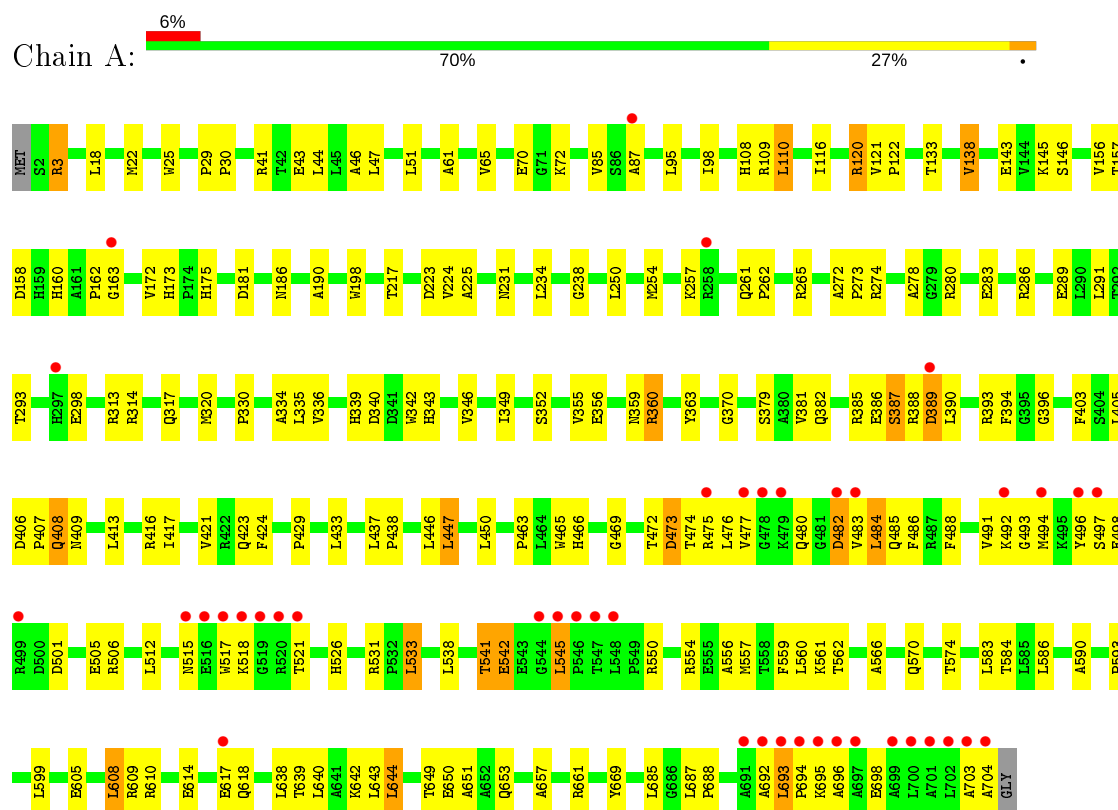
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	137	Total O 137 137	0	0
6	C	4	Total O 4 4	0	0
6	B	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 the various outlier classes 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.

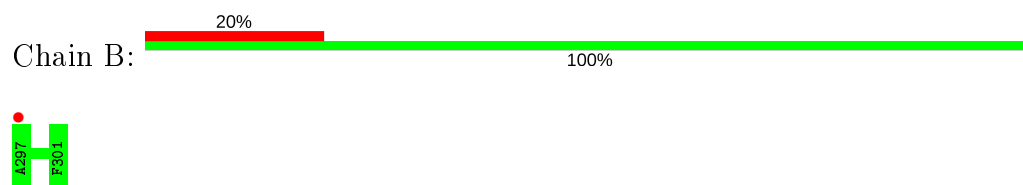
- Molecule 1: Single-stranded-DNA-specific exonuclease



- Molecule 2: DNA (5'-D(*CP*TP*GP*AP*TP*GP*GP*CP*A)-3')



- Molecule 3: ALA-ASP-LEU-PRO-PHE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.22Å 102.22Å 166.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.05 – 2.30 29.05 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.05-2.30) 99.5 (29.05-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10_2155: 000)	Depositor
R, R_{free}	0.226 , 0.239 0.226 , 0.239	Depositor DCC
R_{free} test set	2280 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
Reported twinning fraction	0.050 for -h,-k,l	Depositor
Outliers	0 of 45296 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5723	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.56	0/5469	0.65	0/7470
2	C	0.64	0/204	0.94	0/314
3	B	0.27	0/41	0.39	0/54
All	All	0.56	0/5714	0.66	0/7838

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

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	5342	0	5342	200	0
2	C	182	0	100	9	0
3	B	40	0	35	0	0
4	A	15	0	0	0	0
5	A	2	0	0	0	0
6	A	137	0	0	2	0
6	B	1	0	0	0	0
6	C	4	0	0	0	0
All	All	5723	0	5477	204	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 18.

All (204) 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:389:ASP:OD2	1:A:416:ARG:NH2	1.72	1.22
1:A:386:GLU:O	1:A:416:ARG:NH1	1.85	1.09
1:A:3:ARG:HH21	1:A:3:ARG:HB2	1.16	1.05
1:A:381:VAL:HG21	1:A:396:GLY:O	1.61	0.99
1:A:3:ARG:HH11	1:A:360:ARG:HH21	1.02	0.98
1:A:330:PRO:O	1:A:360:ARG:NH1	2.01	0.93
1:A:359:ASN:ND2	1:A:429:PRO:HD3	1.82	0.93
1:A:138:VAL:HG22	1:A:158:ASP:OD2	1.69	0.93
1:A:3:ARG:HH11	1:A:360:ARG:NH2	1.69	0.91
1:A:517:TRP:CZ3	1:A:518:LYS:HG3	2.06	0.90
1:A:472:THR:OG1	1:A:473:ASP:OD1	1.89	0.90
1:A:41:ARG:NH1	1:A:181:ASP:OD2	2.04	0.90
1:A:545:LEU:HD12	1:A:545:LEU:H	1.36	0.89
1:A:517:TRP:CE3	1:A:518:LYS:HG3	2.07	0.88
1:A:480:GLN:HB3	1:A:482:ASP:OD1	1.72	0.87
1:A:133:THR:O	1:A:157:THR:OG1	1.93	0.84
1:A:695:LYS:HA	1:A:698:GLU:HB2	1.58	0.84
1:A:649:THR:HG22	1:A:651:ALA:H	1.41	0.84
1:A:538:LEU:O	1:A:541:THR:OG1	1.96	0.83
1:A:550:ARG:NH1	1:A:669:TYR:O	2.12	0.83
1:A:3:ARG:NH1	1:A:360:ARG:HH21	1.76	0.82
1:A:317:GLN:HB2	1:A:346:VAL:HG11	1.62	0.81
2:C:3:DG:H2''	2:C:4:DA:H5''	1.64	0.80
1:A:388:ARG:HG2	1:A:394:PHE:HE2	1.46	0.79
1:A:695:LYS:O	1:A:698:GLU:N	2.16	0.79
1:A:640:LEU:HD12	1:A:640:LEU:O	1.81	0.78
1:A:639:THR:OG1	1:A:642:LYS:HG3	1.83	0.78
1:A:3:ARG:NH2	1:A:3:ARG:HB2	1.95	0.78
1:A:120:ARG:HG3	1:A:120:ARG:HH11	1.49	0.77
1:A:381:VAL:CG2	1:A:396:GLY:O	2.32	0.77
1:A:273:PRO:HG3	2:C:4:DA:H5'	1.66	0.76
1:A:3:ARG:NH1	1:A:360:ARG:NH2	2.33	0.75
1:A:257:LYS:HE3	1:A:274:ARG:NH2	2.02	0.74
1:A:474:THR:OG1	1:A:501:ASP:O	2.03	0.74
1:A:515:ASN:O	1:A:521:THR:HA	1.87	0.73
1:A:545:LEU:HD12	1:A:545:LEU:N	2.03	0.73
1:A:608:LEU:HD13	1:A:685:LEU:HD11	1.71	0.72
1:A:108:HIS:CE1	1:A:110:LEU:HB2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:VAL:HG23	1:A:483:VAL:HB	1.72	0.71
1:A:388:ARG:HG2	1:A:394:PHE:CE2	2.25	0.71
1:A:120:ARG:CG	1:A:120:ARG:HH11	2.04	0.69
1:A:484:LEU:HD23	1:A:485:GLN:N	2.07	0.69
1:A:482:ASP:O	1:A:498:GLU:O	2.10	0.68
1:A:643:LEU:O	1:A:644:LEU:HD12	1.94	0.67
1:A:389:ASP:CG	1:A:416:ARG:HH22	1.97	0.67
1:A:476:LEU:HD11	1:A:501:ASP:HB3	1.77	0.67
1:A:379:SER:OG	1:A:382:GLN:HG2	1.94	0.67
1:A:692:ALA:O	1:A:693:LEU:HB2	1.95	0.67
1:A:506:ARG:HG2	1:A:531:ARG:O	1.95	0.67
1:A:649:THR:HG22	1:A:651:ALA:N	2.08	0.67
1:A:657:ALA:O	1:A:661:ARG:HG3	1.93	0.67
1:A:533:LEU:N	1:A:533:LEU:HD23	2.09	0.66
1:A:485:GLN:NE2	2:C:8:DC:O2	2.28	0.66
1:A:640:LEU:HD11	1:A:644:LEU:HD22	1.77	0.65
1:A:494:MET:CE	1:A:496:TYR:CE2	2.80	0.65
1:A:320:MET:HE1	1:A:343:HIS:HB3	1.79	0.65
1:A:494:MET:CE	1:A:496:TYR:CD2	2.81	0.64
1:A:108:HIS:HE1	1:A:110:LEU:HB2	1.61	0.64
1:A:605:GLU:OE2	1:A:661:ARG:NH1	2.32	0.63
1:A:293:THR:OG1	1:A:298:GLU:OE1	2.11	0.63
1:A:320:MET:HG3	1:A:342:TRP:CD1	2.34	0.63
1:A:346:VAL:HG12	1:A:346:VAL:O	2.00	0.61
1:A:157:THR:HG22	1:A:172:VAL:HB	1.81	0.61
1:A:590:ALA:O	1:A:610:ARG:NH1	2.34	0.61
1:A:643:LEU:C	1:A:644:LEU:HD12	2.21	0.61
1:A:494:MET:HE2	1:A:496:TYR:CD2	2.35	0.60
1:A:359:ASN:CG	1:A:429:PRO:HD3	2.22	0.60
1:A:486:PHE:O	1:A:493:GLY:N	2.34	0.60
1:A:643:LEU:C	1:A:644:LEU:CD1	2.70	0.60
1:A:494:MET:HE1	1:A:496:TYR:CE2	2.37	0.59
1:A:138:VAL:HG13	1:A:158:ASP:HB3	1.84	0.59
1:A:614:GLU:O	1:A:618:GLN:HG2	2.03	0.59
1:A:640:LEU:CD1	1:A:644:LEU:HD22	2.34	0.58
1:A:3:ARG:CB	1:A:3:ARG:HH21	2.04	0.57
1:A:382:GLN:HE22	1:A:385:ARG:HE	1.52	0.57
1:A:476:LEU:CD1	1:A:501:ASP:HB3	2.34	0.57
1:A:505:GLU:HG2	1:A:533:LEU:HD11	1.87	0.57
1:A:498:GLU:HA	1:A:498:GLU:OE1	2.04	0.57
1:A:336:VAL:HG22	1:A:363:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:VAL:HG12	1:A:224:VAL:O	2.05	0.56
1:A:346:VAL:HG13	1:A:349:ILE:HD12	1.87	0.56
1:A:339:HIS:HB3	1:A:342:TRP:CG	2.41	0.55
1:A:484:LEU:HD23	1:A:485:GLN:O	2.06	0.55
1:A:320:MET:HE1	1:A:343:HIS:H	1.72	0.55
1:A:433:LEU:HG	1:A:466:HIS:HB2	1.88	0.55
1:A:494:MET:HE1	1:A:496:TYR:CD2	2.42	0.55
1:A:278:ALA:HB1	1:A:283:GLU:O	2.08	0.54
1:A:695:LYS:O	1:A:696:ALA:C	2.45	0.54
1:A:257:LYS:HE3	1:A:274:ARG:HH21	1.70	0.54
1:A:480:GLN:HA	1:A:480:GLN:OE1	2.07	0.54
1:A:609:ARG:HG2	1:A:687:LEU:HD11	1.90	0.54
1:A:217:THR:OG1	1:A:238:GLY:HA3	2.08	0.54
1:A:557:MET:O	1:A:561:LYS:HG2	2.08	0.53
1:A:482:ASP:O	1:A:498:GLU:N	2.40	0.53
1:A:643:LEU:HG	1:A:644:LEU:CD1	2.37	0.53
1:A:703:ALA:O	1:A:704:ALA:HB2	2.09	0.53
1:A:70:GLU:OE1	1:A:72:LYS:HE3	2.08	0.53
1:A:541:THR:C	1:A:542:GLU:OE1	2.47	0.53
1:A:334:ALA:HB2	1:A:421:VAL:HG21	1.91	0.53
1:A:379:SER:CB	1:A:382:GLN:HG2	2.39	0.53
1:A:320:MET:HE1	1:A:343:HIS:CB	2.38	0.53
1:A:586:LEU:HD11	1:A:593:PRO:HD3	1.91	0.53
1:A:261:GLN:N	1:A:262:PRO:CD	2.72	0.52
1:A:476:LEU:HD12	1:A:476:LEU:N	2.24	0.52
1:A:382:GLN:OE1	1:A:385:ARG:NH2	2.42	0.52
1:A:475:ARG:C	1:A:476:LEU:HD12	2.30	0.52
1:A:95:LEU:O	1:A:98:ILE:HG13	2.08	0.52
1:A:644:LEU:CD1	1:A:644:LEU:N	2.73	0.51
1:A:533:LEU:H	1:A:533:LEU:HD23	1.76	0.51
1:A:517:TRP:CZ3	1:A:518:LYS:CG	2.85	0.51
1:A:693:LEU:N	1:A:694:PRO:CD	2.73	0.51
1:A:505:GLU:C	1:A:533:LEU:HD21	2.32	0.50
1:A:505:GLU:CG	1:A:533:LEU:HD11	2.40	0.50
1:A:61:ALA:O	1:A:65:VAL:HG23	2.11	0.50
1:A:506:ARG:HA	1:A:533:LEU:CD2	2.42	0.50
1:A:387:SER:HA	1:A:416:ARG:NH1	2.27	0.50
1:A:18:LEU:O	1:A:22:MET:HG3	2.11	0.49
1:A:491:VAL:HG12	1:A:492:LYS:N	2.26	0.49
1:A:492:LYS:HE2	2:C:9:DA:C2	2.47	0.49
1:A:496:TYR:O	1:A:497:SER:OG	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:THR:OG1	1:A:156:VAL:HA	2.13	0.49
1:A:320:MET:CE	1:A:343:HIS:H	2.25	0.48
1:A:382:GLN:NE2	1:A:385:ARG:HE	2.10	0.48
1:A:394:PHE:C	1:A:394:PHE:CD1	2.86	0.48
1:A:339:HIS:ND1	1:A:340:ASP:N	2.61	0.48
1:A:225:ALA:O	6:A:901:HOH:O	2.20	0.48
1:A:541:THR:O	1:A:542:GLU:OE1	2.32	0.48
1:A:554:ARG:HA	1:A:557:MET:CE	2.45	0.47
1:A:640:LEU:HD12	1:A:640:LEU:C	2.35	0.47
1:A:85:VAL:HG12	1:A:291:LEU:HD12	1.96	0.47
1:A:438:PRO:HG2	1:A:638:LEU:HD11	1.97	0.47
1:A:87:ALA:HB2	1:A:190:ALA:HA	1.97	0.46
1:A:234:LEU:C	1:A:234:LEU:HD23	2.35	0.46
2:C:5:DT:O2	2:C:5:DT:H2'	2.15	0.46
1:A:482:ASP:HB3	1:A:497:SER:HA	1.98	0.46
1:A:265:ARG:HH22	2:C:5:DT:H3	1.63	0.46
1:A:447:LEU:HG	1:A:512:LEU:HB3	1.97	0.46
1:A:109:ARG:HD3	1:A:280:ARG:HA	1.98	0.46
1:A:484:LEU:CD2	1:A:484:LEU:C	2.84	0.46
1:A:494:MET:HG3	1:A:494:MET:O	2.15	0.46
1:A:562:THR:HG22	1:A:562:THR:O	2.15	0.46
1:A:423:GLN:HG2	1:A:424:PHE:CE1	2.51	0.46
1:A:450:LEU:HD13	1:A:463:PRO:HG2	1.99	0.45
2:C:6:DG:H2''	2:C:7:DG:OP2	2.15	0.45
1:A:643:LEU:C	1:A:644:LEU:HD13	2.37	0.45
1:A:482:ASP:OD1	1:A:482:ASP:N	2.48	0.45
1:A:145:LYS:HE2	1:A:146:SER:N	2.32	0.45
1:A:476:LEU:CD1	1:A:476:LEU:N	2.80	0.45
1:A:649:THR:HG22	1:A:650:GLU:N	2.31	0.44
1:A:492:LYS:HE2	2:C:9:DA:H2	1.83	0.44
1:A:317:GLN:CB	1:A:346:VAL:HG11	2.41	0.44
1:A:405:LEU:O	1:A:405:LEU:HD23	2.17	0.44
1:A:515:ASN:HD21	1:A:517:TRP:HE3	1.65	0.44
2:C:4:DA:H2''	2:C:5:DT:H5''	1.99	0.44
1:A:257:LYS:HA	1:A:257:LYS:HD3	1.68	0.44
1:A:695:LYS:HA	1:A:698:GLU:CB	2.39	0.44
1:A:138:VAL:HG11	1:A:173:HIS:CD2	2.53	0.44
1:A:491:VAL:CG1	1:A:492:LYS:N	2.81	0.44
1:A:160:HIS:O	1:A:162:PRO:HD3	2.18	0.44
1:A:352:SER:O	1:A:356:GLU:HG3	2.17	0.44
1:A:359:ASN:ND2	1:A:429:PRO:CD	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ARG:HA	1:A:533:LEU:HD23	1.99	0.44
1:A:570:GLN:O	1:A:574:THR:HG23	2.18	0.44
1:A:437:LEU:HB2	1:A:465:TRP:CE3	2.53	0.43
1:A:488:PHE:CD1	1:A:488:PHE:C	2.92	0.43
1:A:643:LEU:HB3	1:A:644:LEU:HD13	1.99	0.43
1:A:29:PRO:N	1:A:30:PRO:HD2	2.33	0.43
1:A:413:LEU:O	1:A:417:ILE:HG12	2.19	0.43
1:A:280:ARG:CZ	1:A:349:ILE:HD11	2.48	0.43
1:A:473:ASP:OD1	1:A:473:ASP:N	2.51	0.43
1:A:390:LEU:HA	1:A:409:ASN:HD22	1.84	0.43
1:A:583:LEU:HD12	1:A:584:THR:H	1.83	0.42
1:A:695:LYS:C	1:A:698:GLU:H	2.23	0.42
1:A:51:LEU:HD22	1:A:198:TRP:CE2	2.53	0.42
1:A:408:GLN:OE1	1:A:408:GLN:HA	2.19	0.42
1:A:186:ASN:O	1:A:231:ASN:ND2	2.48	0.42
1:A:394:PHE:O	1:A:394:PHE:CD1	2.72	0.42
1:A:556:ALA:O	1:A:559:PHE:HB2	2.20	0.42
1:A:280:ARG:HD2	1:A:313:ARG:HD2	2.02	0.42
1:A:339:HIS:HB3	1:A:342:TRP:CD1	2.55	0.42
1:A:370:GLY:HA3	1:A:403:PHE:CZ	2.54	0.42
1:A:560:LEU:HD21	1:A:566:ALA:HB2	2.02	0.42
1:A:649:THR:O	1:A:653:GLN:HG3	2.20	0.42
1:A:121:VAL:N	1:A:122:PRO:CD	2.83	0.41
1:A:687:LEU:HB3	1:A:688:PRO:HD2	2.00	0.41
1:A:554:ARG:HA	1:A:557:MET:HE3	2.01	0.41
1:A:116:ILE:O	1:A:143:GLU:HG2	2.20	0.41
1:A:25:TRP:HH2	1:A:46:ALA:HB2	1.86	0.41
1:A:484:LEU:CD2	1:A:485:GLN:O	2.68	0.41
1:A:506:ARG:HG2	1:A:531:ARG:C	2.41	0.41
1:A:272:ALA:N	1:A:273:PRO:CD	2.84	0.41
1:A:390:LEU:CA	1:A:409:ASN:HD22	2.34	0.41
1:A:560:LEU:CD2	1:A:566:ALA:HB2	2.51	0.41
1:A:649:THR:CG2	1:A:650:GLU:N	2.83	0.41
1:A:406:ASP:OD1	1:A:407:PRO:N	2.54	0.41
1:A:43:GLU:O	1:A:47:LEU:HB2	2.21	0.41
1:A:163:GLY:HA3	6:A:992:HOH:O	2.21	0.40
1:A:491:VAL:HG12	1:A:492:LYS:O	2.21	0.40
1:A:355:VAL:HG22	1:A:360:ARG:O	2.21	0.40
1:A:389:ASP:OD1	1:A:389:ASP:N	2.48	0.40
1:A:469:GLY:HA3	1:A:488:PHE:CZ	2.56	0.40
1:A:250:LEU:O	1:A:254:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:NH2	1:A:289:GLU:OE1	2.43	0.40
1:A:120:ARG:CG	1:A:120:ARG:NH1	2.72	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	701/705 (99%)	693 (99%)	7 (1%)	1 (0%)	51	64
3	B	3/5 (60%)	3 (100%)	0	0	100	100
All	All	704/710 (99%)	696 (99%)	7 (1%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	693	LEU

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	541/543 (100%)	513 (95%)	28 (5%)	23	32
3	B	4/4 (100%)	4 (100%)	0	100	100
All	All	545/547 (100%)	517 (95%)	28 (5%)	24	33

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	44	LEU
1	A	110	LEU
1	A	120	ARG
1	A	138	VAL
1	A	175	HIS
1	A	223	ASP
1	A	314	ARG
1	A	335	LEU
1	A	360	ARG
1	A	387	SER
1	A	389	ASP
1	A	393	ARG
1	A	408	GLN
1	A	446	LEU
1	A	447	LEU
1	A	473	ASP
1	A	482	ASP
1	A	484	LEU
1	A	526	HIS
1	A	533	LEU
1	A	541	THR
1	A	542	GLU
1	A	545	LEU
1	A	599	LEU
1	A	608	LEU
1	A	617	GLU
1	A	644	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	ASN
1	A	409	ASN

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	802	-	4,4,4	0.14	0	6,6,6	0.24	0
4	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	801	-	4,4,4	0.13	0	6,6,6	0.05	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.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	703/705 (99%)	0.22	42 (5%) 21 28	32, 50, 114, 188	0
2	C	9/9 (100%)	1.69	3 (33%) 0 0	48, 66, 131, 136	0
3	B	5/5 (100%)	1.37	1 (20%) 1 1	58, 65, 88, 90	0
All	All	717/719 (99%)	0.25	46 (6%) 19 25	32, 51, 116, 188	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	704	ALA	10.3
1	A	692	ALA	8.9
1	A	693	LEU	8.2
1	A	697	ALA	8.1
1	A	694	PRO	7.2
1	A	479	LYS	6.7
1	A	702	LEU	6.2
1	A	520	ARG	6.0
1	A	475	ARG	5.8
1	A	516	GLU	5.8
1	A	699	ALA	5.2
1	A	517	TRP	5.2
2	C	7	DG	4.9
1	A	518	LYS	4.9
1	A	519	GLY	4.7
1	A	499	ARG	4.5
1	A	703	ALA	4.4
1	A	691	ALA	4.3
1	A	483	VAL	4.3
1	A	701	ALA	4.0
2	C	6	DG	4.0
1	A	696	ALA	3.3
1	A	478	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	545	LEU	3.1
1	A	547	THR	2.9
1	A	548	LEU	2.8
1	A	521	THR	2.8
1	A	482	ASP	2.8
1	A	163	GLY	2.7
1	A	700	LEU	2.7
1	A	87	ALA	2.6
1	A	544	GLY	2.6
1	A	477	VAL	2.6
3	B	297	ALA	2.6
1	A	492	LYS	2.5
1	A	515	ASN	2.4
1	A	496	TYR	2.4
1	A	695	LYS	2.4
1	A	497	SER	2.3
1	A	546	PRO	2.3
1	A	258	ARG	2.3
1	A	617	GLU	2.2
2	C	8	DC	2.2
1	A	389	ASP	2.2
1	A	297	HIS	2.1
1	A	494	MET	2.1

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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	803	5/5	0.93	0.14	103,105,105,105	0
4	SO4	A	802	5/5	0.94	0.16	74,74,76,77	0
5	MN	A	804	1/1	0.95	0.14	74,74,74,74	0
5	MN	A	805	1/1	0.95	0.15	49,49,49,49	0
4	SO4	A	801	5/5	0.98	0.06	74,74,74,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.