Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:46 PM GMT

PDB ID	:	1H79
Title	:	STRUCTURAL BASIS FOR ALLOSTERIC SUBSTRATE SPECIFICITY REGULATION IN CLASS III RIBONUCLEOTIDE REDUCTASES: NRDD IN COMPLEX WITH DTTP
Authors	:	Larsson, K.-M.; Andersson, J.; Sjoeberg, B.-M.; Nordlund, P.; Logan, D.T.
Deposited on	:	2001-07-04
Resolution	:	2.90 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:

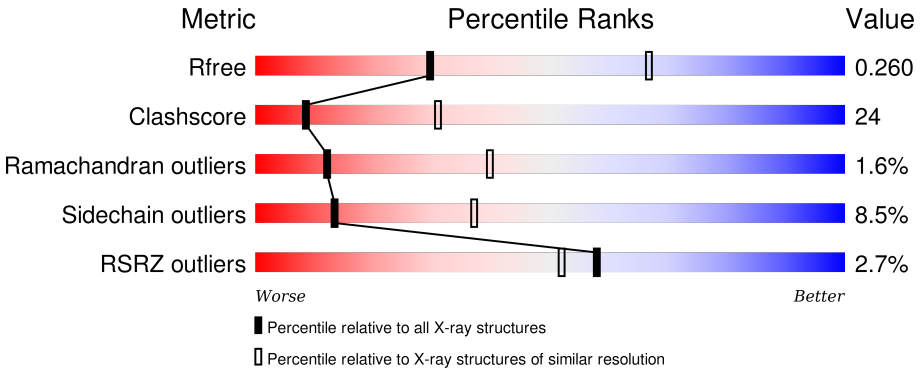
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	605	2% 54% 33% 5% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4479 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.

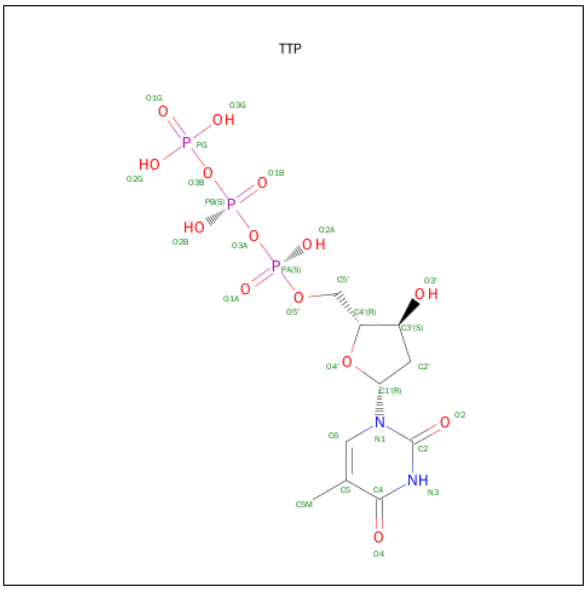
- Molecule 1 is a protein called ANAEROBIC RIBONUCLEOTIDE-TRIPHOSPHATE REDUCTASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4395	2797	740	829	29	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	580	ALA	GLY	ENGINEERED MUTATION	UNP Q9T0V5

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	29	10	2	14	3	0	0
			Total	C	N	O	P		
2	A	1	29	10	2	14	3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 5 is water.

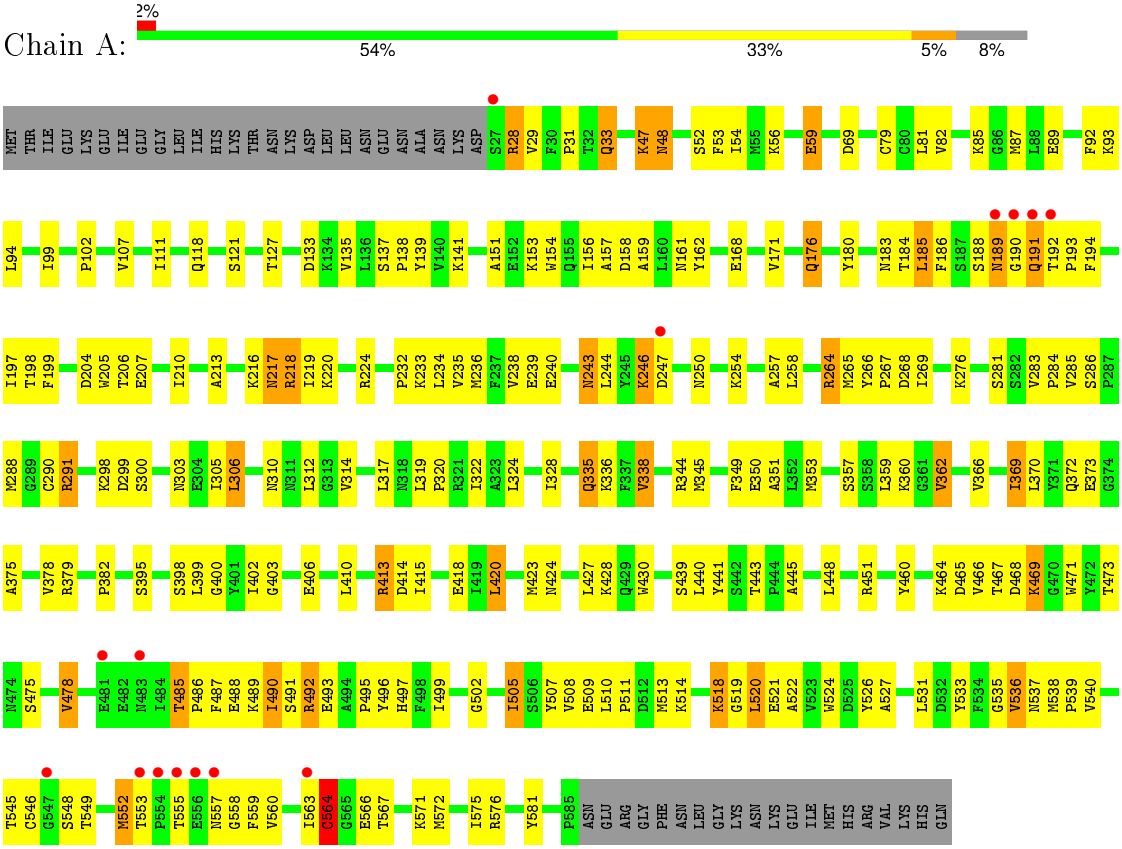
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	24	Total O 24 24	0	0

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: ANAEROBIC RIBONUCLEOTIDE-TRIPHOSPHATE REDUCTASE LARGE CHAIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.10Å 98.10Å 243.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.99-2.90) 99.0 (19.99-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.14 (at 2.88Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.261 0.223 , 0.260	Depositor DCC
R_{free} test set	2270 reflections (8.48%)	DCC
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 26785 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4479	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: MG, TTP, FE2

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	0.38	0/4493	0.64	2/6083 (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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	268	ASP	N-CA-C	-5.56	95.98	111.00
1	A	328	ILE	N-CA-C	-5.13	97.16	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain

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	4395	0	4345	211	0
2	A	58	0	26	1	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	24	0	0	1	0
All	All	4479	0	4371	211	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 24.

All (211) 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:560:VAL:HG12	1:A:567:THR:HG22	1.44	0.97
1:A:492:ARG:HH11	1:A:492:ARG:HG2	1.29	0.95
1:A:240:GLU:HG3	1:A:244:LEU:HD23	1.48	0.95
1:A:29:VAL:HG12	1:A:31:PRO:HD2	1.53	0.89
1:A:370:LEU:HA	1:A:375:ALA:HB3	1.61	0.82
1:A:478:VAL:HG11	1:A:489:LYS:HG3	1.61	0.81
1:A:118:GLN:HB3	1:A:369:ILE:HG12	1.63	0.81
1:A:486:PRO:O	1:A:490:ILE:HG23	1.80	0.81
1:A:555:THR:HG22	1:A:557:ASN:H	1.47	0.80
1:A:236:MET:HE1	1:A:257:ALA:HB2	1.69	0.74
1:A:490:ILE:HD12	1:A:527:ALA:HA	1.69	0.74
1:A:99:ILE:HG23	2:A:1586:TTP:H1'	1.70	0.74
1:A:233:LYS:NZ	1:A:290:CYS:SG	2.62	0.73
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.53	0.73
1:A:518:LYS:H	1:A:518:LYS:NZ	1.86	0.72
1:A:94:LEU:HD11	1:A:118:GLN:HG3	1.71	0.72
1:A:151:ALA:HA	1:A:156:ILE:CG1	2.22	0.69
1:A:233:LYS:HG3	1:A:266:TYR:CZ	2.28	0.69
1:A:276:LYS:HG2	1:A:281:SER:O	1.93	0.69
1:A:546:CYS:HB3	1:A:564:CYS:HB2	1.74	0.68
1:A:240:GLU:CD	1:A:240:GLU:H	1.97	0.67
1:A:218:ARG:HD2	1:A:264:ARG:HG2	1.78	0.65
1:A:492:ARG:HG2	1:A:492:ARG:NH1	2.03	0.65
1:A:540:VAL:HG23	1:A:575:ILE:HB	1.78	0.65
1:A:420:LEU:HB3	1:A:499:ILE:HG21	1.78	0.65
1:A:369:ILE:HD12	1:A:370:LEU:H	1.60	0.65
1:A:359:LEU:O	1:A:362:VAL:HG13	1.97	0.65
1:A:28:ARG:CD	1:A:28:ARG:H	2.10	0.64
1:A:418:GLU:H	1:A:418:GLU:CD	2.00	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:O	1:A:219:ILE:HG13	1.98	0.63
1:A:518:LYS:H	1:A:518:LYS:HZ2	1.45	0.63
1:A:204:ASP:HB3	1:A:207:GLU:HG3	1.79	0.63
1:A:102:PRO:HG3	1:A:111:ILE:HD12	1.78	0.63
1:A:478:VAL:CG1	1:A:489:LYS:HG3	2.29	0.63
1:A:540:VAL:O	1:A:540:VAL:HG23	1.99	0.62
1:A:218:ARG:NH2	1:A:232:PRO:O	2.31	0.62
1:A:469:LYS:HE2	1:A:471:TRP:O	1.98	0.62
1:A:198:THR:HG22	1:A:235:VAL:HB	1.81	0.62
1:A:233:LYS:HE3	1:A:266:TYR:OH	1.99	0.62
1:A:299:ASP:HB3	1:A:305:ILE:HD12	1.81	0.62
1:A:151:ALA:HA	1:A:156:ILE:HG12	1.80	0.62
1:A:137:SER:HB3	1:A:138:PRO:HD3	1.80	0.62
1:A:48:ASN:N	1:A:48:ASN:HD22	1.96	0.62
1:A:372:GLN:NE2	1:A:382:PRO:HG3	2.14	0.61
1:A:285:VAL:HG22	1:A:306:LEU:HD21	1.83	0.61
1:A:204:ASP:OD1	1:A:205:TRP:N	2.33	0.61
1:A:158:ASP:HB3	1:A:161:ASN:HB3	1.83	0.61
1:A:478:VAL:HG13	1:A:489:LYS:HE2	1.81	0.61
1:A:85:LYS:O	1:A:89:GLU:HG3	2.00	0.60
1:A:52:SER:O	1:A:56:LYS:HG2	2.02	0.60
1:A:28:ARG:N	1:A:28:ARG:HD3	2.17	0.60
1:A:345:MET:HE1	1:A:423:MET:CE	2.31	0.60
1:A:28:ARG:H	1:A:28:ARG:HD3	1.66	0.60
1:A:219:ILE:HD12	1:A:220:LYS:N	2.16	0.59
1:A:513:MET:HG3	1:A:538:MET:HE1	1.83	0.59
1:A:224:ARG:HG2	1:A:224:ARG:HH11	1.66	0.59
1:A:552:MET:HG2	1:A:559:PHE:HB3	1.83	0.59
1:A:29:VAL:HG12	1:A:31:PRO:CD	2.28	0.58
1:A:509:GLU:O	1:A:510:LEU:HD12	2.04	0.58
1:A:406:GLU:OE2	1:A:473:THR:HG23	2.04	0.58
1:A:258:LEU:HD12	1:A:520:LEU:HD13	1.84	0.58
1:A:402:ILE:HG13	1:A:403:GLY:N	2.18	0.58
1:A:555:THR:HB	1:A:558:GLY:O	2.04	0.57
1:A:539:PRO:HB2	1:A:576:ARG:HH21	1.69	0.57
1:A:312:LEU:HD13	1:A:395:SER:HB3	1.86	0.57
1:A:264:ARG:O	1:A:265:MET:HB3	2.04	0.57
1:A:345:MET:HE1	1:A:423:MET:HE3	1.87	0.57
1:A:243:ASN:HD22	1:A:243:ASN:N	2.03	0.57
1:A:424:ASN:O	1:A:428:LYS:HG2	2.04	0.57
1:A:539:PRO:CB	1:A:576:ARG:HH21	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:THR:C	1:A:186:PHE:H	2.07	0.56
1:A:497:HIS:ND1	1:A:531:LEU:HB2	2.20	0.56
1:A:540:VAL:CG2	1:A:575:ILE:HB	2.36	0.56
1:A:539:PRO:HA	1:A:576:ARG:HE	1.70	0.56
1:A:199:PHE:HE1	1:A:236:MET:HE2	1.70	0.56
1:A:468:ASP:OD1	1:A:469:LYS:N	2.39	0.56
1:A:490:ILE:HD11	1:A:526:TYR:CD2	2.41	0.55
1:A:505:ILE:HG12	1:A:533:TYR:CD2	2.42	0.55
1:A:198:THR:HG21	1:A:286:SER:HB3	1.88	0.55
1:A:238:VAL:HA	1:A:243:ASN:HD21	1.72	0.55
1:A:314:VAL:HG22	1:A:398:SER:HB2	1.87	0.55
1:A:158:ASP:CB	1:A:161:ASN:HB3	2.37	0.55
1:A:239:GLU:H	1:A:243:ASN:HD21	1.53	0.54
1:A:189:ASN:C	1:A:191:GLN:H	2.10	0.54
1:A:59:GLU:OE1	1:A:59:GLU:HA	2.06	0.54
1:A:176:GLN:HB2	1:A:217:ASN:HD21	1.72	0.54
1:A:349:PHE:HB2	1:A:430:TRP:CZ2	2.43	0.54
1:A:349:PHE:CZ	1:A:353:MET:HG3	2.42	0.54
1:A:509:GLU:C	1:A:510:LEU:HD12	2.29	0.53
1:A:93:LYS:O	1:A:373:GLU:HG3	2.08	0.53
1:A:283:VAL:HG13	1:A:284:PRO:HD2	1.89	0.53
1:A:505:ILE:HD12	1:A:507:TYR:CE1	2.43	0.53
1:A:492:ARG:HH11	1:A:492:ARG:CG	2.12	0.53
1:A:299:ASP:OD1	1:A:303:ASN:N	2.40	0.52
1:A:92:PHE:HB2	1:A:373:GLU:HB3	1.90	0.52
1:A:218:ARG:O	1:A:264:ARG:HD3	2.09	0.52
1:A:514:LYS:NZ	1:A:549:THR:O	2.42	0.52
1:A:490:ILE:HD12	1:A:527:ALA:CA	2.40	0.52
1:A:47:LYS:C	1:A:48:ASN:HD22	2.11	0.52
1:A:188:SER:O	1:A:190:GLY:N	2.43	0.52
1:A:564:CYS:SG	1:A:566:GLU:HB2	2.50	0.52
1:A:239:GLU:H	1:A:243:ASN:ND2	2.08	0.52
1:A:464:LYS:O	1:A:465:ASP:HB2	2.10	0.52
1:A:324:LEU:HB3	1:A:460:TYR:CE2	2.45	0.52
1:A:335:GLN:O	1:A:338:VAL:HG23	2.10	0.52
1:A:246:LYS:HD2	1:A:246:LYS:H	1.75	0.51
1:A:176:GLN:O	1:A:180:TYR:HD1	1.93	0.51
1:A:511:PRO:O	1:A:513:MET:HG2	2.11	0.50
1:A:264:ARG:O	1:A:265:MET:CB	2.59	0.50
1:A:415:ILE:O	1:A:418:GLU:HG2	2.11	0.50
1:A:520:LEU:HD21	1:A:536:VAL:HG11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD11	1:A:118:GLN:CG	2.41	0.49
1:A:369:ILE:HD12	1:A:370:LEU:N	2.25	0.49
1:A:48:ASN:ND2	1:A:48:ASN:N	2.60	0.49
1:A:319:LEU:HB2	1:A:320:PRO:HD3	1.94	0.49
1:A:448:LEU:HD12	1:A:451:ARG:HB3	1.94	0.49
1:A:176:GLN:HG3	1:A:217:ASN:HD21	1.78	0.48
1:A:466:VAL:HG12	1:A:467:THR:HG23	1.94	0.48
1:A:199:PHE:HE1	1:A:236:MET:CE	2.27	0.48
1:A:553:THR:HB	1:A:560:VAL:HG23	1.94	0.48
1:A:370:LEU:HA	1:A:375:ALA:CB	2.37	0.48
1:A:559:PHE:HB2	1:A:572:MET:HE3	1.95	0.48
1:A:545:THR:HG23	1:A:571:LYS:HD2	1.95	0.48
1:A:495:PRO:O	1:A:499:ILE:CD1	2.62	0.47
1:A:497:HIS:CE1	1:A:531:LEU:HB2	2.49	0.47
1:A:413:ARG:HH11	1:A:413:ARG:HB2	1.79	0.47
1:A:176:GLN:CB	1:A:217:ASN:HD21	2.27	0.47
1:A:183:ASN:HB2	5:A:2009:HOH:O	2.14	0.47
1:A:188:SER:C	1:A:190:GLY:N	2.68	0.47
1:A:81:LEU:HG	1:A:288:MET:HG2	1.96	0.47
1:A:188:SER:C	1:A:190:GLY:H	2.18	0.47
1:A:545:THR:CG2	1:A:571:LYS:HD2	2.45	0.47
1:A:218:ARG:HG3	1:A:264:ARG:HG2	1.96	0.47
1:A:400:GLY:HA2	1:A:441:TYR:O	2.15	0.47
1:A:82:VAL:CG1	1:A:87:MET:HE1	2.45	0.47
1:A:485:THR:HG23	1:A:488:GLU:HB2	1.96	0.47
1:A:505:ILE:HG12	1:A:533:TYR:CG	2.50	0.46
1:A:28:ARG:CD	1:A:28:ARG:N	2.76	0.46
1:A:158:ASP:O	1:A:159:ALA:C	2.53	0.46
1:A:322:ILE:HA	1:A:344:ARG:NH1	2.30	0.46
1:A:410:LEU:HD21	1:A:466:VAL:HG21	1.98	0.46
1:A:369:ILE:O	1:A:375:ALA:HB3	2.15	0.46
1:A:576:ARG:HH11	1:A:576:ARG:HG3	1.81	0.46
1:A:372:GLN:HE22	1:A:382:PRO:HG3	1.80	0.46
1:A:414:ASP:C	1:A:414:ASP:OD1	2.55	0.46
1:A:33:GLN:HA	1:A:33:GLN:NE2	2.26	0.45
1:A:191:GLN:HB2	1:A:191:GLN:HE21	1.62	0.45
1:A:548:SER:HB2	1:A:563:ILE:HD11	1.97	0.45
1:A:243:ASN:HD22	1:A:243:ASN:H	1.62	0.45
1:A:538:MET:HB2	1:A:539:PRO:HD2	1.98	0.45
1:A:269:ILE:HD13	1:A:524:TRP:CG	2.52	0.45
1:A:420:LEU:HD12	1:A:420:LEU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASP:HA	1:A:210:ILE:HG21	1.98	0.45
1:A:518:LYS:H	1:A:518:LYS:HZ3	1.64	0.45
1:A:496:TYR:HA	1:A:499:ILE:HD13	1.99	0.45
1:A:189:ASN:C	1:A:191:GLN:N	2.70	0.45
1:A:507:TYR:HA	1:A:535:GLY:O	2.16	0.45
1:A:349:PHE:HB2	1:A:430:TRP:CE2	2.51	0.44
1:A:439:SER:OG	1:A:502:GLY:CA	2.65	0.44
1:A:545:THR:HG21	1:A:566:GLU:OE1	2.17	0.44
1:A:205:TRP:CE2	1:A:206:THR:HG23	2.53	0.44
1:A:291:ARG:HD3	1:A:505:ILE:HB	1.98	0.44
1:A:94:LEU:CD1	1:A:118:GLN:HG3	2.43	0.44
1:A:254:LYS:HE2	1:A:521:GLU:HG3	1.99	0.44
1:A:424:ASN:HB3	1:A:428:LYS:HE2	1.99	0.44
1:A:176:GLN:HG3	1:A:217:ASN:ND2	2.33	0.44
1:A:234:LEU:HB2	1:A:266:TYR:HB3	2.00	0.44
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.20	0.44
1:A:53:PHE:HZ	1:A:350:GLU:HG2	1.83	0.44
1:A:563:ILE:O	1:A:563:ILE:HG13	2.17	0.44
1:A:508:VAL:HG13	1:A:510:LEU:HD13	2.00	0.44
1:A:443:THR:HG22	1:A:445:ALA:H	1.82	0.44
1:A:156:ILE:HG21	1:A:162:TYR:CG	2.53	0.44
1:A:254:LYS:O	1:A:258:LEU:CD2	2.66	0.43
1:A:487:PHE:O	1:A:491:SER:HB2	2.19	0.43
1:A:499:ILE:HD12	1:A:499:ILE:N	2.34	0.43
1:A:485:THR:HG23	1:A:488:GLU:CB	2.48	0.43
1:A:519:GLY:O	1:A:522:ALA:HB3	2.17	0.43
1:A:378:VAL:C	1:A:379:ARG:HG2	2.37	0.43
1:A:265:MET:SD	1:A:537:ASN:HA	2.59	0.43
1:A:138:PRO:O	1:A:141:LYS:HB2	2.19	0.43
1:A:236:MET:CE	1:A:257:ALA:HB2	2.44	0.43
1:A:487:PHE:HD2	1:A:526:TYR:CD2	2.37	0.43
1:A:345:MET:CE	1:A:423:MET:HG2	2.49	0.43
1:A:185:LEU:HB3	1:A:193:PRO:HG2	2.01	0.43
1:A:546:CYS:SG	1:A:548:SER:HB3	2.60	0.42
1:A:439:SER:OG	1:A:502:GLY:HA3	2.19	0.42
1:A:54:ILE:HD13	1:A:351:ALA:HA	2.01	0.42
1:A:107:VAL:O	1:A:111:ILE:HG13	2.19	0.42
1:A:184:THR:O	1:A:186:PHE:N	2.52	0.42
1:A:171:VAL:HG12	1:A:213:ALA:CB	2.50	0.42
1:A:254:LYS:O	1:A:258:LEU:HD23	2.20	0.42
1:A:418:GLU:N	1:A:418:GLU:CD	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASN:HB3	1:A:250:ASN:HB2	2.02	0.41
1:A:266:TYR:HB3	1:A:267:PRO:HA	2.01	0.41
1:A:298:LYS:HA	1:A:303:ASN:O	2.20	0.41
1:A:69:ASP:OD1	1:A:69:ASP:N	2.53	0.41
1:A:487:PHE:HB3	1:A:526:TYR:CE2	2.56	0.41
1:A:518:LYS:N	1:A:518:LYS:HZ2	2.16	0.41
1:A:153:LYS:HE3	1:A:154:TRP:CZ2	2.56	0.41
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.93	0.41
1:A:243:ASN:O	1:A:254:LYS:HD2	2.20	0.41
1:A:410:LEU:CD2	1:A:466:VAL:HG21	2.51	0.41
1:A:465:ASP:N	1:A:468:ASP:OD2	2.36	0.41
1:A:369:ILE:O	1:A:375:ALA:CB	2.69	0.41
1:A:478:VAL:HG12	1:A:493:GLU:OE2	2.21	0.41
1:A:559:PHE:HB2	1:A:572:MET:CE	2.51	0.41
1:A:153:LYS:HE3	1:A:154:TRP:CE2	2.56	0.41
1:A:357:SER:HA	1:A:360:LYS:HD3	2.02	0.41
1:A:79:CYS:O	1:A:310:ASN:HB2	2.21	0.41
1:A:135:VAL:O	1:A:138:PRO:HD2	2.21	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	557/605 (92%)	505 (91%)	43 (8%)	9 (2%)	12 40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	564	CYS
1	A	157	ALA

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Mol	Chain	Res	Type
1	A	246	LYS
1	A	185	LEU
1	A	192	THR
1	A	300	SER
1	A	475	SER
1	A	191	GLN

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	482/524 (92%)	441 (92%)	41 (8%)	13 37

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	33	GLN
1	A	47	LYS
1	A	48	ASN
1	A	59	GLU
1	A	121	SER
1	A	127	THR
1	A	168	GLU
1	A	176	GLN
1	A	194	PHE
1	A	197	ILE
1	A	217	ASN
1	A	218	ARG
1	A	243	ASN
1	A	247	ASP
1	A	264	ARG
1	A	291	ARG
1	A	306	LEU
1	A	317	LEU
1	A	335	GLN

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Mol	Chain	Res	Type
1	A	338	VAL
1	A	362	VAL
1	A	366	VAL
1	A	369	ILE
1	A	399	LEU
1	A	413	ARG
1	A	420	LEU
1	A	427	LEU
1	A	440	LEU
1	A	469	LYS
1	A	478	VAL
1	A	485	THR
1	A	490	ILE
1	A	492	ARG
1	A	505	ILE
1	A	518	LYS
1	A	520	LEU
1	A	536	VAL
1	A	552	MET
1	A	564	CYS
1	A	581	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	48	ASN
1	A	98	GLN
1	A	176	GLN
1	A	189	ASN
1	A	191	GLN
1	A	217	ASN
1	A	243	ASN
1	A	255	GLN
1	A	274	ASN
1	A	342	ASN
1	A	372	GLN
1	A	392	ASN
1	A	426	HIS
1	A	429	GLN
1	A	537	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TTP	A	1586	3	21,30,30	2.28	3 (14%)	31,47,47	2.08	7 (22%)
2	TTP	A	1589	-	21,30,30	2.27	3 (14%)	31,47,47	2.17	7 (22%)

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	TTP	A	1586	3	-	0/18/34/34	0/2/2/2
2	TTP	A	1589	-	-	0/18/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1586	TTP	C2'-C1'	-6.01	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1589	TTP	C2'-C1'	-5.99	1.35	1.52
2	A	1586	TTP	C4-N3	4.31	1.41	1.33
2	A	1589	TTP	C4-N3	4.41	1.41	1.33
2	A	1589	TTP	C6-N1	5.89	1.43	1.35
2	A	1586	TTP	C6-N1	6.06	1.44	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1589	TTP	C5-C4-N3	-3.82	120.89	125.14
2	A	1586	TTP	C5-C4-N3	-3.79	120.92	125.14
2	A	1589	TTP	PB-O3A-PA	-3.64	122.50	132.73
2	A	1586	TTP	PB-O3A-PA	-3.61	122.60	132.73
2	A	1586	TTP	PB-O3B-PG	-2.91	122.90	132.67
2	A	1589	TTP	PB-O3B-PG	-2.74	123.48	132.67
2	A	1589	TTP	C4'-O4'-C1'	2.15	114.90	109.47
2	A	1586	TTP	C4'-O4'-C1'	2.20	115.03	109.47
2	A	1586	TTP	C3'-C2'-C1'	3.31	110.37	102.40
2	A	1589	TTP	C3'-C2'-C1'	3.61	111.09	102.40
2	A	1586	TTP	O4'-C1'-N1	5.77	117.71	107.72
2	A	1586	TTP	C4-N3-C2	5.99	120.42	115.25
2	A	1589	TTP	C4-N3-C2	6.01	120.44	115.25
2	A	1589	TTP	O4'-C1'-N1	6.54	119.04	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1586	TTP	1	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	559/605 (92%)	-0.32	15 (2%) 58 52	26, 48, 92, 101	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLN	5.7
1	A	556	GLU	4.9
1	A	27	SER	4.2
1	A	555	THR	3.7
1	A	557	ASN	3.3
1	A	189	ASN	3.0
1	A	192	THR	2.9
1	A	554	PRO	2.9
1	A	483	ASN	2.7
1	A	553	THR	2.6
1	A	481	GLU	2.4
1	A	563	ILE	2.4
1	A	190	GLY	2.4
1	A	247	ASP	2.0
1	A	547	GLY	2.0

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

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
2	TTP	A	1589	29/29	0.92	0.19	0.01	45,66,79,80	29
2	TTP	A	1586	29/29	0.96	0.12	-0.81	44,55,65,66	0
4	FE2	A	1588	1/1	0.97	0.04	-2.20	74,74,74,74	0
3	MG	A	1587	1/1	0.94	0.06	-	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.