

Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 01:08 PM EDT

PDB ID	:	5CNV
Title	:	Crystal structure of the dATP inhibited E. coli class Ia ribonucleotide reduc-
		tase complex bound to GDP and TTP at 3.20 Angstroms resolution
Authors	:	Chen, P.YT.; Zimanyi, C.M.; Funk, M.A.; Drennan, C.L.
Deposited on	:	2015-07-18
Resolution	:	3.20 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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	:	2.35.1
buster-report	:	1.1.7(2018)
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.20 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.



Matria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of 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 <=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	А	761	.% 8 5%	11%	·
1	В	761	2% 88 %	9%	·
1	С	761	84%	12%	·
1	D	761	% 8 6%	10%	•
2	Е	375	2% 8 6%	8%	6%



Mol	Chain	Length	Quality of chain		
2	F	375	83%	12%	5%
2	G	375	86%	9%	5%
2	Н	375	82%	13%	·



 $\mathbf{2}$

Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 35522 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.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
1	1 A	726	Total	С	Ν	Ο	S	0	0	0
	750	5854	3718	1005	1107	24	0	0	0	
1	1 B	739	Total	С	Ν	Ο	S	0	0	0
		132	5829	3703	1000	1102	24	0	0	0
1	C	794	Total	С	Ν	Ο	S	0	0	0
	104	5841	3709	1003	1105	24	0	0	0	
1 D	734	Total	С	Ν	Ο	S	0	0	0	
		5841	3709	1003	1105	24	0	0	0	

• Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 1 subunit alpha.

• Molecule 2 is a protein called Ribonucleoside-diphosphate reductase 1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	250	Total	С	Ν	0	\mathbf{S}	0	0	0
	552	2867	1831	473	550	13	0	0		
0	2 F	257	Total	С	Ν	0	S	0	0	0
		557	2923	1864	484	562	13	0	0	
0	C	357	Total	С	Ν	0	S	0	0	0
2 G	G		2907	1856	479	559	13	0	0	0
2 H	250	Total	С	Ν	0	S	0	0	0	
	п	359	2931	1869	485	564	13	0	0	

• Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
2	Δ	1	Total	С	Ν	Ο	Р	0	0
D A	L	28	10	5	11	2	0	0	
2	3 B	1	Total	С	Ν	Ο	Р	0	0
0		1	28	10	5	11	2	0	0
2	С	1	Total	С	Ν	Ο	Р	0	0
0	U	1	28	10	5	11	2	0	0
2	D	1	Total	С	Ν	Ο	Р	0	0
3	D		28	10	5	11	2	U	0

• Molecule 4 is 2'-DEOXYADENOSINE-5'-DIPHOSPHATE (three-letter code: DAT) (formula: $C_{10}H_{15}N_5O_9P_2$).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
4	Δ	1	Total	С	Ν	0	Р	0	0	
4	Π	T	26	10	5	9	2	0	0	
4	В	1	Total	С	Ν	Ο	Р	0	0	
4	4 D	1	26	10	5	9	2	0	0	
4	С	1	Total	С	Ν	Ο	Р	0	0	
4	U	1	26	10	5	9	2	0	0	
4	П	1	Total	С	Ν	Ο	Р	0	0	
4	D		26	10	5	9	2	U	U	

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	2	Total Mg 2 2	0	0
5	В	2	Total Mg 2 2	0	0
5	С	2	Total Mg 2 2	0	0
5	D	2	Total Mg 2 2	0	0

• Molecule 6 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	А	1	Total 29	C 10	N 2	0 14	Р 3	0	0



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
6	٨	1	Total	С	Ν	Ο	Р	0	0	
	A	1	29	10	2	14	3	0	0	
6	В	1	Total	С	Ν	Ο	Р	0	0	
0	D	1	29	10	2	14	3	0	0	
6	В	B	1	Total	С	Ν	Ο	Р	0	0
	D	1	29	10	2	14	3	0	0	
6	С	1	Total	С	Ν	Ο	Р	0	0	
0	U		29	10	2	14	3	0	0	
6	С	1	Total	С	Ν	Ο	Р	0	0	
0	U	1	29	10	2	14	3	0	0	
6	Л	1	Total	С	Ν	Ο	Р	0	0	
0	D		29	10	2	14	3	0	0	
6	р	1	Total	С	N	0	Р	0	0	
	D	1	29	10	2	14	3	0	0	

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• Molecule 7 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe₂O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Е	1	TotalFeO321	0	0
7	F	1	TotalFeO321	0	0
7	G	1	TotalFeO321	0	0
7	Н	1	$\begin{array}{ccc} \text{Total} & \text{Fe} & \text{O} \\ 3 & 2 & 1 \end{array}$	0	0



• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	9	Total O 9 9	0	0
8	В	5	Total O 5 5	0	0
8	С	13	Total O 13 13	0	0
8	D	12	Total O 12 12	0	0
8	Е	4	Total O 4 4	0	0
8	F	7	Total O 7 7	0	0
8	G	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0
8	Н	6	Total O 6 6	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Ribonucleoside-diphosphate reductase 1 subunit alpha



• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



ASP SER SER SER ALA ALA ALA ALA ALA CYS CYS

P454 V226 1453 V227 1453 V226 1461 V226 1228 E209 1226 V269 1226 V269 1226 V269 1226 V269 1226 V269 1226 V269 1512 V269 1512 V289 K506 V289 K506 V289 K510 V289 K510 V289 K500 V289 K500 V289 K500 V338 K51 V338 K51 V338 K51 V338 K51

 \bullet Molecule 1: Ribonucleoside-diphosphate reduct as 1 subunit alpha



• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

Chain G:

86%



A1

ASN VAL VAL VAL ALA ALA ALA GLU GLU GLU CAL VAL VAL CAL UAL

• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	274.78Å 157.75Å 165.77Å	Depositor
a, b, c, α , β , γ	90.00° 119.49° 90.00°	Depositor
$\mathbf{Posolution} \left(\overset{\circ}{\mathbf{A}} \right)$	49.73 - 3.20	Depositor
Resolution (A)	49.73 - 3.16	EDS
% Data completeness	98.5 (49.73-3.20)	Depositor
(in resolution range)	95.9 (49.73-3.16)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.02 (at 3.19 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
P. P.	0.190 , 0.219	Depositor
n, n_{free}	0.191 , 0.220	DCC
R_{free} test set	5047 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	78.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 24.8	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35522	wwPDB-VP
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: DAT, TTP, MG, GDP, FEO

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).

Mal	Chain	Bond	lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.26	0/5982	0.42	0/8104
1	В	0.24	0/5957	0.42	0/8070
1	С	0.27	0/5969	0.44	0/8086
1	D	0.26	0/5969	0.43	0/8086
2	Ε	0.24	0/2931	0.39	0/3977
2	F	0.27	0/2987	0.44	0/4050
2	G	0.27	0/2971	0.42	0/4031
2	Н	0.25	0/2995	0.41	0/4062
All	All	0.26	0/35761	0.42	0/48466

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	А	5854	0	5769	54	0
1	В	5829	0	5750	41	0
1	С	5841	0	5759	59	0
1	D	5841	0	5759	50	0
2	Е	2867	0	2781	17	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2923	0	2850	27	0
2	G	2907	0	2822	19	0
2	Н	2931	0	2847	32	0
3	А	28	0	12	5	0
3	В	28	0	12	3	0
3	С	28	0	12	1	0
3	D	28	0	12	2	0
4	А	26	0	12	3	0
4	В	26	0	12	2	0
4	С	26	0	12	2	0
4	D	26	0	12	1	0
5	А	2	0	0	0	0
5	В	2	0	0	0	0
5	С	2	0	0	0	0
5	D	2	0	0	0	0
6	А	58	0	26	5	0
6	В	58	0	26	3	0
6	С	58	0	26	4	0
6	D	58	0	26	3	0
7	Е	3	0	0	0	0
7	F	3	0	0	0	0
7	G	3	0	0	0	0
7	Н	3	0	0	1	0
8	А	9	0	0	1	0
8	В	5	0	0	1	0
8	С	13	0	0	2	0
8	D	12	0	0	0	0
8	Е	4	0	0	2	0
8	F	7	0	0	0	0
8	G	5	0	0	0	0
8	Н	6	0	0	0	0
All	All	35522	0	34537	286	0

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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 (286) 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)
4:A:802:DAT:O1B	8:A:901:HOH:O	2.05	0.74
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.72	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:24:ARG:HH12	6:D:804:TTP:H4'	1.56	0.70
1:B:437:ASN:ND2	3:B:801:GDP:O3'	2.25	0.69
1:C:49:PHE:HE2	2:H:297:ILE:HD11	1.57	0.69
4:B:802:DAT:O3B	8:B:901:HOH:O	2.10	0.68
1:B:229:GLU:OE2	1:B:260:ARG:NH1	2.26	0.68
2:H:42:LYS:HE3	2:H:342:ASP:HB3	1.76	0.68
1:C:221:GLN:NE2	8:C:902:HOH:O	2.27	0.67
1:A:229:GLU:OE2	1:A:260:ARG:NH1	2.28	0.67
1:C:24:ARG:HH12	6:C:804:TTP:H4'	1.60	0.66
1:D:222:PHE:CD2	1:D:492:LEU:HD11	2.31	0.66
1:B:206:SER:HB3	1:B:466:ALA:HB3	1.78	0.66
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.77	0.65
1:C:222:PHE:CD2	1:C:492:LEU:HD11	2.31	0.65
1:D:258:ALA:HB3	1:D:304:LEU:HD21	1.78	0.64
1:C:710:PRO:HA	2:H:362:ASP:HB3	1.78	0.64
1:B:195:ARG:NH1	1:B:480:GLU:OE1	2.30	0.64
1:C:206:SER:HB3	1:C:466:ALA:HB3	1.79	0.64
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.80	0.63
1:C:26:LEU:HB3	1:C:38:ILE:HD12	1.79	0.62
1:C:55:THR:HG21	4:C:802:DAT:O2B	1.99	0.62
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.82	0.62
1:A:206:SER:HB3	1:A:466:ALA:HB3	1.83	0.61
1:C:463:THR:HG21	1:C:492:LEU:HD23	1.84	0.60
1:D:227:LEU:HB2	1:D:460:ALA:HB3	1.83	0.60
2:G:153:ILE:HD13	2:G:203:LEU:HD13	1.83	0.60
1:A:268:ILE:HD11	1:A:275:HIS:HA	1.83	0.60
1:A:710:PRO:HA	2:G:362:ASP:HB3	1.84	0.60
1:D:229:GLU:OE2	1:D:260:ARG:NH1	2.35	0.59
1:A:438:LEU:HD23	3:A:801:GDP:H2'	1.84	0.59
1:C:532:SER:HA	1:C:677:GLY:HA3	1.84	0.59
2:F:199:SER:HA	2:F:275:LEU:HD21	1.84	0.59
1:C:458:GLU:OE2	1:C:510:ARG:NH1	2.35	0.59
1:D:49:PHE:HE2	2:F:297:ILE:HD11	1.68	0.58
1:B:222:PHE:CD2	1:B:492:LEU:HD11	2.38	0.58
1:C:59:HIS:HB2	4:C:802:DAT:H4'	1.86	0.58
1:A:24:ARG:HH12	6:A:804:TTP:H4'	1.68	0.58
1:A:222:PHE:CD2	1:A:492:LEU:HD11	2.38	0.58
1:C:89:LEU:HD11	1:C:152:GLU:HB2	1.86	0.58
1:D:89:LEU:HD11	1:D:152:GLU:HB2	1.85	0.58
1:C:222:PHE:HD2	1:C:492:LEU:HD11	1.68	0.57
2:G:199:SER:HA	2:G:275:LEU:HD21	1.87	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:292:CYS:HB2	6:B:805:TTP:N3	2.20	0.57
1:B:24:ARG:HH12	6:B:804:TTP:H4'	1.69	0.57
1:A:458:GLU:OE2	1:A:510:ARG:NH1	2.38	0.56
2:G:81:THR:O	2:G:85:SER:HB2	2.05	0.56
2:G:191:LYS:HG3	2:G:268:CYS:SG	2.45	0.56
1:A:226:VAL:HG22	1:A:461:LEU:HD22	1.88	0.55
1:A:320:LYS:HE2	1:A:411:ARG:HB2	1.87	0.55
1:C:292:CYS:HB2	6:D:805:TTP:N3	2.21	0.55
1:D:222:PHE:HD2	1:D:492:LEU:HD11	1.71	0.55
2:H:252:LEU:HB3	2:H:261:MET:HG2	1.87	0.55
1:B:532:SER:HA	1:B:677:GLY:HA3	1.89	0.55
1:B:44:ARG:HG3	1:B:69:LEU:HD21	1.89	0.55
1:A:59:HIS:HB2	4:A:802:DAT:H4'	1.89	0.55
1:A:26:LEU:HB3	1:A:38:ILE:HD12	1.89	0.54
1:B:268:ILE:HD11	1:B:275:HIS:HA	1.90	0.54
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.89	0.53
1:A:89:LEU:HD11	1:A:152:GLU:HB2	1.90	0.53
1:D:321:ASN:OD1	1:D:329:ARG:NE	2.41	0.53
2:E:185:SER:HB3	2:E:188:GLU:HB2	1.91	0.53
1:A:208:PRO:HD2	1:A:211:ILE:HD12	1.91	0.52
1:C:139:ARG:NH1	1:C:201:SER:OG	2.43	0.52
1:D:433:VAL:HG11	1:D:443:ALA:HB1	1.91	0.52
1:B:621:PRO:HG2	3:B:801:GDP:O2A	2.09	0.52
1:C:320:LYS:HE2	1:C:411:ARG:HB2	1.91	0.52
1:A:463:THR:HG21	1:A:492:LEU:HD23	1.92	0.52
1:D:621:PRO:HG2	3:D:801:GDP:O1A	2.09	0.52
1:D:59:HIS:HD2	1:D:88:HIS:HB2	1.75	0.52
2:H:32:LYS:N	2:H:103:GLU:OE2	2.41	0.52
1:C:522:TYR:CZ	1:C:526:LYS:HD3	2.45	0.51
2:G:360:GLN:HG3	2:G:361:ILE:HG12	1.93	0.51
1:D:438:LEU:HD23	3:D:801:GDP:H2'	1.93	0.51
2:F:317:GLN:HB2	2:F:323:LEU:HD21	1.91	0.50
1:A:295:GLY:HA3	1:B:274:PHE:O	2.11	0.50
1:D:26:LEU:HD21	1:D:62:ILE:HD12	1.91	0.50
2:F:169:LEU:HD12	2:G:169:LEU:HD12	1.93	0.50
1:A:451:ASP:H	1:A:454:ASP:HB2	1.77	0.50
1:D:55:THR:HG21	4:D:802:DAT:O1B	2.11	0.50
2:G:317:GLN:HB2	2:G:323:LEU:HD21	1.93	0.50
2:F:311:ILE:O	2:F:315:ARG:HG2	2.12	0.50
1:D:206:SER:HB3	1:D:466:ALA:HB3	1.94	0.49
2:E:3:THR:HG22	2:E:5:PHE:H	1.76	0.49



	louis page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:463:THR:HG21	1:D:492:LEU:HD23	1.93	0.49
2:E:79:TYR:CZ	2:E:83:LEU:HD11	2.48	0.49
2:H:366:ASP:OD2	2:H:369:ASP:HB2	2.12	0.49
6:A:805:TTP:N3	1:B:292:CYS:HB2	2.27	0.49
1:B:451:ASP:H	1:B:454:ASP:HB2	1.77	0.49
1:D:21:LYS:NZ	6:D:804:TTP:O3G	2.45	0.49
1:B:320:LYS:HE2	1:B:411:ARG:HB2	1.95	0.49
1:C:640:GLY:HA2	1:C:668:LEU:HD13	1.94	0.49
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.94	0.49
1:D:155:TYR:HE1	1:D:209:THR:HG23	1.77	0.49
1:A:619:LEU:HB2	1:A:693:ILE:HG23	1.94	0.49
1:B:55:THR:HG21	4:B:802:DAT:O2B	2.12	0.49
1:A:522:TYR:CZ	1:A:526:LYS:HD3	2.48	0.48
1:C:490:ASP:OD1	1:C:613:ASN:ND2	2.46	0.48
1:A:353:ILE:HG13	1:A:395:ALA:HB2	1.94	0.48
1:B:619:LEU:HB2	1:B:693:ILE:HG23	1.94	0.48
1:C:268:ILE:HD11	1:C:275:HIS:HA	1.94	0.48
2:G:277:VAL:O	2:G:281:GLN:HG2	2.12	0.48
1:C:42:GLU:HB3	2:H:297:ILE:HG23	1.95	0.48
2:F:19:PHE:CE2	2:F:190:LYS:HG2	2.48	0.48
1:B:463:THR:HG21	1:B:492:LEU:HD23	1.94	0.48
2:H:115:GLU:CD	7:H:501:FEO:O	2.46	0.48
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.96	0.48
1:B:268:ILE:HB	1:B:273:ALA:HB3	1.96	0.48
1:C:24:ARG:NH1	6:C:804:TTP:H4'	2.27	0.48
1:C:438:LEU:HD23	3:C:801:GDP:H2'	1.95	0.48
2:E:16:PRO:O	2:E:100:SER:OG	2.25	0.48
1:D:26:LEU:HB3	1:D:38:ILE:HD12	1.96	0.48
1:C:34:HIS:CD2	1:C:35:ASN:HB2	2.48	0.48
2:E:24:ASN:OD1	2:E:24:ASN:N	2.42	0.48
1:D:522:TYR:CZ	1:D:526:LYS:HD3	2.49	0.48
2:F:191:LYS:HG3	2:F:268:CYS:SG	2.54	0.48
1:A:274:PHE:O	1:B:295:GLY:HA3	2.14	0.47
1:B:26:LEU:HB3	1:B:38:ILE:HD12	1.95	0.47
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.96	0.47
1:D:444:LEU:HD22	1:D:512:THR:HG21	1.95	0.47
1:A:552:LEU:HD23	1:A:616:LEU:HD12	1.96	0.47
1:D:176:VAL:HG22	1:D:215:VAL:HB	1.95	0.47
2:E:199:SER:HA	2:E:275:LEU:HD21	1.95	0.47
1:A:292:CYS:HB2	6:B:805:TTP:C2	2.49	0.47
2:H:16:PRO:O	2:H:100:SER:OG	2.27	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:35:ILE:HG12	2:F:247:HIS:CG	2.49	0.47
2:F:79:TYR:CZ	2:F:83:LEU:HD11	2.50	0.47
1:C:269:ARG:NH2	8:C:904:HOH:O	2.46	0.47
1:C:451:ASP:H	1:C:454:ASP:HB2	1.79	0.47
1:A:298:ARG:HD3	3:A:801:GDP:C2	2.50	0.47
1:B:208:PRO:HD2	1:B:211:ILE:HD12	1.97	0.47
2:H:317:GLN:HB2	2:H:323:LEU:HD21	1.97	0.46
1:A:621:PRO:HG2	3:A:801:GDP:O2A	2.15	0.46
1:B:305:PHE:CZ	1:B:436:SER:HB3	2.50	0.46
1:C:211:ILE:HA	1:C:215:VAL:HG23	1.98	0.46
1:D:59:HIS:CD2	1:D:88:HIS:HB2	2.50	0.46
2:H:139:ASP:O	2:H:143:ASN:HB2	2.15	0.46
1:D:451:ASP:H	1:D:454:ASP:HB2	1.80	0.46
1:B:124:THR:HG23	1:B:186:ARG:HH22	1.81	0.46
1:C:520:PHE:HB3	1:C:635:ILE:HA	1.97	0.46
2:F:172:GLU:HG3	2:F:184:VAL:O	2.15	0.46
2:H:149:ARG:HG2	2:H:282:GLN:OE1	2.15	0.46
1:B:37:SER:HB3	1:B:40:GLN:HB2	1.98	0.46
2:F:196:CYS:O	2:F:200:VAL:HG23	2.15	0.46
1:A:220:ARG:HA	1:A:222:PHE:CZ	2.51	0.45
2:H:309:GLU:OE1	2:H:328:ARG:NH2	2.50	0.45
1:A:439:CYS:SG	3:A:801:GDP:H3'	2.56	0.45
1:A:371:ASP:HB3	1:A:374:GLU:HB3	1.97	0.45
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.98	0.45
1:C:295:GLY:HA3	1:D:274:PHE:O	2.16	0.45
1:D:125:GLU:HG2	1:D:129:LYS:HE2	1.98	0.45
2:H:253:ARG:NH1	2:H:320:GLY:HA3	2.31	0.45
1:A:247:TYR:OH	1:A:461:LEU:HD11	2.16	0.45
1:C:137:HIS:HA	1:C:170:GLN:HG3	1.98	0.45
1:C:466:ALA:HB2	1:C:620:MET:HE1	1.99	0.45
2:F:60:ILE:HD12	2:F:60:ILE:H	1.82	0.45
2:G:19:PHE:CE2	2:G:190:LYS:HG2	2.52	0.45
2:H:19:PHE:CE2	2:H:190:LYS:HG2	2.52	0.45
2:H:24:ASN:OD1	2:H:24:ASN:N	2.48	0.45
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.98	0.45
1:C:208:PRO:HD2	1:C:211:ILE:HD12	1.98	0.45
1:C:307:PRO:HA	1:C:338:GLN:HB2	1.98	0.45
2:F:46:PHE:CE2	2:F:236:ARG:HG2	2.53	0.45
2:F:252:LEU:HD22	2:F:261:MET:HG2	1.98	0.44
2:F:9:LYS:HD2	2:G:142:THR:CG2	2.47	0.44
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.99	0.44



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:322:ASN:HA	1:A:331:ARG:HE	1.81	0.44	
1:C:444:LEU:HD22	1:C:512:THR:HG21	2.00	0.44	
1:D:211:ILE:HA	1:D:215:VAL:HG23	1.99	0.44	
2:F:80:GLN:HB3	2:F:122:TYR:CZ	2.52	0.44	
2:H:190:LYS:HB3	2:H:261:MET:HE1	1.99	0.44	
1:A:556:ASN:ND2	1:A:610:GLY:O	2.49	0.44	
2:H:79:TYR:CZ	2:H:83:LEU:HD11	2.52	0.44	
1:A:211:ILE:HA	1:A:215:VAL:HG23	2.00	0.44	
1:D:640:GLY:HA2	1:D:668:LEU:HD13	1.99	0.44	
1:A:621:PRO:HD3	1:A:694:SER:OG	2.17	0.44	
6:A:805:TTP:O4	1:B:249:SER:HB2	2.16	0.44	
1:B:226:VAL:HG22	1:B:461:LEU:HD22	1.98	0.44	
1:D:294:GLN:CD	1:D:294:GLN:H	2.21	0.44	
2:F:304:LEU:O	2:F:308:VAL:HG23	2.18	0.44	
1:A:307:PRO:HA	1:A:338:GLN:HB2	1.99	0.44	
1:C:285:PHE:O	1:C:289:VAL:HG23	2.18	0.44	
1:B:63:ILE:HG12	1:B:84:LEU:HB3	2.00	0.44	
1:D:139:ARG:NH1	1:D:201:SER:OG	2.51	0.44	
1:A:55:THR:HG21	4:A:802:DAT:O3B	2.18	0.43	
1:D:268:ILE:HD11	1:D:275:HIS:HA	1.99	0.43	
1:A:696:ASN:HD22	1:A:733:ASN:HD21	1.66	0.43	
1:B:220:ARG:HA	1:B:222:PHE:CZ	2.52	0.43	
1:D:135:ILE:HD11	1:D:174:ILE:HG21	2.00	0.43	
2:E:6:SER:N	8:E:602:HOH:O	2.51	0.43	
2:F:129:ILE:HG13	2:F:130:VAL:HG13	1.99	0.43	
2:E:129:ILE:HG13	2:E:130:VAL:HG13	2.01	0.43	
2:G:304:LEU:O	2:G:308:VAL:HG23	2.18	0.43	
2:H:149:ARG:HD3	2:H:282:GLN:HB3	2.00	0.43	
1:C:232:ASP:O	6:C:805:TTP:H5'2	2.18	0.43	
2:E:143:ASN:HB3	2:E:146:ILE:HB	1.99	0.43	
1:C:447:LYS:NZ	1:C:505:ARG:HH22	2.17	0.43	
1:D:305:PHE:CZ	1:D:436:SER:HB3	2.54	0.43	
2:H:191:LYS:HG3	2:H:268:CYS:SG	2.59	0.43	
2:H:199:SER:HA	2:H:275:LEU:HD21	1.99	0.43	
1:A:195:ARG:HB3	1:A:484:LEU:HD21	2.00	0.43	
1:A:312:GLU:O	1:A:316:LEU:HG	2.19	0.43	
6:A:804:TTP:H6	6:A:804:TTP:H2'2	1.71	0.43	
2:H:49:ARG:O	2:H:52:GLU:HG2	2.18	0.43	
1:B:209:THR:OG1	3:B:801:GDP:O3B	2.35	0.43	
1:C:305:PHE:CZ	1:C:436:SER:HB3	2.54	0.43	
1:C:348:LEU:O	2:H:371:SER:OG	2.37	0.43	



	, and pagetti	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:G:196:CYS:O	2:G:200:VAL:HG23	2.18	0.43	
6:C:805:TTP:O4	1:D:249:SER:HB2	2.18	0.42	
1:D:116:ASP:OD1	1:D:117:ASN:N	2.53	0.42	
1:D:227:LEU:HD11	1:D:437:ASN:HB3	2.00	0.42	
2:F:191:LYS:HE3	2:F:268:CYS:SG	2.58	0.42	
2:G:198:MET:HG3	2:G:272:CYS:SG	2.59	0.42	
1:D:578:LEU:HD11	1:D:603:ARG:HB2	2.01	0.42	
2:E:252:LEU:HD22	2:E:261:MET:HG3	2.00	0.42	
1:A:232:ASP:O	6:A:805:TTP:H5'2	2.19	0.42	
1:C:9:LYS:HD3	1:C:15:GLU:HG2	2.00	0.42	
1:C:647:SER:HB3	1:C:650:GLY:O	2.19	0.42	
2:H:111:TRP:O	2:H:115:GLU:HG2	2.19	0.42	
2:H:311:ILE:O	2:H:315:ARG:HG2	2.19	0.42	
1:C:298:ARG:HE	1:C:298:ARG:HB2	1.62	0.42	
2:F:26:ALA:N	2:G:85:SER:OG	2.50	0.42	
1:A:305:PHE:CZ	1:A:436:SER:HB3	2.54	0.42	
1:B:578:LEU:HD11	1:B:603:ARG:HB2	2.01	0.42	
1:C:556:ASN:O	1:C:560:LYS:HG3	2.20	0.42	
1:D:208:PRO:HD2	1:D:211:ILE:HD12	2.01	0.42	
1:D:244:ILE:HG12	1:D:254:ILE:HG21	2.02	0.42	
2:G:311:ILE:O	2:G:315:ARG:HG2	2.19	0.42	
1:D:42:GLU:HB3	2:F:297:ILE:HG23	2.02	0.42	
2:E:116:THR:HB	2:H:106:THR:HG23	2.02	0.42	
2:H:198:MET:HG3	2:H:272:CYS:SG	2.59	0.42	
1:B:23:HIS:CD2	2:E:300:ASN:HD22	2.38	0.42	
1:B:208:PRO:HB2	1:B:210:PRO:HD2	2.01	0.42	
1:B:211:ILE:HA	1:B:215:VAL:HG23	2.01	0.42	
1:C:226:VAL:HG22	1:C:461:LEU:HD22	2.01	0.42	
2:E:35:ILE:HG12	2:E:247:HIS:CG	2.55	0.42	
2:G:163:MET:HB3	2:G:189:LEU:HD13	2.02	0.42	
2:E:84:ASP:HA	2:E:87:GLN:HB2	2.02	0.42	
2:F:82:LEU:HD22	2:F:146:ILE:HG23	2.01	0.42	
2:F:139:ASP:O	2:F:143:ASN:HB2	2.20	0.42	
1:A:34:HIS:CD2	1:A:35:ASN:HB2	2.55	0.41	
1:C:195:ARG:HD2	1:C:480:GLU:OE1	2.19	0.41	
1:C:420:CYS:O	1:C:424:SER:HB3	2.20	0.41	
2:E:63:GLN:HA	2:E:70:LYS:HE3	2.02	0.41	
1:D:265:GLY:HA2	1:D:274:PHE:CZ	2.56	0.41	
1:D:560:LYS:HG2	1:D:609:HIS:CG	2.55	0.41	
1:C:229:GLU:OE2	1:C:260:ARG:NH1	2.54	0.41	
1:C:312:GLU:O	1:C:316:LEU:HG	2.20	0.41	



A to any 1	A t and D	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:H:53:VAL:HG11	2:H:230:ILE:HG13	2.01	0.41	
1:B:578:LEU:HD13	1:B:599:TRP:HE3	1.84	0.41	
1:C:544:PHE:CE1	1:C:685:MET:HG2	2.56	0.41	
2:F:149:ARG:HD3	2:F:282:GLN:HB3	2.02	0.41	
1:C:559:ALA:HB2	1:C:612:ARG:N	2.35	0.41	
1:A:682:VAL:HG11	1:A:695:ALA:HB2	2.03	0.41	
2:H:35:ILE:HG12	2:H:247:HIS:CD2	2.55	0.41	
2:H:35:ILE:HG12	2:H:247:HIS:CG	2.56	0.41	
2:H:196:CYS:O	2:H:200:VAL:HG23	2.21	0.41	
1:B:466:ALA:HB2	1:B:620:MET:HE1	2.03	0.41	
1:D:520:PHE:HB3	1:D:635:ILE:HA	2.02	0.41	
2:F:126:ILE:O	2:F:130:VAL:HG22	2.20	0.41	
2:F:311:ILE:HD12	2:F:311:ILE:HA	1.95	0.41	
2:H:160:LEU:HD21	2:H:193:LEU:HD23	2.02	0.41	
1:A:215:VAL:O	1:A:216:ARG:HB3	2.21	0.41	
1:A:425:PRO:HG3	1:A:615:THR:HG22	2.02	0.41	
1:C:338:GLN:NE2	1:C:434:ARG:O	2.52	0.41	
1:D:208:PRO:HB2	1:D:210:PRO:HD2	2.02	0.41	
1:D:425:PRO:HG3	1:D:615:THR:HG22	2.03	0.41	
2:E:95:LEU:O	2:E:99:ILE:HG13	2.21	0.41	
1:A:159:ASN:HB3	1:A:162:THR:HB	2.02	0.41	
1:C:35:ASN:ND2	1:C:73:ASP:O	2.52	0.41	
1:D:710:PRO:HA	2:F:362:ASP:HB3	2.02	0.41	
2:E:238:GLU:OE1	8:E:601:HOH:O	2.22	0.41	
2:G:185:SER:HB3	2:G:188:GLU:HB2	2.03	0.41	
1:A:298:ARG:HD3	3:A:801:GDP:N1	2.36	0.40	
1:B:522:TYR:CZ	1:B:526:LYS:HD3	2.56	0.40	
1:B:135:ILE:HD11	1:B:174:ILE:HG21	2.04	0.40	
1:D:329:ARG:HD3	1:D:329:ARG:HA	1.88	0.40	
1:C:522:TYR:O	1:C:526:LYS:HG3	2.21	0.40	
1:D:215:VAL:O	1:D:216:ARG:HB3	2.21	0.40	
2:G:129:ILE:HG13	2:G:130:VAL:HG13	2.03	0.40	
1:A:27:ASP:OD1	1:A:38:ILE:HG13	2.22	0.40	
1:A:140:ASP:OD1	1:A:169:ALA:HB3	2.22	0.40	
1:A:444:LEU:HD22	1:A:512:THR:HG21	2.02	0.40	
1:B:636:GLU:OE1	1:B:678:TYR:OH	2.35	0.40	
1:C:700:ASP:HB3	1:C:703:ARG:HD2	2.03	0.40	
1:D:406:ARG:HA	1:D:412:ILE:HB	2.03	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	Perce	ntiles
1	А	734/761~(96%)	713 (97%)	20 (3%)	1 (0%)	51	83
1	В	730/761~(96%)	710 (97%)	19 (3%)	1 (0%)	51	83
1	С	732/761~(96%)	710 (97%)	21 (3%)	1 (0%)	51	83
1	D	732/761~(96%)	712 (97%)	19 (3%)	1 (0%)	51	83
2	Е	348/375~(93%)	343~(99%)	5 (1%)	0	100	100
2	F	353/375~(94%)	346~(98%)	7 (2%)	0	100	100
2	G	353/375~(94%)	348~(99%)	5 (1%)	0	100	100
2	Н	355/375~(95%)	349~(98%)	6 (2%)	0	100	100
All	All	4337/4544 (95%)	4231 (98%)	102 (2%)	4 (0%)	51	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	216	ARG
1	В	216	ARG
1	С	216	ARG
1	D	216	ARG

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	А	628/651~(96%)	625~(100%)	3~(0%)	88 95	



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	В	627/651~(96%)	626 (100%)	1 (0%)	93 98		
1	\mathbf{C}	628/651~(96%)	626 (100%)	2(0%)	92 96		
1	D	628/651~(96%)	624~(99%)	4 (1%)	86 94		
2	Ε	315/340~(93%)	313~(99%)	2(1%)	86 94		
2	F	324/340~(95%)	319~(98%)	5(2%)	65 85		
2	G	320/340~(94%)	318~(99%)	2(1%)	86 94		
2	Н	323/340~(95%)	322 (100%)	1 (0%)	92 96		
All	All	3793/3964~(96%)	3773 (100%)	20~(0%)	88 95		

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All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	17	ILE
1	А	48	GLN
1	А	505	ARG
1	В	620	MET
1	С	17	ILE
1	С	620	MET
1	D	219	THR
1	D	294	GLN
1	D	505	ARG
1	D	620	MET
2	Е	208	PHE
2	Е	261	MET
2	F	25	VAL
2	F	183	THR
2	F	203	LEU
2	F	208	PHE
2	F	360	GLN
2	G	85	SER
2	G	208	PHE
2	Н	208	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	696	ASN
1	В	183	ASN



Continued from previous page...

Mol	Chain	Res	Type
1	В	437	ASN
1	В	713	GLN
2	Н	278	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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).

Mal	Turne	Chain	Chain Deg Li		Bo	Bond lengths		Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FEO	G	501	2,8	0,2,2	-	-	-		
6	TTP	А	804	5	26,30,30	1.26	5 (19%)	39,47,47	1.98	7 (17%)
4	DAT	В	802	5	24,28,28	0.90	1 (4%)	28,43,43	1.25	2 (7%)
6	TTP	D	804	5	26,30,30	1.24	4 (15%)	39,47,47	2.04	7 (17%)
4	DAT	С	802	5	24,28,28	0.91	1 (4%)	28,43,43	1.17	2 (7%)
4	DAT	D	802	5	24,28,28	0.89	1 (4%)	28,43,43	1.22	2 (7%)
7	FEO	Е	501	2,8	0,2,2	-	-	-		
4	DAT	А	802	5	24,28,28	0.86	1 (4%)	28,43,43	1.25	2 (7%)
7	FEO	F	501	2,8	0,2,2	-	-	-		



Mal	Type	Chain	Dog	Box Link Bond lengths			Bond angles			
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
6	TTP	А	805	5	26,30,30	1.24	5 (19%)	39,47,47	1.86	6 (15%)
6	TTP	С	805	5	26,30,30	1.28	6 (23%)	39,47,47	1.99	7 (17%)
6	TTP	D	805	5	26,30,30	1.26	5 (19%)	39,47,47	1.92	6 (15%)
3	GDP	С	801	-	24,30,30	0.99	2 (8%)	30,47,47	1.24	4 (13%)
6	TTP	В	805	5	26,30,30	1.27	5 (19%)	39,47,47	1.88	<mark>6 (15%)</mark>
7	FEO	Н	501	2,8	0,2,2	-	-	-		
3	GDP	А	801	-	24,30,30	0.97	1 (4%)	30,47,47	1.17	4 (13%)
3	GDP	В	801	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)
6	TTP	С	804	5	26,30,30	1.20	5 (19%)	39,47,47	2.00	8 (20%)
6	TTP	В	804	5	26,30,30	1.26	5 (19%)	39,47,47	1.96	<u>6 (15%)</u>
3	GDP	D	801	-	24,30,30	0.96	1 (4%)	30,47,47	1.26	5 (16%)

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
6	TTP	А	804	5	-	11/22/34/34	0/2/2/2
3	GDP	А	801	-	-	6/12/32/32	0/3/3/3
4	DAT	В	802	5	-	2/12/28/28	0/3/3/3
3	GDP	В	801	-	-	5/12/32/32	0/3/3/3
6	TTP	С	804	5	-	7/22/34/34	0/2/2/2
6	TTP	D	804	5	-	8/22/34/34	0/2/2/2
6	TTP	А	805	5	-	7/22/34/34	0/2/2/2
4	DAT	С	802	5	-	4/12/28/28	0/3/3/3
4	DAT	D	802	5	-	3/12/28/28	0/3/3/3
6	TTP	С	805	5	-	3/22/34/34	0/2/2/2
6	TTP	D	805	5	-	7/22/34/34	0/2/2/2
3	GDP	С	801	-	-	3/12/32/32	0/3/3/3
3	GDP	D	801	-	-	5/12/32/32	0/3/3/3
6	TTP	В	804	5	-	12/22/34/34	0/2/2/2
6	TTP	В	805	5	-	3/22/34/34	0/2/2/2
4	DAT	А	802	5	-	3/12/28/28	0/3/3/3

All (49) bond length outliers are listed below:



51	IN	V
50	JIN	v

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
6	D	805	TTP	C6-C5	2.89	1.39	1.34
6	С	805	TTP	C4-N3	-2.88	1.33	1.38
6	А	805	TTP	C6-C5	2.84	1.39	1.34
6	В	805	TTP	C6-C5	2.81	1.39	1.34
6	D	805	TTP	C4-N3	-2.79	1.33	1.38
6	В	804	TTP	C6-C5	2.78	1.39	1.34
6	В	805	TTP	C4-N3	-2.76	1.33	1.38
6	D	804	TTP	C6-C5	2.74	1.39	1.34
6	А	804	TTP	C6-C5	2.68	1.39	1.34
6	С	805	TTP	C6-C5	2.66	1.39	1.34
6	А	805	TTP	C4-N3	-2.56	1.34	1.38
6	В	804	TTP	C4-N3	-2.56	1.34	1.38
4	D	802	DAT	C5-C4	2.56	1.47	1.40
6	А	804	TTP	C4-C5	2.55	1.49	1.44
4	С	802	DAT	C5-C4	2.54	1.47	1.40
4	В	802	DAT	C5-C4	2.52	1.47	1.40
6	В	804	TTP	C4-C5	2.51	1.48	1.44
6	С	804	TTP	C4-N3	-2.50	1.34	1.38
6	D	804	TTP	C4-N3	-2.44	1.34	1.38
4	А	802	DAT	C5-C4	2.43	1.47	1.40
6	С	805	TTP	C6-N1	-2.38	1.34	1.38
6	А	804	TTP	C4-N3	-2.38	1.34	1.38
6	В	805	TTP	C4-C5	2.38	1.48	1.44
6	D	804	TTP	C4-C5	2.37	1.48	1.44
6	С	804	TTP	C6-N1	-2.36	1.34	1.38
6	С	804	TTP	C6-C5	2.33	1.38	1.34
3	А	801	GDP	C6-N1	-2.33	1.34	1.37
6	В	805	TTP	C6-N1	-2.32	1.34	1.38
3	D	801	GDP	C6-N1	-2.32	1.34	1.37
3	С	801	GDP	C6-N1	-2.27	1.34	1.37
6	D	805	TTP	C2-N3	-2.26	1.33	1.38
6	А	804	TTP	C6-N1	-2.26	1.34	1.38
6	А	805	TTP	C6-N1	-2.25	1.34	1.38
6	D	805	TTP	C4-C5	2.24	1.48	1.44
6	С	805	TTP	C2-N3	-2.23	1.34	1.38
6	А	804	TTP	C2-N1	2.22	1.42	1.38
6	С	805	TTP	C4-C5	2.22	1.48	1.44
6	D	804	TTP	C6-N1	-2.22	1.34	1.38
6	D	805	TTP	C6-N1	-2.21	1.34	1.38
6	В	804	TTP	C6-N1	-2.21	1.34	1.38
6	А	805	TTP	C4-C5	2.20	1.48	1.44
3	B	801	GDP	C6-N1	-2.19	1.34	1.37
6	С	804	TTP	C2-N1	2.16	1.41	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
6	С	804	TTP	C4-C5	2.15	1.48	1.44
6	В	805	TTP	C2-N3	-2.06	1.34	1.38
6	В	804	TTP	C2-N3	-2.04	1.34	1.38
3	С	801	GDP	O4'-C1'	2.03	1.43	1.41
6	А	805	TTP	C2-N3	-2.03	1.34	1.38
6	С	805	TTP	C2-N1	2.01	1.41	1.38

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	А	804	TTP	C4-N3-C2	-5.53	120.19	127.35
6	С	805	TTP	C4-N3-C2	-5.51	120.21	127.35
6	D	804	TTP	C4-N3-C2	-5.42	120.33	127.35
6	В	804	TTP	C4-N3-C2	-5.39	120.37	127.35
6	D	805	TTP	C4-N3-C2	-5.35	120.42	127.35
6	В	805	TTP	C4-N3-C2	-5.34	120.44	127.35
6	С	804	TTP	C4-N3-C2	-5.30	120.48	127.35
6	С	805	TTP	N3-C2-N1	5.19	121.77	114.89
6	А	805	TTP	C4-N3-C2	-5.15	120.68	127.35
6	D	805	TTP	C5-C4-N3	5.11	119.68	115.31
6	В	805	TTP	N3-C2-N1	5.09	121.64	114.89
6	А	804	TTP	N3-C2-N1	4.97	121.49	114.89
6	В	804	TTP	N3-C2-N1	4.94	121.45	114.89
6	D	805	TTP	N3-C2-N1	4.88	121.37	114.89
6	D	804	TTP	N3-C2-N1	4.83	121.31	114.89
6	А	805	TTP	N3-C2-N1	4.82	121.29	114.89
6	А	804	TTP	C5-C6-N1	-4.66	118.54	123.34
6	С	805	TTP	C5-C4-N3	4.66	119.29	115.31
6	С	804	TTP	N3-C2-N1	4.64	121.05	114.89
6	С	804	TTP	C5-C4-N3	4.58	119.22	115.31
6	D	804	TTP	C5-C6-N1	-4.54	118.67	123.34
6	В	804	TTP	C5-C6-N1	-4.50	118.71	123.34
6	D	804	TTP	C5-C4-N3	4.48	119.14	115.31
6	В	804	TTP	C5-C4-N3	4.48	119.14	115.31
6	С	804	TTP	O4-C4-C5	-4.48	119.71	124.90
6	А	805	TTP	C5-C4-N3	4.45	119.11	115.31
6	В	805	TTP	C5-C4-N3	4.35	119.02	115.31
6	В	805	TTP	C5-C6-N1	-4.32	118.90	123.34
6	С	805	TTP	C5-C6-N1	-4.31	118.90	123.34
6	D	804	TTP	O4-C4-C5	-4.27	119.95	124.90
6	А	804	TTP	C5-C4-N3	4.22	118.91	115.31
6	A	805	TTP	O4-C4-C5	-4.13	120.12	124.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	А	804	TTP	O4-C4-C5	-4.09	120.16	124.90
6	D	805	TTP	C5-C6-N1	-4.08	119.14	123.34
6	D	805	TTP	O4-C4-C5	-3.97	120.30	124.90
6	А	805	TTP	C5-C6-N1	-3.96	119.26	123.34
6	В	804	TTP	O4-C4-C5	-3.85	120.43	124.90
6	С	804	TTP	C5-C6-N1	-3.78	119.45	123.34
6	С	805	TTP	O4-C4-C5	-3.73	120.58	124.90
6	В	805	TTP	O4-C4-C5	-3.47	120.88	124.90
4	А	802	DAT	N3-C2-N1	-3.33	123.47	128.68
4	D	802	DAT	N3-C2-N1	-3.30	123.52	128.68
4	В	802	DAT	C4-C5-N7	-3.26	106.00	109.40
4	С	802	DAT	N3-C2-N1	-3.22	123.64	128.68
4	В	802	DAT	N3-C2-N1	-3.18	123.72	128.68
6	А	804	TTP	O2-C2-N1	-3.16	118.58	122.79
6	D	804	TTP	PB-O3B-PG	-3.14	122.04	132.83
6	D	804	TTP	O2-C2-N1	-3.10	118.67	122.79
6	В	804	TTP	O2-C2-N1	-3.05	118.74	122.79
3	В	801	GDP	C3'-C2'-C1'	2.93	105.38	100.98
4	С	802	DAT	C4-C5-N7	-2.91	106.37	109.40
4	D	802	DAT	C4-C5-N7	-2.90	106.38	109.40
4	А	802	DAT	C4-C5-N7	-2.89	106.39	109.40
3	В	801	GDP	PA-O3A-PB	-2.83	123.13	132.83
3	D	801	GDP	PA-O3A-PB	-2.77	123.31	132.83
6	С	804	TTP	O2-C2-N1	-2.69	119.21	122.79
6	А	805	TTP	O2-C2-N1	-2.65	119.27	122.79
6	D	805	TTP	O2-C2-N1	-2.60	119.33	122.79
3	А	801	GDP	C3'-C2'-C1'	2.58	104.86	100.98
6	\mathbf{C}	805	TTP	O2-C2-N1	-2.58	119.36	122.79
3	D	801	GDP	C5-C6-N1	2.55	118.45	113.95
6	В	805	TTP	O2-C2-N1	-2.55	119.40	122.79
6	\mathbf{C}	805	TTP	PB-O3B-PG	-2.47	124.34	132.83
3	С	801	GDP	C5-C6-N1	2.41	118.20	113.95
3	С	801	GDP	C3'-C2'-C1'	2.39	104.58	100.98
3	D	801	GDP	C3'-C2'-C1'	2.39	104.57	100.98
3	В	801	GDP	C5-C6-N1	2.38	118.16	113.95
6	\mathbf{C}	804	TTP	PB-O3B-PG	-2.32	124.87	132.83
3	С	801	GDP	PA-O3A-PB	-2.31	124.91	132.83
3	C	801	GDP	C8-N7-C5	$2.3\overline{0}$	107.37	102.99
3	А	801	GDP	C5-C6-N1	2.29	118.00	113.95
3	А	801	GDP	C8-N7-C5	2.27	107.32	102.99
3	D	801	GDP	C8-N7-C5	$2.2\overline{2}$	$107.2\overline{2}$	102.99
3	В	801	GDP	C8-N7-C5	2.19	107.16	102.99



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	А	804	TTP	C5M-C5-C6	-2.16	119.97	122.85
3	D	801	GDP	O6-C6-C5	-2.10	120.27	124.37
3	А	801	GDP	PA-O3A-PB	-2.09	125.65	132.83
6	С	804	TTP	C5M-C5-C4	2.04	121.01	118.77

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	801	GDP	C5'-O5'-PA-O1A
3	А	801	GDP	C5'-O5'-PA-O2A
3	В	801	GDP	PA-O3A-PB-O2B
3	В	801	GDP	PA-O3A-PB-O3B
3	В	801	GDP	O4'-C4'-C5'-O5'
3	В	801	GDP	C3'-C4'-C5'-O5'
3	С	801	GDP	PA-O3A-PB-O3B
3	D	801	GDP	C5'-O5'-PA-O1A
3	D	801	GDP	C5'-O5'-PA-O2A
4	С	802	DAT	C5'-O5'-PA-O2A
6	А	804	TTP	C5'-O5'-PA-O2A
6	А	805	TTP	C5'-O5'-PA-O2A
6	А	805	TTP	PB-O3B-PG-O3G
6	В	804	TTP	C5'-O5'-PA-O1A
6	В	804	TTP	PB-O3B-PG-O2G
6	В	804	TTP	PB-O3B-PG-O3G
6	В	805	TTP	C5'-O5'-PA-O1A
6	С	805	TTP	PB-O3B-PG-O3G
6	D	804	TTP	C5'-O5'-PA-O1A
6	D	804	TTP	C5'-O5'-PA-O2A
6	D	805	TTP	C5'-O5'-PA-O1A
3	А	801	GDP	O4'-C4'-C5'-O5'
4	В	802	DAT	O4'-C4'-C5'-O5'
4	В	802	DAT	C3'-C4'-C5'-O5'
4	D	802	DAT	O4'-C4'-C5'-O5'
6	D	805	TTP	PA-O3A-PB-O1B
4	D	802	DAT	C3'-C4'-C5'-O5'
6	D	804	TTP	C2'-C1'-N1-C6
3	A	801	GDP	C3'-C4'-C5'-O5'
6	A	804	TTP	C2'-C1'-N1-C6
6	А	804	TTP	PB-O3B-PG-O1G
6	A	805	TTP	PB-O3B-PG-O2G
4	С	802	DAT	C5'-O5'-PA-O3A



Mol	Chain	Res	Type	Atoms
6	А	804	TTP	C5'-O5'-PA-O3A
6	А	805	TTP	C5'-O5'-PA-O3A
6	В	804	TTP	C5'-O5'-PA-O3A
6	D	804	TTP	C5'-O5'-PA-O3A
6	D	805	TTP	C5'-O5'-PA-O3A
4	А	802	DAT	PB-O3A-PA-O2A
4	D	802	DAT	PB-O3A-PA-O2A
6	А	805	TTP	PA-O3A-PB-O2B
6	В	804	TTP	PB-O3A-PA-O2A
6	С	804	TTP	PB-O3A-PA-O2A
4	А	802	DAT	C5'-O5'-PA-O1A
4	С	802	DAT	C5'-O5'-PA-O1A
6	А	805	TTP	C5'-O5'-PA-O1A
6	В	804	TTP	C5'-O5'-PA-O2A
6	В	805	TTP	C5'-O5'-PA-O2A
6	D	805	TTP	C5'-O5'-PA-O2A
6	D	804	TTP	C2'-C1'-N1-C2
6	D	804	TTP	O4'-C1'-N1-C6
6	В	804	TTP	C4'-C5'-O5'-PA
3	D	801	GDP	O4'-C4'-C5'-O5'
3	D	801	GDP	PB-O3A-PA-O2A
4	А	802	DAT	PB-O3A-PA-O1A
6	С	804	TTP	PB-O3A-PA-O1A
6	D	805	TTP	PA-O3A-PB-O2B
6	А	804	TTP	O4'-C1'-N1-C6
6	А	804	TTP	O4'-C1'-N1-C2
6	D	804	TTP	O4'-C1'-N1-C2
6	А	804	TTP	C2'-C1'-N1-C2
6	D	804	TTP	O4'-C4'-C5'-O5'
6	В	804	TTP	PB-O3A-PA-O1A
6	С	804	TTP	PA-O3A-PB-O1B
6	D	805	TTP	PG-O3B-PB-O1B
3	В	801	GDP	PA-O3A-PB-O1B
6	В	804	TTP	O4'-C1'-N1-C6
6	А	804	TTP	O4'-C4'-C5'-O5'
6	В	804	TTP	O4'-C4'-C5'-O5'
4	С	802	DAT	PA-O3A-PB-O2B
6	А	804	TTP	PB-O3B-PG-O2G
6	А	804	TTP	PB-O3B-PG-O3G
6	С	804	TTP	C2'-C1'-N1-C6
3	А	801	GDP	C5'-O5'-PA-O3A
3	С	801	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	D	801	GDP	C5'-O5'-PA-O3A
6	В	805	TTP	C5'-O5'-PA-O3A
6	С	804	TTP	O4'-C4'-C5'-O5'
6	А	805	TTP	PA-O3A-PB-O1B
6	С	804	TTP	PA-O3A-PB-O2B
6	С	805	TTP	PA-O3A-PB-O1B
6	С	805	TTP	PA-O3A-PB-O2B
6	D	805	TTP	PG-O3B-PB-O2B
6	А	804	TTP	C5'-O5'-PA-O1A
6	С	804	TTP	O4'-C1'-N1-C6
3	А	801	GDP	PA-O3A-PB-O1B
3	С	801	GDP	PA-O3A-PB-O1B
6	В	804	TTP	PB-O3B-PG-O1G
6	В	804	TTP	C2'-C1'-N1-C6

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There are no ring outliers.

17	monomers	are	invol	ved	in	35	short	contacts:
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	А	804	TTP	2	0
4	В	802	DAT	2	0
6	D	804	TTP	2	0
4	С	802	DAT	2	0
4	D	802	DAT	1	0
4	А	802	DAT	3	0
6	А	805	TTP	3	0
6	С	805	TTP	2	0
6	D	805	TTP	1	0
3	С	801	GDP	1	0
6	В	805	TTP	2	0
7	Н	501	FEO	1	0
3	А	801	GDP	5	0
3	В	801	GDP	3	0
6	С	804	TTP	2	0
6	В	804	TTP	1	0
3	D	801	GDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.



Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.































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, 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	$\langle RSRZ \rangle$	#RSRZ>2		$OWAB(Å^2)$	Q < 0.9
1	А	736/761~(96%)	-0.09	9 (1%) 79	67	59, 75, 88, 104	0
1	В	732/761~(96%)	0.15	12 (1%) 72	59	75, 91, 101, 108	0
1	С	734/761~(96%)	-0.30	0 100	100	47, 58, 74, 93	0
1	D	734/761~(96%)	-0.29	4 (0%) 91	86	47, 61, 85, 110	0
2	Е	352/375~(93%)	0.10	6 (1%) 70	57	65, 86, 101, 117	0
2	F	357/375~(95%)	-0.38	1 (0%) 94	92	42, 54, 73, 95	0
2	G	357/375~(95%)	-0.35	1 (0%) 94	92	39, 52, 77, 98	0
2	Н	359/375~(95%)	-0.11	7 (1%) 66	53	58, 71, 92, 116	0
All	All	4361/4544 (95%)	-0.15	40 (0%) 84	75	39, 69, 97, 117	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Н	179	GLY	4.2
2	Ε	1	ALA	3.6
1	D	14	THR	3.5
2	F	341	SER	3.4
1	В	128	PHE	3.2
1	А	2	ASN	3.0
1	В	706	SER	3.0
1	В	382	TYR	2.8
1	В	708	LYS	2.7
1	D	4	ASN	2.6
2	Ε	170	LEU	2.6
1	В	107	VAL	2.6
1	D	16	ARG	2.6
1	А	49	PHE	2.5
2	Н	363	SER	2.5
2	Н	182	VAL	2.5



Mol	Chain	Res	Type	RSRZ
2	Е	363	SER	2.5
1	В	378	LEU	2.4
1	В	379	TYR	2.4
1	В	131	MET	2.4
1	В	364	LEU	2.4
2	Н	343	ASN	2.3
1	В	105	HIS	2.3
1	А	456	ASN	2.3
1	В	190	LEU	2.2
2	Н	181	THR	2.2
1	В	692	SER	2.2
2	Н	341	SER	2.2
1	А	388	ILE	2.2
2	Е	375	LEU	2.1
1	А	48	GLN	2.1
1	А	3	GLN	2.1
1	А	5	LEU	2.1
1	D	10	ARG	2.1
2	Е	60	ILE	2.1
2	Е	114	SER	2.1
1	А	610	GLY	2.1
2	Н	183	THR	2.1
1	А	4	ASN	2.1
2	G	372	ASN	2.0

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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 monosaccharides 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, 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	$B-factors(Å^2)$	Q<0.9
6	TTP	А	804	29/29	0.83	0.25	73,84,94,98	29
5	MG	В	806	1/1	0.86	0.11	81,81,81,81	0
6	TTP	С	804	29/29	0.88	0.18	68,73,80,82	29
5	MG	D	803	1/1	0.89	0.03	95,95,95,95	0
6	TTP	В	804	29/29	0.91	0.17	96,101,104,105	29
3	GDP	В	801	28/28	0.91	0.31	81,84,87,88	0
6	TTP	D	804	29/29	0.91	0.21	79,89,100,102	29
5	MG	А	803	1/1	0.92	0.06	93,93,93,93	0
5	MG	В	803	1/1	0.92	0.05	102,102,102,102	0
4	DAT	А	802	26/26	0.93	0.25	74,81,88,89	0
5	MG	А	806	1/1	0.94	0.06	81,81,81,81	0
4	DAT	В	802	26/26	0.94	0.20	96,100,104,105	0
5	MG	С	803	1/1	0.95	0.07	73,73,73,73	0
4	DAT	D	802	26/26	0.95	0.27	84,92,98,99	0
3	GDP	D	801	28/28	0.96	0.18	$52,\!55,\!58,\!59$	0
6	TTP	А	805	29/29	0.96	0.14	78,81,84,86	0
4	DAT	С	802	26/26	0.96	0.16	66, 69, 75, 77	0
6	TTP	В	805	29/29	0.96	0.15	79,81,84,88	0
3	GDP	А	801	28/28	0.96	0.32	66,69,72,73	0
6	TTP	С	805	29/29	0.96	0.15	53,56,61,65	0
5	MG	D	806	1/1	0.96	0.04	54,54,54,54	0
5	MG	С	806	1/1	0.97	0.12	59,59,59,59	0
3	GDP	С	801	28/28	0.97	0.26	49,53,56,57	0
6	TTP	D	805	29/29	0.97	0.13	$50,\!53,\!56,\!59$	0
7	FEO	Е	501	$\overline{3/3}$	0.98	0.16	73,73,75,81	0
7	FEO	F	501	3/3	0.98	0.15	47,47,47,49	0
7	FEO	G	501	3/3	0.99	0.17	43,43,45,47	0
7	FEO	Н	501	3/3	0.99	0.17	$\overline{62,\!62,\!62,\!63}$	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





























































6.5 Other polymers (i)

There are no such residues in this entry.

