



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:25 PM UTC

PDB ID : 2G88 / pdb_00002g88
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Deposited on : 2006-03-02
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

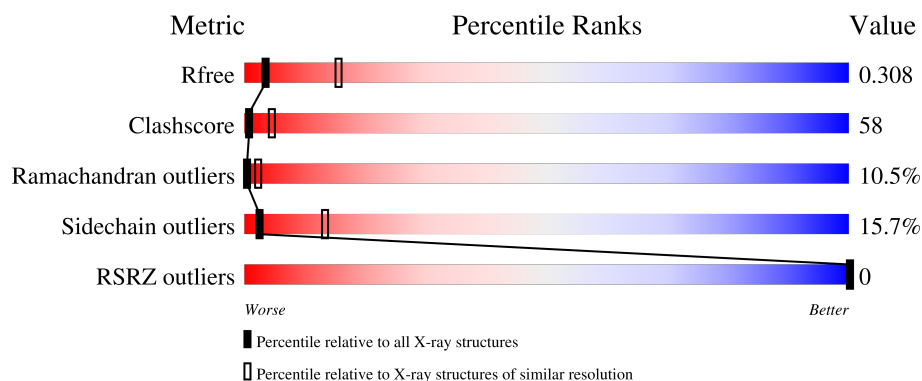
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. 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	349	29% 43% 17% 7% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DTP	A	833	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	A	1322	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2581 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.

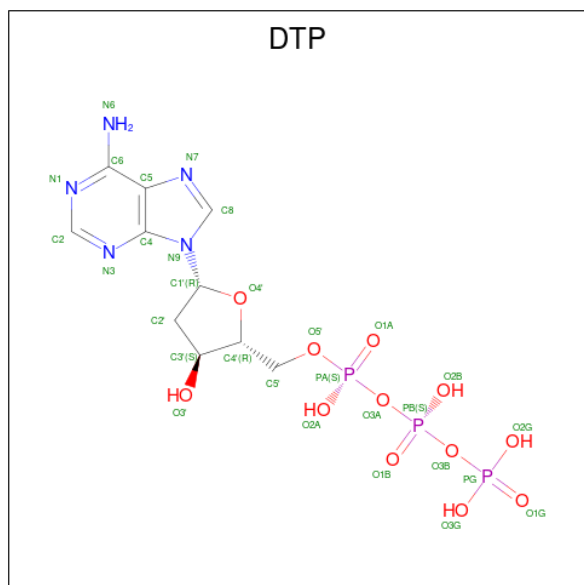
- Molecule 1 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2399	1504	421	468	6			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

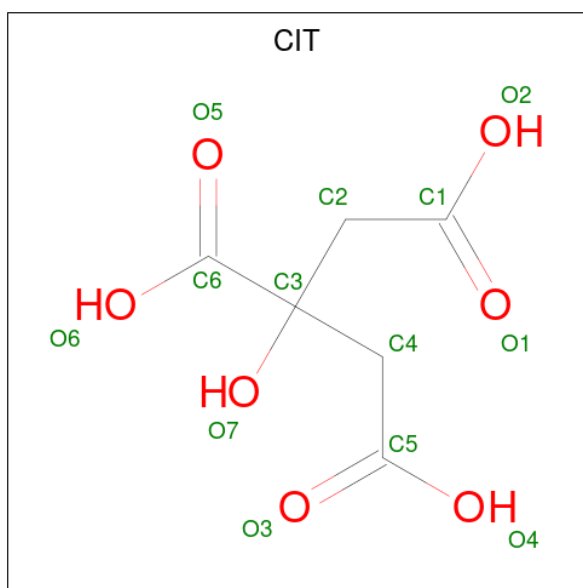
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

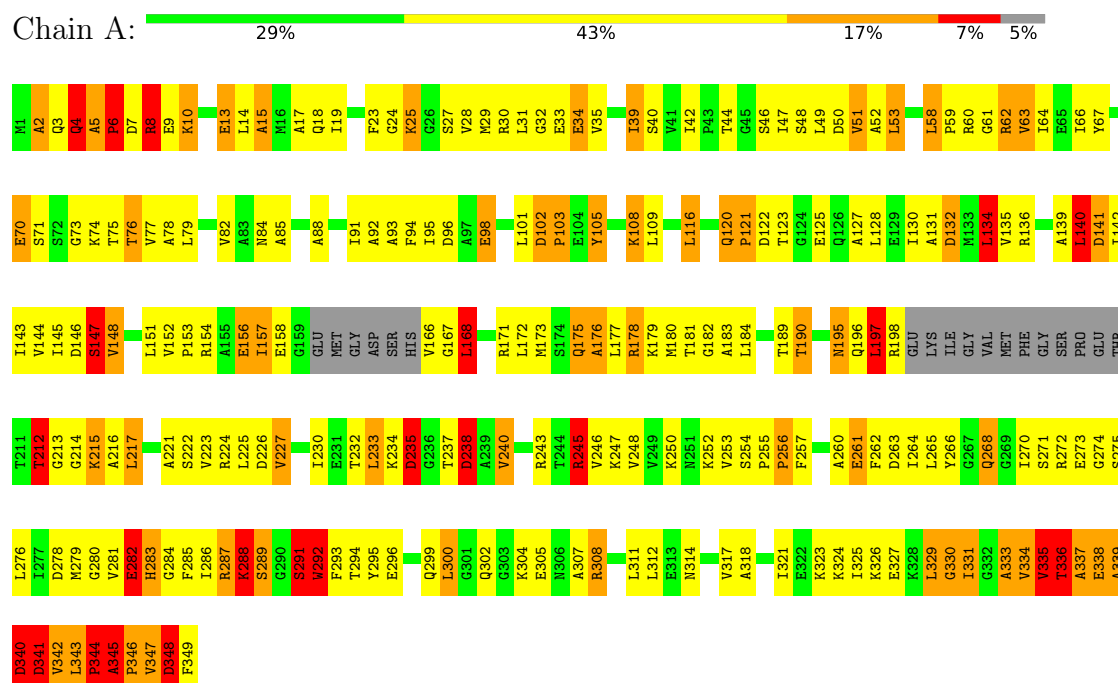
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		

3 Residue-property plots

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: Protein recA



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	108.21 Å 108.21 Å 72.97 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.40 – 3.20 25.40 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (25.40-3.20) 96.4 (25.40-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 3.17 Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.237 , 0.309 0.234 , 0.308	Depositor DCC
R_{free} test set	829 reflections (10.59%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.440 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2581	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, MG, DTP

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	0.77	1/2427 (0.0%)	1.67	78/3284 (2.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ARG	CA-CB	6.52	1.63	1.53

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ALA	CA-C-N	-15.02	101.06	119.84
1	A	345	ALA	C-N-CA	-15.02	101.06	119.84
1	A	291	SER	N-CA-C	-14.31	80.31	110.80
1	A	245	ARG	N-CA-CB	12.28	129.72	110.56
1	A	337	ALA	N-CA-C	12.00	127.50	112.86
1	A	345	ALA	N-CA-C	11.59	135.43	109.81
1	A	292	TRP	N-CA-C	11.48	135.25	110.80
1	A	245	ARG	CA-CB-CG	11.42	136.93	114.10
1	A	287	ARG	N-CA-C	11.38	127.81	109.94
1	A	343	LEU	N-CA-C	10.69	133.43	109.81
1	A	289	SER	N-CA-C	10.44	125.91	111.92
1	A	343	LEU	CA-C-N	10.38	132.81	119.84
1	A	343	LEU	C-N-CA	10.38	132.81	119.84
1	A	333	ALA	N-CA-C	10.01	132.12	110.80
1	A	340	ASP	N-CA-C	9.94	131.98	110.80
1	A	334	VAL	N-CA-C	9.92	126.34	112.35
1	A	344	PRO	N-CA-C	9.79	132.65	112.47
1	A	329	LEU	N-CA-C	-9.18	93.90	109.24
1	A	168	LEU	N-CA-C	9.07	130.13	110.80
1	A	347	VAL	N-CA-C	8.70	121.56	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	LYS	N-CA-C	-8.49	103.97	112.97
1	A	333	ALA	CA-C-N	8.11	133.40	120.82
1	A	333	ALA	C-N-CA	8.11	133.40	120.82
1	A	234	LYS	N-CA-C	7.79	121.59	108.90
1	A	346	PRO	N-CA-C	-7.75	96.51	112.47
1	A	245	ARG	CB-CG-CD	7.63	128.84	111.30
1	A	222	SER	N-CA-C	-7.60	102.82	112.93
1	A	238	ASP	N-CA-C	-7.26	95.33	110.80
1	A	197	LEU	N-CA-C	7.24	126.23	110.80
1	A	342	VAL	N-CA-C	7.13	124.17	109.34
1	A	134	LEU	N-CA-C	-7.11	104.42	113.23
1	A	240	VAL	N-CA-C	7.07	121.94	112.04
1	A	335	VAL	N-CA-C	7.00	123.90	109.34
1	A	348	ASP	CA-C-N	6.88	134.08	121.70
1	A	348	ASP	C-N-CA	6.88	134.08	121.70
1	A	8	ARG	N-CA-C	6.77	120.46	110.30
1	A	213	GLY	N-CA-C	-6.70	97.30	113.18
1	A	53	LEU	N-CA-C	-6.66	105.12	113.18
1	A	121	PRO	N-CA-C	6.55	121.94	111.26
1	A	288	LYS	CA-C-N	6.29	131.53	122.35
1	A	288	LYS	C-N-CA	6.29	131.53	122.35
1	A	105	TYR	N-CA-C	-6.28	104.31	112.23
1	A	30	ARG	N-CA-C	-6.27	99.02	109.24
1	A	346	PRO	CA-C-N	-6.06	115.33	122.36
1	A	346	PRO	C-N-CA	-6.06	115.33	122.36
1	A	334	VAL	CB-CA-C	-6.04	103.13	111.65
1	A	349	PHE	N-CA-C	-6.04	94.09	111.00
1	A	282	GLU	CB-CG-CD	6.02	122.84	112.60
1	A	178	ARG	N-CA-C	-6.01	106.08	113.41
1	A	102	ASP	CA-C-N	5.98	127.31	119.84
1	A	102	ASP	C-N-CA	5.98	127.31	119.84
1	A	167	GLY	CA-C-N	5.87	132.75	121.54
1	A	167	GLY	C-N-CA	5.87	132.75	121.54
1	A	336	THR	CA-C-N	5.83	132.20	123.05
1	A	336	THR	C-N-CA	5.83	132.20	123.05
1	A	308	ARG	N-CA-C	-5.80	105.04	111.71
1	A	88	ALA	N-CA-C	-5.69	104.75	112.26
1	A	13	GLU	CA-CB-CG	5.60	125.30	114.10
1	A	148	VAL	N-CA-C	-5.59	105.41	113.07
1	A	35	VAL	N-CA-C	5.58	116.80	109.21
1	A	196	GLN	N-CA-C	5.56	118.41	110.68
1	A	4	GLN	N-CA-C	-5.49	99.10	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASP	N-CA-C	5.48	122.48	110.80
1	A	217	LEU	N-CA-C	-5.39	104.81	111.33
1	A	349	PHE	N-CA-CB	5.38	119.64	110.50
1	A	235	ASP	N-CA-C	5.20	121.88	110.80
1	A	348	ASP	N-CA-C	5.20	121.88	110.80
1	A	156	GLU	N-CA-C	5.20	117.35	111.11
1	A	13	GLU	CB-CA-C	5.15	119.34	110.79
1	A	284	GLY	N-CA-C	5.14	122.93	115.32
1	A	181	THR	N-CA-C	-5.14	106.70	112.87
1	A	287	ARG	CA-C-N	5.13	131.34	121.54
1	A	287	ARG	C-N-CA	5.13	131.34	121.54
1	A	227	VAL	N-CA-C	5.12	115.22	107.75
1	A	120	GLN	CA-C-N	5.07	125.36	119.93
1	A	120	GLN	C-N-CA	5.07	125.36	119.93
1	A	58	LEU	N-CA-C	-5.05	103.17	110.40
1	A	98	GLU	N-CA-C	-5.04	107.53	113.97

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	2399	0	2356	282	0
2	A	1	0	0	0	0
3	A	60	0	24	17	0
4	A	13	0	4	4	0
5	A	108	0	0	5	0
All	All	2581	0	2384	284	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 58.

All (284) 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:291:SER:HB3	1:A:302:GLN:HG3	1.27	1.12
1:A:326:LYS:HG2	1:A:331:ILE:HD12	1.36	1.07
1:A:330:GLY:O	1:A:331:ILE:HG13	1.54	1.07
1:A:279:MET:HE1	3:A:833:DTP:H2'1	1.31	1.05
1:A:286:ILE:HD11	1:A:321:ILE:HD13	1.44	0.97
1:A:289:SER:HA	1:A:292:TRP:O	1.65	0.95
1:A:279:MET:CE	3:A:833:DTP:H2'1	1.97	0.94
1:A:237:THR:O	1:A:238:ASP:CG	2.11	0.93
1:A:5:ALA:HB1	1:A:6:PRO:CD	2.00	0.91
1:A:291:SER:CB	1:A:302:GLN:HG3	2.03	0.88
1:A:131:ALA:O	1:A:135:VAL:HG23	1.74	0.87
1:A:78:ALA:O	1:A:82:VAL:HG23	1.75	0.85
1:A:130:ILE:O	1:A:134:LEU:HB2	1.76	0.85
1:A:64:ILE:HG23	1:A:223:VAL:HB	1.60	0.82
1:A:2:ALA:O	1:A:5:ALA:HB3	1.80	0.81
1:A:3:GLN:O	1:A:4:GLN:HG3	1.80	0.81
1:A:125:GLU:CD	1:A:154:ARG:H	1.87	0.81
1:A:335:VAL:HG13	1:A:336:THR:N	1.96	0.81
1:A:157:ILE:HG13	1:A:157:ILE:O	1.79	0.81
1:A:323:LYS:NZ	1:A:335:VAL:HG11	1.95	0.80
1:A:329:LEU:O	1:A:330:GLY:O	2.00	0.79
1:A:127:ALA:O	1:A:131:ALA:HB2	1.84	0.78
1:A:330:GLY:O	1:A:331:ILE:CG1	2.31	0.77
1:A:5:ALA:CB	1:A:6:PRO:CD	2.64	0.75
1:A:95:ILE:HG21	1:A:127:ALA:HB1	1.69	0.75
1:A:335:VAL:CG1	1:A:336:THR:N	2.49	0.74
1:A:136:ARG:HH21	1:A:179:LYS:HG2	1.53	0.74
1:A:73:GLY:O	1:A:77:VAL:HG23	1.89	0.73
1:A:136:ARG:NH2	1:A:179:LYS:HG2	2.03	0.73
1:A:335:VAL:CG1	1:A:336:THR:H	2.01	0.73
1:A:265:LEU:HB2	1:A:268:GLN:HB2	1.71	0.72
1:A:245:ARG:HB3	1:A:261:GLU:HG3	1.72	0.72
1:A:5:ALA:HB1	1:A:6:PRO:HD3	1.72	0.71
1:A:25:LYS:N	4:A:1322:CIT:O5	2.23	0.71
1:A:237:THR:O	1:A:238:ASP:OD1	2.09	0.70
1:A:5:ALA:HB1	1:A:6:PRO:HD2	1.74	0.69
1:A:279:MET:SD	3:A:833:DTP:H2'1	2.32	0.69
1:A:105:TYR:O	1:A:109:LEU:HG	1.93	0.69
1:A:184:LEU:HD23	1:A:189:THR:HB	1.75	0.69
1:A:314:ASN:O	1:A:317:VAL:HG12	1.93	0.69
1:A:76:THR:HG22	1:A:77:VAL:N	2.09	0.68
1:A:283:HIS:CE1	3:A:833:DTP:O3'	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:H	1:A:39:ILE:HD12	1.59	0.68
1:A:51:VAL:HG12	1:A:331:ILE:HD11	1.76	0.67
1:A:344:PRO:O	1:A:345:ALA:HB2	1.93	0.67
1:A:102:ASP:HB3	3:A:832:DTP:HN62	1.59	0.67
1:A:345:ALA:C	1:A:346:PRO:O	2.34	0.66
1:A:323:LYS:HZ2	1:A:335:VAL:CG1	2.07	0.66
1:A:3:GLN:C	1:A:4:GLN:HG3	2.19	0.66
1:A:4:GLN:HG2	5:A:504:HOH:O	1.96	0.66
1:A:327:GLU:OE2	1:A:335:VAL:HG13	1.95	0.66
1:A:171:ARG:O	1:A:175:GLN:HG3	1.96	0.66
1:A:91:ILE:HB	1:A:140:LEU:HA	1.78	0.66
1:A:285:PHE:CE1	1:A:325:ILE:HG12	2.31	0.65
1:A:285:PHE:CD1	1:A:325:ILE:HG12	2.32	0.65
1:A:305:GLU:O	1:A:308:ARG:HB3	1.97	0.65
1:A:215:LYS:HG3	1:A:215:LYS:O	1.96	0.65
1:A:279:MET:HE1	3:A:833:DTP:C2'	2.19	0.65
1:A:323:LYS:HZ2	1:A:335:VAL:HG11	1.61	0.64
1:A:44:THR:CB	1:A:49:LEU:HD23	2.28	0.63
1:A:286:ILE:HD11	1:A:321:ILE:CD1	2.26	0.62
1:A:102:ASP:HB3	3:A:832:DTP:N6	2.15	0.62
1:A:96:ASP:HB3	1:A:120:GLN:HG2	1.82	0.62
1:A:272:ARG:O	1:A:275:SER:HB2	2.00	0.62
1:A:71:SER:H	3:A:832:DTP:PG	2.22	0.62
1:A:283:HIS:CE1	1:A:329:LEU:HD21	2.35	0.62
1:A:289:SER:CA	1:A:292:TRP:O	2.45	0.61
1:A:23:PHE:HB2	1:A:27:SER:OG	2.00	0.61
1:A:64:ILE:HG23	1:A:223:VAL:CB	2.31	0.60
1:A:323:LYS:CE	1:A:335:VAL:HG11	2.30	0.60
1:A:345:ALA:CB	5:A:499:HOH:O	2.49	0.60
1:A:327:GLU:OE2	1:A:336:THR:HA	2.02	0.60
1:A:32:GLY:O	1:A:346:PRO:HD3	2.01	0.60
1:A:53:LEU:HD21	1:A:225:LEU:HD21	1.84	0.59
1:A:136:ARG:NH1	1:A:183:ALA:HB2	2.17	0.59
1:A:24:GLY:HA3	4:A:1322:CIT:O6	2.03	0.59
1:A:264:ILE:HG12	1:A:270:ILE:HG12	1.83	0.59
1:A:3:GLN:O	1:A:4:GLN:CG	2.50	0.59
1:A:168:LEU:O	1:A:172:LEU:HG	2.03	0.59
1:A:279:MET:HE3	1:A:279:MET:O	2.03	0.58
1:A:321:ILE:O	1:A:325:ILE:HG13	2.03	0.58
1:A:227:VAL:HG22	1:A:246:VAL:HG22	1.85	0.58
1:A:337:ALA:HA	5:A:404:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:HG2	1:A:287:ARG:HH11	1.66	0.58
1:A:125:GLU:OE2	1:A:154:ARG:N	2.36	0.58
1:A:230:ILE:HD11	1:A:245:ARG:N	2.19	0.58
1:A:14:LEU:O	1:A:17:ALA:HB3	2.03	0.57
1:A:63:VAL:HG13	1:A:221:ALA:HA	1.86	0.57
1:A:197:LEU:O	1:A:198:ARG:CB	2.53	0.57
1:A:276:LEU:H	1:A:276:LEU:HD22	1.69	0.57
1:A:327:GLU:HG3	1:A:336:THR:CB	2.35	0.57
1:A:254:SER:OG	1:A:255:PRO:HD2	2.05	0.57
1:A:108:LYS:NZ	1:A:108:LYS:HB3	2.19	0.57
1:A:335:VAL:HG23	5:A:456:HOH:O	2.05	0.57
1:A:47:ILE:CG2	1:A:279:MET:HG2	2.35	0.56
1:A:76:THR:HG21	1:A:270:ILE:HG13	1.87	0.56
1:A:2:ALA:O	1:A:5:ALA:CB	2.53	0.56
1:A:307:ALA:O	1:A:311:LEU:HD13	2.04	0.56
1:A:75:THR:O	1:A:79:LEU:N	2.34	0.56
1:A:48:SER:OG	3:A:833:DTP:H8	2.06	0.56
1:A:64:ILE:CD1	1:A:223:VAL:HB	2.35	0.56
1:A:102:ASP:CB	3:A:832:DTP:HN62	2.19	0.56
1:A:127:ALA:HB3	1:A:151:LEU:HD12	1.88	0.56
1:A:33:GLU:HG2	1:A:34:GLU:H	1.71	0.55
1:A:66:ILE:HG22	1:A:74:LYS:HG2	1.88	0.55
1:A:70:GLU:HG3	3:A:832:DTP:O3G	2.07	0.55
1:A:180:MET:HG2	1:A:184:LEU:HD11	1.88	0.55
1:A:47:ILE:HD11	1:A:326:LYS:HG3	1.89	0.55
1:A:47:ILE:O	1:A:50:ASP:HB2	2.07	0.55
1:A:76:THR:CG2	1:A:270:ILE:HG13	2.37	0.55
1:A:121:PRO:HG3	1:A:127:ALA:HB2	1.89	0.55
1:A:214:GLY:C	1:A:216:ALA:H	2.14	0.55
1:A:147:SER:O	1:A:151:LEU:CD2	2.54	0.55
1:A:5:ALA:CB	1:A:6:PRO:HD2	2.35	0.55
1:A:76:THR:O	1:A:77:VAL:C	2.49	0.55
1:A:96:ASP:O	1:A:121:PRO:HD2	2.07	0.55
1:A:74:LYS:HB2	3:A:832:DTP:O2B	2.07	0.55
1:A:92:ALA:O	1:A:116:LEU:HD23	2.07	0.55
1:A:140:LEU:H	1:A:140:LEU:HD22	1.71	0.54
1:A:327:GLU:HG3	1:A:336:THR:CA	2.37	0.54
1:A:140:LEU:HD22	1:A:140:LEU:N	2.21	0.54
1:A:281:VAL:C	1:A:283:HIS:H	2.14	0.54
1:A:153:PRO:HG3	1:A:172:LEU:CD1	2.37	0.54
1:A:335:VAL:HG12	1:A:336:THR:H	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ALA:HB3	1:A:143:ILE:HG13	1.88	0.54
1:A:212:THR:HG22	1:A:212:THR:O	2.07	0.54
1:A:94:PHE:HE2	1:A:146:ASP:HB2	1.72	0.54
1:A:153:PRO:CA	1:A:172:LEU:HD11	2.38	0.54
1:A:180:MET:HG2	1:A:184:LEU:CD1	2.38	0.53
1:A:330:GLY:O	1:A:331:ILE:CB	2.56	0.53
1:A:8:ARG:HB3	1:A:10:LYS:HE3	1.90	0.53
1:A:91:ILE:HD12	1:A:139:ALA:O	2.08	0.53
1:A:29:MET:HE1	1:A:254:SER:CA	2.38	0.53
1:A:64:ILE:HD12	1:A:223:VAL:HB	1.91	0.53
1:A:33:GLU:HG2	1:A:34:GLU:N	2.23	0.53
1:A:323:LYS:NZ	1:A:335:VAL:CG1	2.64	0.52
1:A:67:TYR:HA	1:A:195:ASN:O	2.09	0.52
1:A:153:PRO:CB	1:A:172:LEU:HD11	2.39	0.52
1:A:224:ARG:HB2	1:A:250:LYS:HB3	1.90	0.52
1:A:132:ASP:O	1:A:135:VAL:N	2.40	0.52
1:A:46:SER:O	1:A:47:ILE:C	2.53	0.52
1:A:142:ILE:HA	1:A:190:THR:O	2.09	0.52
1:A:329:LEU:C	1:A:330:GLY:O	2.53	0.51
1:A:44:THR:HB	1:A:49:LEU:HD23	1.92	0.51
1:A:175:GLN:O	1:A:178:ARG:N	2.30	0.51
1:A:148:VAL:HG12	1:A:148:VAL:O	2.09	0.51
1:A:125:GLU:OE2	1:A:153:PRO:HA	2.11	0.51
1:A:323:LYS:HE3	1:A:335:VAL:HG11	1.94	0.50
1:A:153:PRO:HG3	1:A:172:LEU:HD11	1.92	0.50
1:A:156:GLU:C	1:A:158:GLU:H	2.18	0.50
1:A:84:ASN:O	1:A:85:ALA:C	2.55	0.50
1:A:276:LEU:HD22	1:A:276:LEU:N	2.27	0.50
1:A:340:ASP:O	1:A:341:ASP:CB	2.60	0.50
1:A:67:TYR:OH	1:A:226:ASP:HB2	2.12	0.50
1:A:148:VAL:HB	1:A:195:ASN:OD1	2.12	0.50
1:A:67:TYR:CZ	1:A:226:ASP:HB2	2.47	0.50
1:A:254:SER:O	1:A:255:PRO:C	2.54	0.50
1:A:178:ARG:HG2	1:A:178:ARG:HH11	1.77	0.49
1:A:140:LEU:H	1:A:140:LEU:CD2	2.25	0.49
1:A:308:ARG:O	1:A:312:LEU:HG	2.11	0.49
1:A:276:LEU:O	1:A:280:GLY:N	2.45	0.49
4:A:1322:CIT:O4	4:A:1322:CIT:O7	2.26	0.49
1:A:70:GLU:HA	3:A:832:DTP:O2G	2.11	0.49
1:A:39:ILE:H	1:A:39:ILE:CD1	2.21	0.49
1:A:94:PHE:CE1	1:A:101:LEU:HD13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:MET:C	1:A:182:GLY:N	2.70	0.49
1:A:293:PHE:HE2	1:A:304:LYS:N	2.10	0.49
1:A:47:ILE:HG21	1:A:279:MET:HG2	1.94	0.49
1:A:292:TRP:CD1	1:A:292:TRP:H	2.29	0.49
1:A:62:ARG:HH21	1:A:62:ARG:HG3	1.78	0.49
1:A:344:PRO:O	1:A:345:ALA:CB	2.59	0.49
1:A:40:SER:HB2	1:A:60:ARG:HD2	1.94	0.49
1:A:61:GLY:HA2	1:A:184:LEU:O	2.12	0.49
1:A:240:VAL:O	1:A:266:TYR:HD2	1.95	0.49
1:A:240:VAL:C	1:A:266:TYR:HD2	2.20	0.48
1:A:327:GLU:CD	1:A:336:THR:HA	2.38	0.48
1:A:60:ARG:HA	1:A:190:THR:HG22	1.94	0.48
1:A:345:ALA:O	1:A:346:PRO:C	2.47	0.48
1:A:75:THR:O	1:A:78:ALA:HB3	2.13	0.48
1:A:142:ILE:HG23	1:A:142:ILE:O	2.12	0.48
1:A:153:PRO:O	1:A:154:ARG:C	2.56	0.48
1:A:60:ARG:HH12	1:A:141:ASP:CG	2.21	0.48
1:A:29:MET:HE1	1:A:254:SER:HA	1.96	0.48
1:A:335:VAL:O	1:A:337:ALA:N	2.47	0.48
1:A:276:LEU:H	1:A:276:LEU:CD2	2.26	0.48
1:A:125:GLU:OE2	1:A:125:GLU:N	2.46	0.47
1:A:75:THR:O	1:A:76:THR:C	2.57	0.47
1:A:345:ALA:HB3	5:A:499:HOH:O	2.14	0.47
1:A:67:TYR:CD1	1:A:67:TYR:C	2.91	0.47
1:A:265:LEU:CD2	1:A:271:SER:HB2	2.45	0.47
1:A:226:ASP:OD2	1:A:226:ASP:C	2.57	0.47
1:A:327:GLU:CG	1:A:336:THR:HA	2.44	0.47
1:A:74:LYS:N	3:A:832:DTP:O2B	2.48	0.47
1:A:263:ASP:HB2	1:A:271:SER:HB3	1.97	0.47
1:A:265:LEU:O	1:A:266:TYR:C	2.57	0.47
1:A:125:GLU:OE1	1:A:154:ARG:N	2.46	0.47
1:A:283:HIS:ND1	3:A:833:DTP:O3'	2.48	0.47
1:A:49:LEU:HD13	1:A:246:VAL:HG11	1.97	0.47
1:A:153:PRO:HG2	1:A:168:LEU:CB	2.45	0.47
1:A:70:GLU:HG3	1:A:71:SER:H	1.81	0.46
1:A:153:PRO:HA	1:A:172:LEU:HD11	1.98	0.46
1:A:128:LEU:O	1:A:131:ALA:HB3	2.16	0.46
1:A:347:VAL:O	1:A:348:ASP:CB	2.63	0.46
1:A:145:ILE:N	1:A:145:ILE:HD12	2.31	0.46
1:A:175:GLN:O	1:A:176:ALA:C	2.59	0.46
1:A:180:MET:HE3	1:A:180:MET:HB2	1.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HG21	1:A:28:VAL:CG2	2.46	0.46
1:A:78:ALA:C	1:A:82:VAL:HG23	2.41	0.46
1:A:136:ARG:HH21	1:A:179:LYS:CG	2.25	0.46
1:A:327:GLU:HG3	1:A:336:THR:HA	1.98	0.46
1:A:148:VAL:HG13	1:A:173:MET:SD	2.56	0.45
1:A:132:ASP:CA	1:A:180:MET:HE2	2.46	0.45
1:A:31:LEU:O	1:A:255:PRO:CB	2.65	0.45
1:A:153:PRO:CG	1:A:172:LEU:HD11	2.46	0.45
1:A:74:LYS:HB2	1:A:74:LYS:NZ	2.31	0.45
1:A:74:LYS:O	1:A:75:THR:C	2.58	0.45
1:A:230:ILE:HD12	1:A:243:ARG:CG	2.47	0.45
1:A:323:LYS:HZ1	1:A:335:VAL:HG21	1.81	0.45
1:A:47:ILE:HG23	1:A:279:MET:HG2	1.99	0.45
1:A:295:TYR:O	1:A:296:GLU:C	2.60	0.44
1:A:64:ILE:HG23	1:A:223:VAL:CG1	2.48	0.44
1:A:144:VAL:C	1:A:145:ILE:HD12	2.42	0.44
1:A:281:VAL:HG23	1:A:282:GLU:N	2.30	0.44
1:A:289:SER:C	1:A:291:SER:O	2.61	0.44
1:A:333:ALA:HB1	1:A:334:VAL:HG23	1.99	0.44
1:A:265:LEU:N	1:A:265:LEU:HD22	2.32	0.44
1:A:122:ASP:O	1:A:123:THR:HG23	2.16	0.44
1:A:175:GLN:O	1:A:177:LEU:N	2.50	0.44
1:A:325:ILE:C	1:A:327:GLU:H	2.25	0.44
1:A:136:ARG:HG2	1:A:136:ARG:HH11	1.82	0.44
1:A:226:ASP:O	1:A:246:VAL:HA	2.18	0.44
1:A:230:ILE:HD12	1:A:243:ARG:HG3	1.99	0.44
1:A:248:VAL:O	1:A:248:VAL:HG13	2.18	0.43
1:A:224:ARG:HD3	1:A:250:LYS:HD3	2.00	0.43
1:A:3:GLN:O	1:A:4:GLN:CB	2.66	0.43
1:A:70:GLU:HG3	1:A:71:SER:N	2.32	0.43
1:A:121:PRO:CG	1:A:127:ALA:HB2	2.48	0.43
1:A:152:VAL:HA	1:A:153:PRO:HD3	1.81	0.43
1:A:67:TYR:C	1:A:74:LYS:HD3	2.43	0.43
1:A:327:GLU:OE2	1:A:335:VAL:CG1	2.64	0.43
1:A:180:MET:C	1:A:182:GLY:H	2.25	0.43
1:A:281:VAL:C	1:A:283:HIS:N	2.76	0.43
1:A:98:GLU:CG	1:A:147:SER:HB2	2.49	0.43
1:A:264:ILE:HA	1:A:270:ILE:HA	2.00	0.43
1:A:49:LEU:CD1	1:A:246:VAL:HG11	2.49	0.43
1:A:147:SER:O	1:A:151:LEU:HD21	2.19	0.43
1:A:285:PHE:CE1	1:A:325:ILE:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:PHE:O	1:A:300:LEU:HB2	2.18	0.43
1:A:278:ASP:O	1:A:282:GLU:HB2	2.20	0.42
1:A:333:ALA:HB1	1:A:334:VAL:H	1.23	0.42
1:A:294:THR:HA	1:A:299:GLN:HA	2.00	0.42
1:A:23:PHE:CB	1:A:27:SER:OG	2.66	0.42
1:A:216:ALA:O	1:A:217:LEU:C	2.62	0.42
1:A:253:VAL:HG12	1:A:253:VAL:O	2.18	0.42
1:A:279:MET:HE1	3:A:833:DTP:O3'	2.18	0.42
3:A:833:DTP:N3	3:A:833:DTP:H5'1	2.34	0.42
1:A:148:VAL:HA	1:A:151:LEU:HD23	2.01	0.42
1:A:289:SER:CB	1:A:293:PHE:CD1	3.03	0.42
1:A:323:LYS:O	1:A:324:LYS:C	2.63	0.42
1:A:52:ALA:HB2	1:A:260:ALA:HB2	2.01	0.42
1:A:102:ASP:HA	1:A:103:PRO:HD2	1.80	0.42
1:A:24:GLY:HA3	4:A:1322:CIT:C6	2.50	0.42
1:A:256:PRO:HG2	1:A:257:PHE:CD2	2.55	0.41
1:A:53:LEU:HD13	1:A:58:LEU:HD23	2.02	0.41
1:A:59:PRO:HB2	1:A:62:ARG:HD3	2.02	0.41
1:A:156:GLU:C	1:A:158:GLU:N	2.78	0.41
1:A:42:ILE:HD11	1:A:190:THR:HG21	2.03	0.41
1:A:177:LEU:CD2	1:A:217:LEU:HA	2.50	0.41
1:A:287:ARG:HG2	1:A:287:ARG:NH1	2.34	0.41
1:A:265:LEU:CB	1:A:268:GLN:HB2	2.45	0.41
1:A:262:PHE:CE1	1:A:270:ILE:HG12	2.56	0.41
1:A:15:ALA:O	1:A:18:GLN:N	2.54	0.41
1:A:273:GLU:O	1:A:274:GLY:C	2.63	0.41
1:A:317:VAL:HG13	1:A:318:ALA:N	2.35	0.41
1:A:326:LYS:HE2	1:A:331:ILE:HD13	2.03	0.41
1:A:157:ILE:O	1:A:157:ILE:CG1	2.61	0.41
1:A:232:THR:O	1:A:233:LEU:C	2.63	0.40
1:A:288:LYS:HB3	1:A:289:SER:H	1.43	0.40
1:A:338:GLU:O	1:A:339:ALA:HB2	2.21	0.40
1:A:47:ILE:CG2	1:A:48:SER:N	2.85	0.40
1:A:64:ILE:HD13	1:A:223:VAL:HB	2.03	0.40
1:A:325:ILE:C	1:A:327:GLU:N	2.80	0.40
1:A:132:ASP:HA	1:A:135:VAL:HB	2.04	0.40
1:A:31:LEU:O	1:A:255:PRO:HB3	2.22	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	325/349 (93%)	233 (72%)	58 (18%)	34 (10%)	0 2

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	4	GLN
1	A	5	ALA
1	A	168	LEU
1	A	197	LEU
1	A	235	ASP
1	A	238	ASP
1	A	292	TRP
1	A	330	GLY
1	A	331	ILE
1	A	336	THR
1	A	344	PRO
1	A	6	PRO
1	A	140	LEU
1	A	175	GLN
1	A	176	ALA
1	A	212	THR
1	A	233	LEU
1	A	288	LYS
1	A	335	VAL
1	A	338	GLU
1	A	339	ALA
1	A	341	ASP
1	A	345	ALA
1	A	348	ASP
1	A	9	GLU
1	A	141	ASP
1	A	340	ASP

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Mol	Chain	Res	Type
1	A	343	LEU
1	A	15	ALA
1	A	147	SER
1	A	103	PRO
1	A	342	VAL
1	A	256	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	235/275 (86%)	198 (84%)	37 (16%)	2 13

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	7	ASP
1	A	8	ARG
1	A	10	LYS
1	A	13	GLU
1	A	25	LYS
1	A	34	GLU
1	A	39	ILE
1	A	51	VAL
1	A	62	ARG
1	A	63	VAL
1	A	70	GLU
1	A	76	THR
1	A	108	LYS
1	A	116	LEU
1	A	132	ASP
1	A	134	LEU
1	A	140	LEU
1	A	147	SER
1	A	157	ILE

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Mol	Chain	Res	Type
1	A	166	VAL
1	A	190	THR
1	A	195	ASN
1	A	212	THR
1	A	235	ASP
1	A	245	ARG
1	A	247	LYS
1	A	252	LYS
1	A	261	GLU
1	A	268	GLN
1	A	282	GLU
1	A	283	HIS
1	A	288	LYS
1	A	291	SER
1	A	300	LEU
1	A	335	VAL
1	A	340	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	22	ASN
1	A	37	GLN
1	A	120	GLN
1	A	126	GLN
1	A	186	ASN
1	A	268	GLN
1	A	283	HIS
1	A	302	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is 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$
3	DTP	A	832	-	31,32,32	3.04	15 (48%)	46,50,50	2.30	15 (32%)
3	DTP	A	833	2	31,32,32	2.46	14 (45%)	46,50,50	2.80	14 (30%)
4	CIT	A	1322	-	12,12,12	3.88	6 (50%)	17,17,17	4.88	9 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTP	A	832	-	-	8/22/34/34	0/3/3/3
3	DTP	A	833	2	-	8/22/34/34	0/3/3/3
4	CIT	A	1322	-	-	10/16/16/16	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1322	CIT	C3-C6	9.92	1.63	1.53
3	A	832	DTP	C1'-N9	7.67	1.61	1.46
3	A	832	DTP	C2-N3	6.32	1.45	1.33
4	A	1322	CIT	O7-C3	-6.28	1.31	1.43
3	A	833	DTP	PB-O3A	5.78	1.65	1.59
3	A	832	DTP	C5-N7	-5.64	1.28	1.39
3	A	832	DTP	C4-N3	5.29	1.44	1.34
3	A	833	DTP	PB-O3B	4.93	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	833	DTP	PA-O3A	4.66	1.64	1.59
3	A	832	DTP	C4-N9	4.31	1.46	1.37
3	A	832	DTP	PG-O2G	-4.15	1.39	1.54
3	A	833	DTP	PA-O5'	-3.79	1.44	1.59
4	A	1322	CIT	C2-C3	-3.78	1.49	1.54
3	A	833	DTP	PG-O2G	-3.71	1.41	1.54
3	A	832	DTP	PA-O5'	-3.63	1.45	1.59
3	A	832	DTP	PB-O2B	-3.46	1.39	1.55
3	A	833	DTP	C2'-C3'	-3.42	1.44	1.52
3	A	833	DTP	C8-N9	-3.36	1.31	1.37
3	A	832	DTP	PA-O3A	3.29	1.63	1.59
4	A	1322	CIT	O2-C1	-3.08	1.20	1.30
3	A	833	DTP	PB-O2B	-3.03	1.41	1.55
3	A	832	DTP	C2-N1	2.96	1.39	1.33
3	A	833	DTP	C4-N3	2.60	1.39	1.34
3	A	833	DTP	C4-N9	2.58	1.43	1.37
4	A	1322	CIT	O1-C1	2.58	1.30	1.22
3	A	832	DTP	C5'-C4'	2.51	1.59	1.51
4	A	1322	CIT	O3-C5	2.47	1.30	1.22
3	A	833	DTP	O3'-C3'	-2.43	1.38	1.43
3	A	832	DTP	C8-N9	2.42	1.41	1.37
3	A	832	DTP	PB-O3A	2.35	1.62	1.59
3	A	832	DTP	O3'-C3'	-2.34	1.38	1.43
3	A	833	DTP	C5-N7	-2.17	1.35	1.39
3	A	833	DTP	PA-O2A	-2.13	1.45	1.55
3	A	833	DTP	C2-N3	2.10	1.37	1.33
3	A	832	DTP	C5-C6	2.06	1.46	1.41

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1322	CIT	C2-C3-C6	13.91	140.79	110.03
4	A	1322	CIT	O7-C3-C6	-7.70	98.03	108.96
3	A	833	DTP	C2'-C1'-N9	-7.43	97.16	114.63
3	A	833	DTP	O3A-PA-O1A	-7.31	88.72	110.70
3	A	833	DTP	O2A-PA-O3A	7.18	126.69	107.27
3	A	833	DTP	O4'-C1'-N9	6.99	120.52	107.96
3	A	832	DTP	N3-C4-N9	6.18	137.68	127.17
4	A	1322	CIT	O5-C6-C3	6.13	133.98	122.09
4	A	1322	CIT	C4-C3-C6	-5.69	97.45	110.03
3	A	833	DTP	O3B-PB-O1B	5.22	126.41	110.70
3	A	832	DTP	N9-C8-N7	-4.67	107.30	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1322	CIT	O6-C6-C3	-4.61	104.30	113.14
3	A	833	DTP	O2B-PB-O3B	-4.46	95.21	107.27
3	A	832	DTP	O4'-C1'-N9	-4.40	100.06	107.96
3	A	832	DTP	C5-N7-C8	4.27	110.16	103.45
4	A	1322	CIT	O7-C3-C4	4.25	119.08	109.38
3	A	832	DTP	C5-C4-N3	-4.20	120.94	126.72
3	A	832	DTP	C5-C4-N9	-4.10	101.34	105.81
3	A	832	DTP	O2A-PA-O3A	3.90	117.80	107.27
3	A	833	DTP	O5'-C5'-C4'	3.78	121.86	108.99
4	A	1322	CIT	O7-C3-C2	-3.58	101.21	109.38
3	A	833	DTP	O5'-PA-O1A	-3.51	95.02	108.94
3	A	832	DTP	O4'-C4'-C5'	3.45	120.37	109.33
4	A	1322	CIT	C3-C2-C1	3.37	123.14	113.92
3	A	833	DTP	N3-C4-N9	3.12	132.47	127.17
3	A	833	DTP	C5-C4-N9	-3.05	102.48	105.81
3	A	832	DTP	C6-C5-N7	-3.04	126.23	132.09
3	A	832	DTP	O3A-PA-O1A	-3.04	101.57	110.70
3	A	832	DTP	C4-C5-N7	2.84	113.83	110.58
3	A	833	DTP	O2B-PB-O3A	-2.72	99.93	107.27
4	A	1322	CIT	C4-C3-C2	-2.70	102.40	109.31
3	A	832	DTP	C2'-C3'-C4'	2.57	108.01	102.80
3	A	832	DTP	O5'-C5'-C4'	2.52	117.58	108.99
3	A	833	DTP	O2G-PG-O1G	-2.41	101.46	110.83
3	A	833	DTP	O4'-C4'-C5'	-2.28	102.03	109.33
3	A	832	DTP	C4'-O4'-C1'	2.20	114.74	109.51
3	A	832	DTP	C2'-C1'-N9	2.13	119.63	114.63
3	A	833	DTP	C3'-C2'-C1'	2.07	107.66	102.60

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	833	DTP	PB-O3B-PG-O3G
4	A	1322	CIT	C6-C3-C4-C5
4	A	1322	CIT	O7-C3-C6-O5
4	A	1322	CIT	O7-C3-C6-O6
4	A	1322	CIT	C4-C3-C6-O5
4	A	1322	CIT	C4-C3-C6-O6
3	A	833	DTP	O4'-C4'-C5'-O5'
3	A	833	DTP	O4'-C1'-N9-C8
3	A	832	DTP	PB-O3B-PG-O1G
3	A	833	DTP	PB-O3B-PG-O1G

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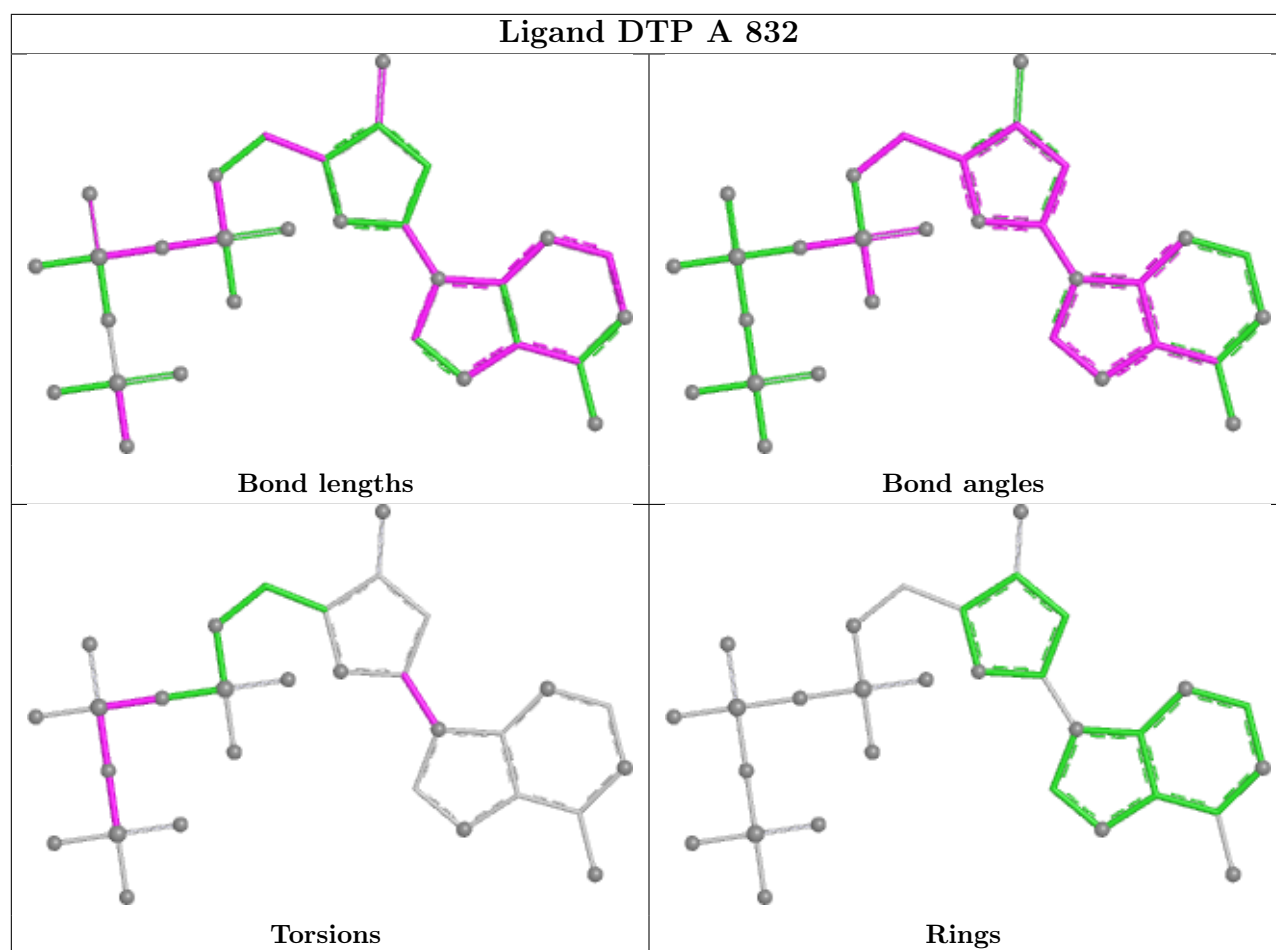
Mol	Chain	Res	Type	Atoms
3	A	832	DTP	PG-O3B-PB-O1B
3	A	832	DTP	PA-O3A-PB-O1B
4	A	1322	CIT	O2-C1-C2-C3
4	A	1322	CIT	O1-C1-C2-C3
3	A	833	DTP	PG-O3B-PB-O1B
4	A	1322	CIT	C3-C4-C5-O4
3	A	832	DTP	PB-O3B-PG-O3G
4	A	1322	CIT	C3-C4-C5-O3
3	A	832	DTP	PA-O3A-PB-O2B
3	A	833	DTP	PB-O3A-PA-O2A
3	A	832	DTP	C2'-C1'-N9-C4
3	A	832	DTP	O4'-C1'-N9-C4
3	A	833	DTP	O4'-C1'-N9-C4
4	A	1322	CIT	O7-C3-C4-C5
3	A	832	DTP	PG-O3B-PB-O2B
3	A	833	DTP	PG-O3B-PB-O2B

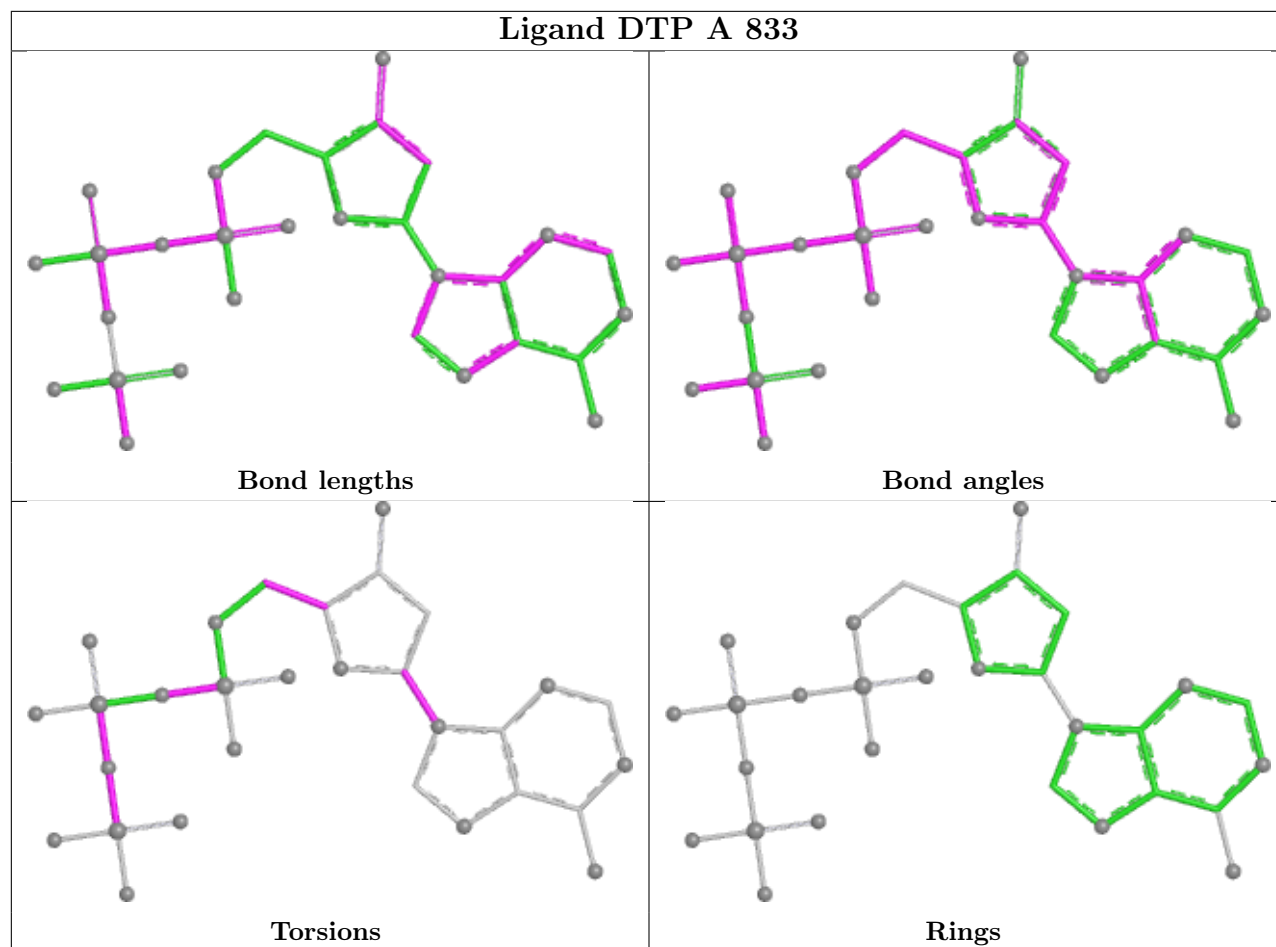
There are no ring outliers.

3 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	832	DTP	8	0
3	A	833	DTP	9	0
4	A	1322	CIT	4	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 than 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, 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	331/349 (94%)	-1.79	0 100 100	5, 41, 96, 100	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

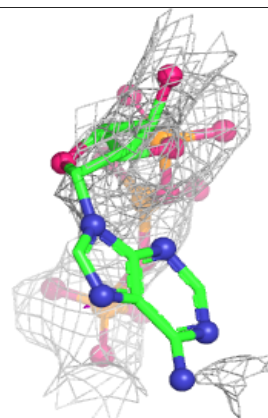
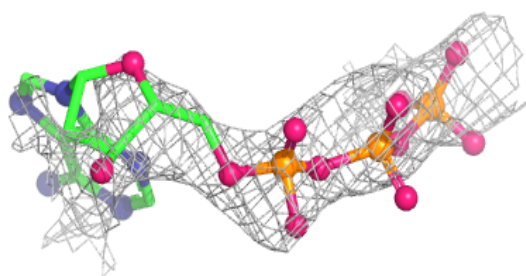
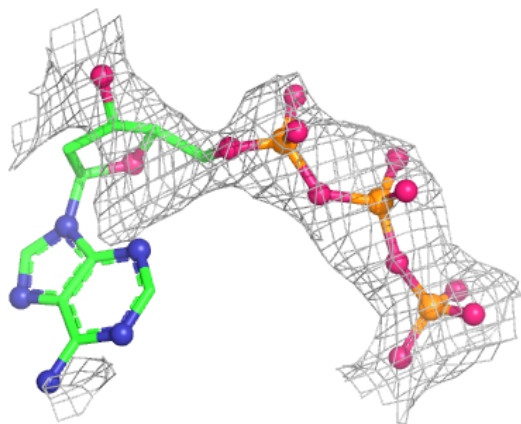
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	2633	1/1	0.99	0.02	40,40,40,40	0
3	DTP	A	833	30/30	0.99	0.04	99,99,99,99	0
4	CIT	A	1322	13/13	0.99	0.03	97,97,97,97	0
3	DTP	A	832	30/30	1.00	0.03	69,69,69,69	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.

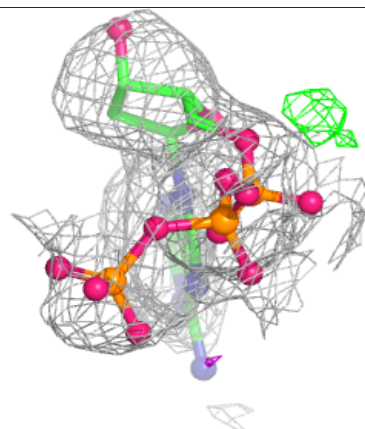
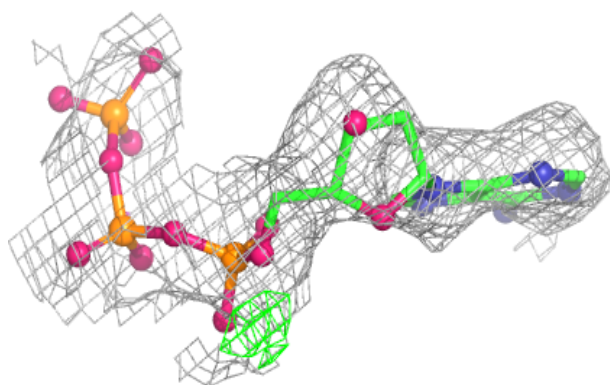
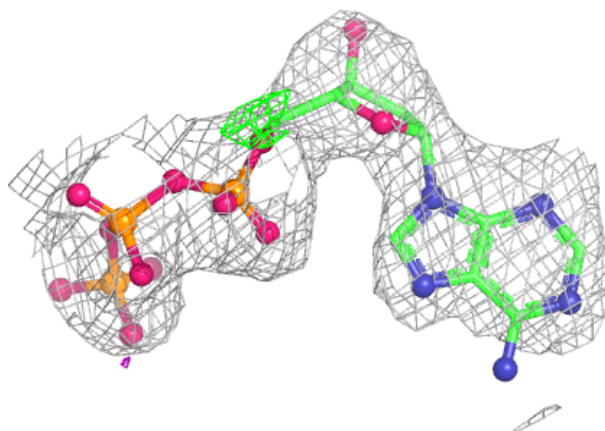
Electron density around DTP A 833:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DTP A 832:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.