



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:47 PM UTC

PDB ID : 4A57 / pdb_00004a57
Title : CRYSTAL STRUCTURE OF TOXOPLASMA GONDII NUCLEOSIDE
TRIPHOSPHATE DIPHOSPHOHYDROLASE 3 (NTPDASE3)
Authors : Krug, U.; Zebisch, M.; Straeter, N.
Deposited on : 2011-10-24
Resolution : 2.00 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
Xtriage (Phenix) : 2.0
EDS : 3.0
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

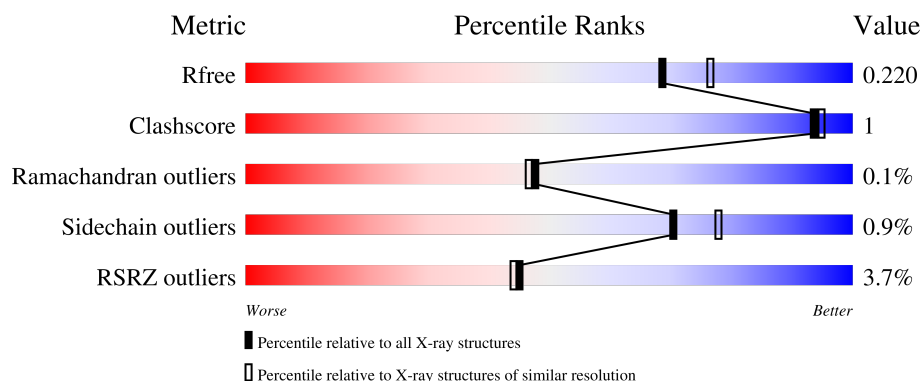
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	611	3% 90% 7% .
1	B	611	6% 92% 5% .
1	C	611	% 91% 5% .
1	D	611	5% 92% 5% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19870 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 NUCLEOSIDE-TRIPHOSPHATASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	6	0
			4640	2916	823	874	27			
1	B	594	Total	C	N	O	S	0	3	0
			4617	2905	813	872	27			
1	C	591	Total	C	N	O	S	0	4	0
			4611	2898	817	869	27			
1	D	595	Total	C	N	O	S	0	2	0
			4624	2905	817	875	27			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	expression tag	UNP Q27893
A	629	GLU	-	expression tag	UNP Q27893
A	630	HIS	-	expression tag	UNP Q27893
A	631	HIS	-	expression tag	UNP Q27893
A	632	HIS	-	expression tag	UNP Q27893
A	633	HIS	-	expression tag	UNP Q27893
A	634	HIS	-	expression tag	UNP Q27893
A	635	HIS	-	expression tag	UNP Q27893
B	25	MET	-	expression tag	UNP Q27893
B	629	GLU	-	expression tag	UNP Q27893
B	630	HIS	-	expression tag	UNP Q27893
B	631	HIS	-	expression tag	UNP Q27893
B	632	HIS	-	expression tag	UNP Q27893
B	633	HIS	-	expression tag	UNP Q27893
B	634	HIS	-	expression tag	UNP Q27893
B	635	HIS	-	expression tag	UNP Q27893
C	25	MET	-	expression tag	UNP Q27893
C	629	GLU	-	expression tag	UNP Q27893
C	630	HIS	-	expression tag	UNP Q27893
C	631	HIS	-	expression tag	UNP Q27893
C	632	HIS	-	expression tag	UNP Q27893

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Chain	Residue	Modelled	Actual	Comment	Reference
C	633	HIS	-	expression tag	UNP Q27893
C	634	HIS	-	expression tag	UNP Q27893
C	635	HIS	-	expression tag	UNP Q27893
D	25	MET	-	expression tag	UNP Q27893
D	629	GLU	-	expression tag	UNP Q27893
D	630	HIS	-	expression tag	UNP Q27893
D	631	HIS	-	expression tag	UNP Q27893
D	632	HIS	-	expression tag	UNP Q27893
D	633	HIS	-	expression tag	UNP Q27893
D	634	HIS	-	expression tag	UNP Q27893
D	635	HIS	-	expression tag	UNP Q27893

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cl 3 3	0	0
2	C	1	Total Cl 1 1	0	0

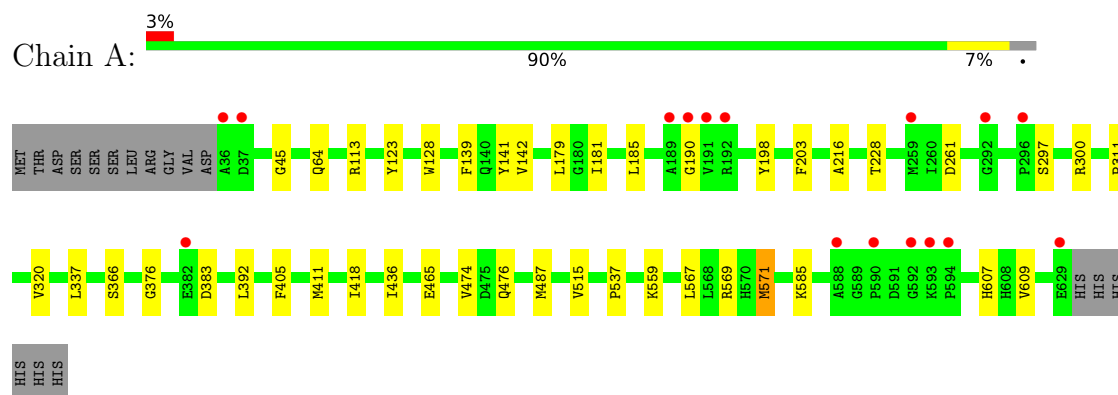
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	451	Total O 452 452	0	1
3	B	306	Total O 307 307	0	1
3	C	366	Total O 366 366	0	0
3	D	248	Total O 249 249	0	1

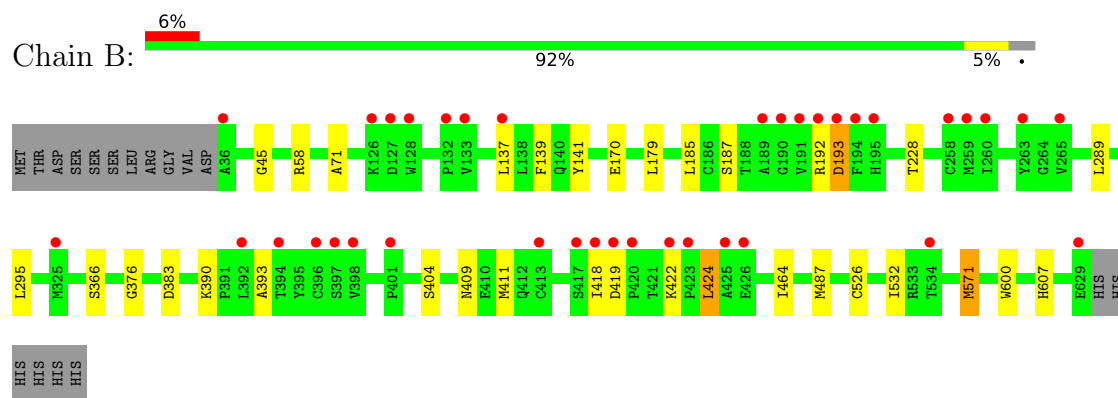
3 Residue-property plots

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.

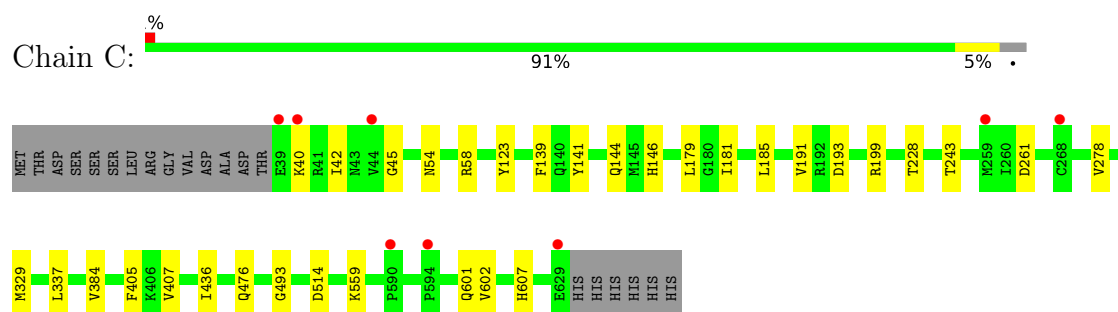
• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1



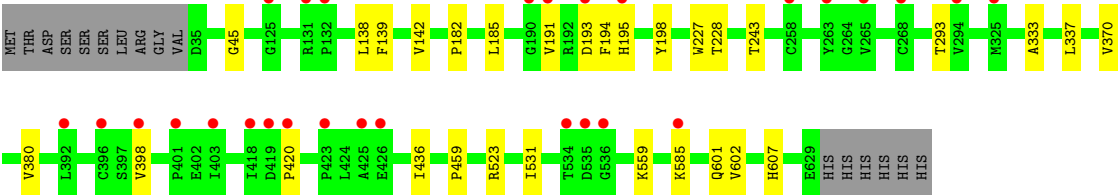
• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1



• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1



• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.96Å 165.94Å 97.51Å 90.00° 97.03° 90.00°	Depositor
Resolution (Å)	39.43 – 2.00 39.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.43-2.00) 97.1 (39.43-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.174 , 0.210 0.179 , 0.220	Depositor DCC
R_{free} test set	1844 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19870	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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:
CL

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	0.85	2/4748 (0.0%)	1.18	9/6424 (0.1%)
1	B	0.83	1/4716 (0.0%)	1.23	9/6384 (0.1%)
1	C	0.84	0/4711	1.18	15/6374 (0.2%)
1	D	0.84	1/4719 (0.0%)	1.20	6/6386 (0.1%)
All	All	0.84	4/18894 (0.0%)	1.20	39/25568 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	571	MET	SD-CE	-6.68	1.62	1.79
1	B	571	MET	SD-CE	-6.32	1.63	1.79
1	A	142	VAL	CA-C	6.18	1.57	1.52
1	D	142	VAL	CA-C	5.08	1.57	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	ASP	N-CA-C	7.88	122.61	112.92
1	A	405	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	383	ASP	CA-CB-CG	6.85	119.45	112.60
1	B	141	TYR	CA-C-N	6.38	124.26	120.24
1	B	141	TYR	C-N-CA	6.38	124.26	120.24
1	C	141	TYR	CA-C-N	6.38	124.26	120.24
1	C	141	TYR	C-N-CA	6.38	124.26	120.24
1	A	320	VAL	N-CA-C	-6.12	99.77	108.58
1	C	601	GLN	N-CA-C	5.93	117.42	111.07
1	C	407	VAL	N-CA-C	5.92	116.57	110.36
1	D	194	PHE	N-CA-C	5.91	118.67	111.82
1	C	193	ASP	N-CA-C	5.77	119.30	112.72
1	A	203	PHE	CA-CB-CG	-5.77	108.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	198	TYR	N-CA-C	5.74	118.02	111.02
1	B	192	ARG	N-CA-C	5.74	118.31	111.71
1	C	146	HIS	CA-C-N	5.73	128.27	120.54
1	C	146	HIS	C-N-CA	5.73	128.27	120.54
1	A	198	TYR	N-CA-C	5.72	117.98	111.11
1	D	193	ASP	N-CA-C	5.67	119.82	113.02
1	A	585	LYS	N-CA-C	-5.61	106.57	113.41
1	C	405	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	261	ASP	CA-CB-CG	5.53	118.13	112.60
1	C	261	ASP	CA-CB-CG	5.53	118.13	112.60
1	C	40	LYS	CA-C-N	5.51	128.69	120.31
1	C	40	LYS	C-N-CA	5.51	128.69	120.31
1	D	601	GLN	N-CA-C	5.50	116.95	111.07
1	C	181	ILE	N-CA-C	5.45	113.54	108.15
1	C	514	ASP	CA-C-N	5.44	127.61	120.60
1	C	514	ASP	C-N-CA	5.44	127.61	120.60
1	B	170	GLU	N-CA-C	5.42	117.19	111.28
1	D	195	HIS	N-CA-C	5.35	119.64	113.38
1	A	181	ILE	N-CA-C	5.34	113.44	108.15
1	A	216	ALA	N-CA-C	5.31	117.48	111.11
1	B	600	TRP	N-CA-C	5.28	118.98	112.54
1	B	383	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	409	ASN	N-CA-C	5.21	117.36	111.11
1	B	424	LEU	N-CA-C	5.16	119.84	111.37
1	D	585	LYS	N-CA-C	-5.04	105.45	112.45
1	C	179	LEU	N-CA-C	5.03	117.65	111.82

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	4640	0	4632	20	0
1	B	4617	0	4600	16	0
1	C	4611	0	4590	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4624	0	4599	10	0
2	A	3	0	0	2	0
2	C	1	0	0	1	0
3	A	452	0	0	0	0
3	B	307	0	0	1	0
3	C	366	0	0	0	0
3	D	249	0	0	1	0
All	All	19870	0	18421	50	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 1.

All (50) 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:B:419:ASP:HB3	1:B:422:LYS:HD3	1.55	0.89
1:A:300[A]:ARG:HG3	1:B:464:ILE:HD12	1.68	0.76
1:A:476:GLN:HG3	2:A:1630:CL:CL	2.30	0.69
1:B:289:LEU:HD11	1:B:295[A]:LEU:HD21	1.75	0.67
1:B:487:MET:HG3	1:B:571:MET:HE1	1.79	0.65
1:A:411:MET:HE1	1:B:411:MET:HE1	1.79	0.64
1:A:487:MET:HG3	1:A:571:MET:HE1	1.79	0.64
1:A:113:ARG:HB2	1:A:190:GLY:O	2.00	0.62
1:B:185:LEU:HB3	1:B:228:THR:HG23	1.88	0.55
1:A:45:GLY:HA3	1:D:139:PHE:O	2.08	0.54
1:D:459:PRO:HD2	3:D:2182:HOH:O	2.09	0.53
1:B:45:GLY:HA3	1:C:139:PHE:O	2.11	0.50
1:D:243:THR:HG23	1:D:602:VAL:HB	1.95	0.48
1:A:185:LEU:HB3	1:A:228:THR:HG23	1.96	0.48
1:C:337:LEU:HD22	1:C:436:ILE:HD13	1.96	0.48
1:D:185:LEU:HB3	1:D:228:THR:HG23	1.95	0.47
1:C:123:TYR:OH	1:C:144:GLN:HG2	2.15	0.46
1:A:64:GLN:HB2	1:A:179:LEU:HD12	1.97	0.46
1:B:376:GLY:HA3	1:B:532:ILE:HD12	1.96	0.46
1:C:54:ASN:HB3	1:C:58:ARG:HE	1.81	0.46
1:C:191:VAL:O	1:C:199:ARG:HD3	2.16	0.46
1:A:411:MET:HE1	1:B:411:MET:CE	2.44	0.45
1:C:476:GLN:HG3	2:C:1630:CL:CL	2.53	0.45
1:A:515:VAL:HG11	1:A:569:ARG:HG3	1.99	0.45
1:D:398:VAL:HG13	1:D:420:PRO:HB2	1.99	0.45
1:C:329:MET:HE3	1:C:493:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:PHE:O	1:C:45:GLY:HA3	2.16	0.45
1:A:311:PRO:HB2	2:A:1631:CL:CL	2.54	0.45
1:A:392:LEU:HB3	1:A:418:ILE:HD13	1.99	0.45
1:A:487:MET:HG3	1:A:571:MET:CE	2.47	0.44
1:B:390:LYS:HE2	1:B:424:LEU:HD21	1.99	0.44
1:D:370:VAL:HG22	1:D:380:VAL:HG22	2.00	0.43
1:A:123:TYR:HB3	1:A:141:TYR:CD2	2.53	0.43
1:A:474:VAL:HG11	1:A:567:LEU:CD2	2.49	0.43
1:B:393:ALA:HA	1:B:418:ILE:HG21	2.01	0.43
1:A:139:PHE:O	1:D:45:GLY:HA3	2.19	0.43
1:D:337:LEU:HD22	1:D:436:ILE:HD13	2.00	0.43
1:D:333:ALA:HA	1:D:559:LYS:HE2	2.01	0.42
1:B:137:LEU:HD23	1:C:42:ILE:HD11	2.02	0.42
1:C:185:LEU:HB3	1:C:228:THR:HG23	2.02	0.42
1:C:243:THR:HG23	1:C:602:VAL:HB	2.01	0.41
1:D:182:PRO:HB3	1:D:227:TRP:CZ3	2.55	0.41
1:A:474:VAL:HG11	1:A:567:LEU:HD23	2.03	0.41
1:A:376:GLY:HA2	1:A:537:PRO:HG3	2.02	0.41
1:A:337:LEU:HD22	1:A:436:ILE:HD13	2.03	0.41
1:B:71:ALA:O	1:B:187:SER:HA	2.20	0.41
1:C:278:VAL:HG12	1:C:329:MET:HE2	2.01	0.41
1:B:411:MET:HE2	1:B:411:MET:HB3	1.96	0.40
1:B:526:CYS:HB3	3:B:2175:HOH:O	2.21	0.40
1:A:300[B]:ARG:HH22	1:A:465:GLU:C	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	598/611 (98%)	588 (98%)	8 (1%)	2 (0%)	36 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	595/611 (97%)	587 (99%)	8 (1%)	0	100	100
1	C	593/611 (97%)	584 (98%)	9 (2%)	0	100	100
1	D	595/611 (97%)	588 (99%)	7 (1%)	0	100	100
All	All	2381/2444 (97%)	2347 (99%)	32 (1%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	TRP
1	A	297	SER

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	511/521 (98%)	507 (99%)	4 (1%)	73	80
1	B	508/521 (98%)	501 (99%)	7 (1%)	59	66
1	C	507/521 (97%)	504 (99%)	3 (1%)	78	85
1	D	508/521 (98%)	502 (99%)	6 (1%)	63	70
All	All	2034/2084 (98%)	2014 (99%)	20 (1%)	70	75

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

Mol	Chain	Res	Type
1	A	366	SER
1	A	559	LYS
1	A	607	HIS
1	A	609	VAL
1	B	58	ARG
1	B	179[A]	LEU
1	B	179[B]	LEU
1	B	193	ASP
1	B	366	SER

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Mol	Chain	Res	Type
1	B	404	SER
1	B	607	HIS
1	C	384	VAL
1	C	559	LYS
1	C	607	HIS
1	D	138	LEU
1	D	191	VAL
1	D	293	THR
1	D	523	ARG
1	D	531	ILE
1	D	607	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	HIS
1	A	267	GLN
1	A	270	ASN
1	B	48	HIS
1	B	348	GLN
1	B	363	GLN
1	B	399	ASN
1	B	412	GLN
1	B	543	ASN
1	C	50	GLN
1	C	195	HIS
1	C	270	ASN
1	C	548	GLN
1	D	270	ASN
1	D	448	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, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	594/611 (97%)	-0.26	16 (2%) 56 55	10, 24, 55, 92	6 (1%)
1	B	594/611 (97%)	0.11	37 (6%) 26 25	16, 30, 64, 126	3 (0%)
1	C	591/611 (96%)	-0.26	8 (1%) 73 73	12, 25, 50, 88	4 (0%)
1	D	595/611 (97%)	0.04	28 (4%) 36 35	12, 31, 60, 81	2 (0%)
All	All	2374/2444 (97%)	-0.09	89 (3%) 45 44	10, 28, 59, 126	15 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	LYS	4.6
1	A	592	GLY	4.4
1	B	36	ALA	4.2
1	A	588	ALA	3.7
1	B	132	PRO	3.6
1	B	128	TRP	3.5
1	A	191	VAL	3.5
1	A	189	ALA	3.5
1	B	418	ILE	3.4
1	B	191	VAL	3.3
1	D	401	PRO	3.3
1	A	36	ALA	3.3
1	C	268	CYS	3.2
1	B	629	GLU	3.2
1	B	190	GLY	3.2
1	D	191	VAL	3.2
1	B	396	CYS	3.2
1	A	590	PRO	3.1
1	B	133	VAL	3.1
1	C	590	PRO	3.1
1	A	192	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	534	THR	3.0
1	B	127	ASP	3.0
1	B	417	SER	3.0
1	B	425	ALA	2.9
1	B	419	ASP	2.9
1	B	263	TYR	2.9
1	A	190	GLY	2.9
1	C	40	LYS	2.9
1	D	403	ILE	2.9
1	D	398	VAL	2.9
1	B	401	PRO	2.8
1	D	418	ILE	2.8
1	A	296	PRO	2.7
1	D	190	GLY	2.7
1	C	39	GLU	2.6
1	D	420	PRO	2.6
1	D	294	VAL	2.6
1	D	125	GLY	2.6
1	B	423	PRO	2.6
1	D	265	VAL	2.5
1	B	413	CYS	2.5
1	D	193	ASP	2.5
1	D	425	ALA	2.5
1	A	259	MET	2.5
1	B	259	MET	2.5
1	D	263	TYR	2.5
1	D	535	ASP	2.5
1	A	629	GLU	2.5
1	B	392	LEU	2.5
1	C	259	MET	2.5
1	A	593	LYS	2.5
1	D	423	PRO	2.4
1	D	258	CYS	2.4
1	B	397	SER	2.4
1	B	422	LYS	2.4
1	D	585	LYS	2.4
1	B	260	ILE	2.4
1	B	265	VAL	2.4
1	D	195	HIS	2.4
1	D	426	GLU	2.3
1	B	192	ARG	2.3
1	B	258	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	594	PRO	2.3
1	B	137	LEU	2.3
1	A	382	GLU	2.3
1	D	131	ARG	2.3
1	D	325	MET	2.3
1	D	419	ASP	2.2
1	A	594	PRO	2.2
1	D	132	PRO	2.2
1	D	268	CYS	2.2
1	D	396	CYS	2.2
1	B	534	THR	2.2
1	C	629	GLU	2.2
1	A	37	ASP	2.2
1	B	195	HIS	2.1
1	B	189	ALA	2.1
1	B	394	THR	2.1
1	D	536	GLY	2.1
1	B	426	GLU	2.1
1	B	420	PRO	2.1
1	B	194	PHE	2.1
1	C	44	VAL	2.1
1	D	392	LEU	2.1
1	B	325	MET	2.0
1	B	193	ASP	2.0
1	B	398	VAL	2.0
1	A	292	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
2	CL	A	1632	1/1	0.86	0.23	36,36,36,36	1
2	CL	A	1631	1/1	0.97	0.14	29,29,29,29	1
2	CL	A	1630	1/1	0.97	0.07	32,32,32,32	0
2	CL	C	1630	1/1	0.98	0.12	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.