



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:43 AM UTC

PDB ID : 5EWN / pdb_00005ewn
Title : Crystal structure of the human astrovirus 1 capsid protein core domain at 2.6 Å resolution
Authors : York, R.L.; Yousefi, P.A.; Bogdanoff, W.; Haile, S.; Tripathi, S.; DuBois, R.M.
Deposited on : 2015-11-20
Resolution : 2.60 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

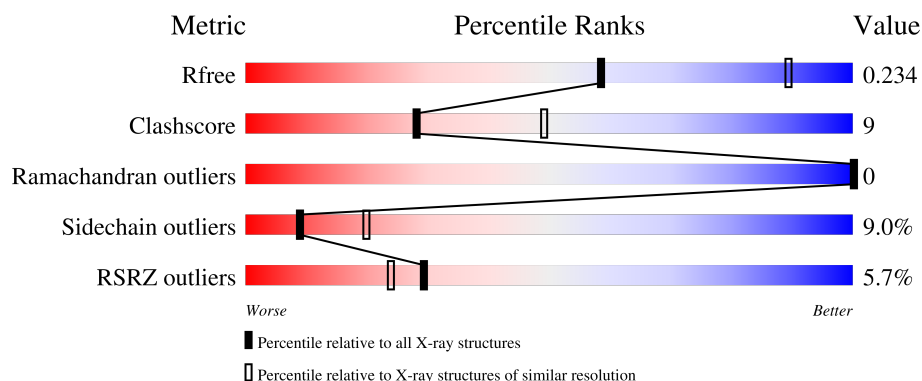
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	375	5% 63% 19% • 14%
1	B	375	5% 62% 19% • 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4883 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 Structural protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	3	0	0
			2413	1523	412	469	9			
1	B	315	Total	C	N	O	S	4	0	0
			2381	1505	409	458	9			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	MET	-	expression tag	UNP Q82452
A	430	ALA	-	expression tag	UNP Q82452
A	431	ALA	-	expression tag	UNP Q82452
A	432	ALA	-	expression tag	UNP Q82452
A	433	GLU	-	expression tag	UNP Q82452
A	434	LEU	-	expression tag	UNP Q82452
A	435	ALA	-	expression tag	UNP Q82452
A	436	LEU	-	expression tag	UNP Q82452
A	437	VAL	-	expression tag	UNP Q82452
A	438	PRO	-	expression tag	UNP Q82452
A	439	ARG	-	expression tag	UNP Q82452
A	440	GLY	-	expression tag	UNP Q82452
A	441	SER	-	expression tag	UNP Q82452
A	442	SER	-	expression tag	UNP Q82452
A	443	ALA	-	expression tag	UNP Q82452
A	444	HIS	-	expression tag	UNP Q82452
A	445	HIS	-	expression tag	UNP Q82452
A	446	HIS	-	expression tag	UNP Q82452
A	447	HIS	-	expression tag	UNP Q82452
A	448	HIS	-	expression tag	UNP Q82452
A	449	HIS	-	expression tag	UNP Q82452
A	450	HIS	-	expression tag	UNP Q82452
A	451	HIS	-	expression tag	UNP Q82452
A	452	HIS	-	expression tag	UNP Q82452
A	453	HIS	-	expression tag	UNP Q82452

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Chain	Residue	Modelled	Actual	Comment	Reference
B	79	MET	-	expression tag	UNP Q82452
B	430	ALA	-	expression tag	UNP Q82452
B	431	ALA	-	expression tag	UNP Q82452
B	432	ALA	-	expression tag	UNP Q82452
B	433	GLU	-	expression tag	UNP Q82452
B	434	LEU	-	expression tag	UNP Q82452
B	435	ALA	-	expression tag	UNP Q82452
B	436	LEU	-	expression tag	UNP Q82452
B	437	VAL	-	expression tag	UNP Q82452
B	438	PRO	-	expression tag	UNP Q82452
B	439	ARG	-	expression tag	UNP Q82452
B	440	GLY	-	expression tag	UNP Q82452
B	441	SER	-	expression tag	UNP Q82452
B	442	SER	-	expression tag	UNP Q82452
B	443	ALA	-	expression tag	UNP Q82452
B	444	HIS	-	expression tag	UNP Q82452
B	445	HIS	-	expression tag	UNP Q82452
B	446	HIS	-	expression tag	UNP Q82452
B	447	HIS	-	expression tag	UNP Q82452
B	448	HIS	-	expression tag	UNP Q82452
B	449	HIS	-	expression tag	UNP Q82452
B	450	HIS	-	expression tag	UNP Q82452
B	451	HIS	-	expression tag	UNP Q82452
B	452	HIS	-	expression tag	UNP Q82452
B	453	HIS	-	expression tag	UNP Q82452

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	B	2	Total Cl 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	50	Total O 50 50	0	0
3	B	35	Total O 35 35	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.24Å 71.10Å 158.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 2.60 48.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.47-2.60) 98.9 (48.47-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.192 , 0.234 0.196 , 0.234	Depositor DCC
R_{free} test set	1209 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.5	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	0.93	EDS
Total number of atoms	4883	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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	1.11	6/2467 (0.2%)	1.05	18/3371 (0.5%)
1	B	1.18	13/2435 (0.5%)	1.06	6/3325 (0.2%)
All	All	1.15	19/4902 (0.4%)	1.05	24/6696 (0.4%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	ARG	C-O	-6.45	1.15	1.23
1	B	402	LEU	C-O	-6.10	1.17	1.24
1	B	290	ASN	C-O	-6.03	1.16	1.23
1	B	285	SER	C-O	-5.99	1.18	1.24
1	B	288	ILE	C-O	-5.79	1.18	1.24
1	B	225	ILE	C-O	-5.77	1.18	1.24
1	A	288	ILE	C-O	-5.73	1.17	1.24
1	B	328	ASN	C-O	-5.58	1.17	1.23
1	A	144	LEU	C-O	-5.34	1.17	1.24
1	B	275	VAL	C-O	-5.34	1.18	1.24
1	B	299	ARG	C-O	-5.26	1.17	1.24
1	B	289	MET	C-O	-5.25	1.17	1.24
1	A	145	THR	C-O	-5.19	1.17	1.24
1	B	275	VAL	CA-C	-5.16	1.48	1.53
1	B	374	GLN	C-O	-5.12	1.18	1.24
1	A	248	GLU	C-O	-5.08	1.17	1.24
1	A	172	SER	C-O	-5.05	1.17	1.23
1	B	95	ASN	C-O	-5.02	1.17	1.24
1	B	319	THR	C-O	-5.02	1.17	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	LEU	N-CA-C	7.75	121.05	108.34
1	A	340	PRO	C-N-CD	7.71	137.55	120.60
1	A	201	GLY	CA-C-N	6.51	126.21	119.64
1	A	201	GLY	C-N-CA	6.51	126.21	119.64
1	A	116	ALA	N-CA-C	-6.49	101.78	110.55
1	A	339	PRO	CA-C-N	-6.42	113.77	120.38
1	A	339	PRO	C-N-CA	-6.42	113.77	120.38
1	A	402	LEU	N-CA-C	6.40	118.84	108.41
1	A	119	SER	N-CA-C	-6.17	100.58	110.14
1	B	275	VAL	N-CA-C	6.13	114.72	107.73
1	B	315	GLY	N-CA-C	-6.07	106.72	114.37
1	B	201	GLY	CA-C-N	6.07	125.77	119.64
1	B	201	GLY	C-N-CA	6.07	125.77	119.64
1	A	258	TYR	N-CA-C	5.82	119.03	109.72
1	A	306	THR	N-CA-C	-5.62	101.03	109.79
1	A	200	GLY	N-CA-C	5.54	117.85	111.36
1	A	338	THR	CA-C-N	-5.41	114.81	120.38
1	A	338	THR	C-N-CA	-5.41	114.81	120.38
1	A	380	LYS	CA-C-N	-5.30	115.12	120.31
1	A	380	LYS	C-N-CA	-5.30	115.12	120.31
1	A	121	GLN	N-CA-C	5.13	117.61	111.71
1	A	398	VAL	CB-CA-C	-5.13	105.08	111.08
1	B	175	GLY	N-CA-C	-5.01	106.68	112.50
1	A	338	THR	O-C-N	5.00	125.43	121.88

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	2413	0	2391	44	0
1	B	2381	0	2363	41	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	50	0	0	0	0
3	B	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4883	0	4754	85	1

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 9.

All (85) 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:328:ASN:OD1	1:A:333:ALA:HB2	1.56	1.04
1:A:317:ARG:NH1	1:A:360:THR:OG1	1.95	1.00
1:B:293:GLU:OE2	1:B:359:ARG:NH1	2.00	0.93
1:A:115:ASP:HB3	1:A:119:SER:HB3	1.49	0.92
1:B:160:VAL:HG12	1:B:225:ILE:HG12	1.53	0.89
1:B:326:VAL:HG13	1:B:402:LEU:HD22	1.53	0.89
1:A:301:VAL:O	1:A:305:SER:OG	1.98	0.81
1:B:280:GLU:OE2	1:B:361:ARG:NH1	2.14	0.78
1:A:140:LEU:HD11	1:A:249:LEU:HD11	1.67	0.77
1:B:140:LEU:HD11	1:B:249:LEU:HD11	1.66	0.77
1:A:230:ARG:HG2	1:A:232:MET:HE3	1.69	0.74
1:A:319:THR:HG22	1:A:356:ILE:HG22	1.72	0.70
1:B:262:PRO:HA	1:B:265:VAL:HG23	1.76	0.67
1:B:326:VAL:HG13	1:B:402:LEU:CD2	2.25	0.66
1:A:338:THR:HG22	1:A:339:PRO:O	1.96	0.65
1:B:89:LEU:HD13	1:B:106:ILE:HD12	1.79	0.64
1:B:273:ASN:HA	1:B:401:THR:HB	1.79	0.63
1:B:330:ALA:HB2	1:B:401:THR:HG23	1.81	0.63
1:B:89:LEU:HD11	1:B:249:LEU:HB2	1.82	0.61
1:A:328:ASN:OD1	1:A:333:ALA:CB	2.43	0.61
1:B:293:GLU:CG	1:B:365:ARG:HE	2.15	0.59
1:A:232:MET:CE	1:A:239:GLN:HA	2.33	0.59
1:A:274:GLN:HA	1:A:274:GLN:OE1	2.00	0.59
1:B:293:GLU:HG2	1:B:365:ARG:HE	1.68	0.59
1:A:232:MET:HE2	1:A:239:GLN:HA	1.84	0.58
1:B:342:PHE:CE2	1:B:382:ALA:HB1	2.39	0.57
1:A:301:VAL:HG11	1:A:367:PHE:HE2	1.70	0.57
1:B:379:ASN:O	1:B:381:PRO:HD3	2.05	0.57
1:B:138:LYS:O	1:B:196:PRO:HG3	2.05	0.56
1:A:96:THR:O	1:A:230:ARG:NH1	2.39	0.56
1:B:114:LYS:HE2	1:B:269:LYS:HB3	1.87	0.55
1:B:140:LEU:HD23	1:B:194:LEU:HD12	1.89	0.55
1:B:162:LEU:HD11	1:B:221:PRO:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASN:OD1	1:A:408:ASN:HB2	2.07	0.54
1:B:272:ASP:CG	1:B:275:VAL:HG22	2.31	0.54
1:B:313:ARG:O	1:B:313:ARG:HG3	2.09	0.53
1:B:323:VAL:HG22	1:B:354:LYS:HD3	1.90	0.52
1:A:159:ARG:NH1	1:A:173:TRP:O	2.44	0.51
1:A:307:THR:O	1:A:309:THR:N	2.41	0.51
1:B:138:LYS:O	1:B:196:PRO:HD3	2.11	0.51
1:A:180:LYS:NZ	1:A:198:ASP:OD1	2.33	0.50
1:B:278:THR:HG22	1:B:290:ASN:HD22	1.77	0.49
1:A:326:VAL:HG13	1:A:402:LEU:HD22	1.95	0.49
1:A:275:VAL:HG12	1:A:400:THR:O	2.14	0.48
1:B:338:THR:HG22	1:B:339:PRO:O	2.13	0.48
1:B:211:THR:HA	1:B:218:THR:HG21	1.96	0.48
1:B:212:ASN:OD1	1:B:408:ASN:HB2	2.14	0.47
1:B:273:ASN:HD22	1:B:401:THR:HB	1.82	0.45
1:A:317:ARG:HG3	1:A:368:TYR:OH	2.17	0.45
1:A:276:PRO:HA	1:A:399:THR:HA	1.99	0.45
1:A:338:THR:HB	1:A:343:ASN:CG	2.43	0.44
1:B:361:ARG:HB2	1:B:364:SER:HB2	1.99	0.44
1:A:291:VAL:CG1	1:A:298:ALA:HB2	2.48	0.44
1:B:270:SER:OG	1:B:271:THR:N	2.50	0.43
1:A:231:THR:O	1:A:232:MET:HE2	2.18	0.43
1:A:317:ARG:NH1	1:A:360:THR:HG1	2.09	0.43
1:A:140:LEU:HD11	1:A:249:LEU:CD1	2.44	0.43
1:B:230:ARG:O	1:B:232:MET:HG2	2.19	0.43
1:B:287:LEU:HD13	1:B:339:PRO:HG2	2.01	0.43
1:B:293:GLU:OE2	1:B:365:ARG:NE	2.51	0.43
1:A:140:LEU:HA	1:A:140:LEU:HD12	1.76	0.43
1:A:338:THR:HG23	1:A:339:PRO:HD2	2.01	0.42
1:A:116:ALA:O	1:A:119:SER:HB2	2.19	0.42
1:B:251:SER:HB3	1:B:253:TRP:CZ3	2.54	0.42
1:B:313:ARG:NH1	1:B:313:ARG:HG2	2.33	0.42
1:B:324:TRP:CZ3	1:B:406:GLN:HB2	2.54	0.42
1:A:324:TRP:CZ3	1:A:406:GLN:HB2	2.54	0.42
1:A:326:VAL:CG1	1:A:402:LEU:HD22	2.49	0.42
1:A:341:PRO:HD2	1:A:342:PHE:CD2	2.55	0.42
1:B:299:ARG:HH11	1:B:299:ARG:HD2	1.71	0.42
1:A:230:ARG:CG	1:A:232:MET:HE3	2.45	0.42
1:A:310:THR:O	1:A:318:THR:HA	2.20	0.42
1:A:371:PRO:HD3	1:A:382:ALA:HB2	2.00	0.42
1:B:326:VAL:CG1	1:B:402:LEU:HD22	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:VAL:HG11	1:A:367:PHE:CE2	2.53	0.42
1:A:359:ARG:HG3	1:A:360:THR:N	2.34	0.41
1:B:370:TYR:CD2	1:B:376:ALA:HA	2.54	0.41
1:A:304:ARG:HD3	1:A:304:ARG:HA	1.82	0.41
1:A:115:ASP:CB	1:A:119:SER:HB3	2.34	0.41
1:A:134:MET:HE2	1:A:206:TRP:HB2	2.01	0.41
1:B:280:GLU:CD	1:B:361:ARG:HH11	2.21	0.41
1:A:370:TYR:CD2	1:A:381:PRO:HA	2.56	0.41
1:A:134:MET:HE2	1:A:206:TRP:CB	2.51	0.40
1:A:291:VAL:HG12	1:A:298:ALA:HB2	2.04	0.40
1:B:379:ASN:C	1:B:381:PRO:HD3	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:MET:O	1:B:361:ARG:NH2[4_565]	2.18	0.02

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	315/375 (84%)	311 (99%)	4 (1%)	0	100	100
1	B	307/375 (82%)	300 (98%)	7 (2%)	0	100	100
All	All	622/750 (83%)	611 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	268/305 (88%)	242 (90%)	26 (10%)	8	17
1	B	265/305 (87%)	243 (92%)	22 (8%)	10	23
All	All	533/610 (87%)	485 (91%)	48 (9%)	9	20

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	THR
1	A	117	THR
1	A	120	THR
1	A	136	LYS
1	A	138	LYS
1	A	171	THR
1	A	172	SER
1	A	180	LYS
1	A	186	VAL
1	A	197	SER
1	A	265	VAL
1	A	278	THR
1	A	285	SER
1	A	291	VAL
1	A	304	ARG
1	A	305	SER
1	A	309	THR
1	A	310	THR
1	A	311	LEU
1	A	329	THR
1	A	337	VAL
1	A	347	LYS
1	A	359	ARG
1	A	380	LYS
1	A	387	SER
1	A	401	THR
1	B	88	THR

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Mol	Chain	Res	Type
1	B	91	THR
1	B	106	ILE
1	B	121	GLN
1	B	136	LYS
1	B	143	LYS
1	B	197	SER
1	B	213	ASP
1	B	236	LYS
1	B	275	VAL
1	B	278	THR
1	B	291	VAL
1	B	302	LEU
1	B	304	ARG
1	B	310	THR
1	B	313	ARG
1	B	364	SER
1	B	365	ARG
1	B	388	THR
1	B	398	VAL
1	B	399	THR
1	B	401	THR

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	83	GLN
1	A	121	GLN
1	A	154	ASN
1	A	261	ASN
1	A	328	ASN
1	A	403	GLN
1	B	154	ASN
1	B	273	ASN
1	B	328	ASN

5.3.3 RNA ⓘ

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 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	321/375 (85%)	0.01	18 (5%) 30 24	13, 36, 80, 98	1 (0%)
1	B	315/375 (84%)	-0.05	18 (5%) 29 24	13, 34, 66, 89	1 (0%)
All	All	636/750 (84%)	-0.02	36 (5%) 29 24	13, 34, 75, 98	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	ALA	5.2
1	A	397	PRO	5.2
1	A	258	TYR	4.7
1	B	389	PRO	3.9
1	B	397	PRO	3.9
1	B	313	ARG	3.8
1	B	274	GLN	3.6
1	A	265	VAL	3.5
1	A	310	THR	3.5
1	B	258	TYR	3.4
1	B	314	ALA	3.3
1	A	213	ASP	3.3
1	B	121	GLN	3.2
1	A	387	SER	3.2
1	B	411	SER	3.2
1	B	115	ASP	3.1
1	A	118	GLY	3.0
1	A	309	THR	2.8
1	A	120	THR	2.7
1	B	337	VAL	2.7
1	B	261	ASN	2.6
1	B	259	ALA	2.6
1	B	398	VAL	2.5
1	A	235	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	311	LEU	2.4
1	A	315	GLY	2.4
1	A	261	ASN	2.3
1	A	263	ASN	2.2
1	A	274	GLN	2.2
1	A	311	LEU	2.2
1	A	358	GLY	2.2
1	B	316	GLU	2.1
1	A	410	PRO	2.1
1	B	235	TYR	2.1
1	B	361	ARG	2.0
1	B	315	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	501	1/1	0.92	0.08	30,30,30,30	0
2	CL	B	502	1/1	0.94	0.07	30,30,30,30	0
2	CL	A	502	1/1	0.96	0.08	30,30,30,30	0
2	CL	B	501	1/1	0.97	0.08	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.