



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:26 PM EDT

PDB ID : 3N4P / pdb_00003n4p
Title : Human cytomegalovirus terminase nuclease domain
Authors : Nadal, M.; Mas, P.J.; Blanco, A.G.; Arnan, C.; Sola, M.; Hart, D.J.; Coll, M.
Deposited on : 2010-05-22
Resolution : 2.15 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

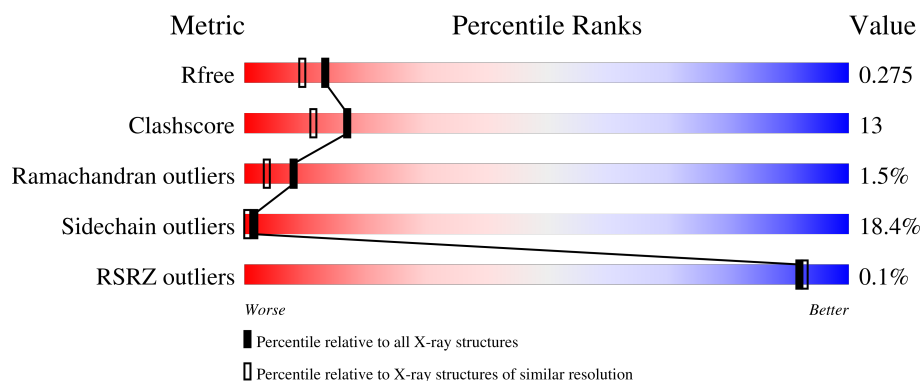
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	279	
1	B	279	
1	C	279	
1	D	279	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7146 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 Terminase subunit UL89 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1736	1113	292	325	6			
1	B	227	Total	C	N	O	S	0	1	0
			1838	1176	315	341	6			
1	C	218	Total	C	N	O	S	0	0	0
			1747	1120	292	329	6			
1	D	212	Total	C	N	O	S	0	1	0
			1720	1103	290	321	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	MET	-	expression tag	UNP P16732
A	397	GLY	-	expression tag	UNP P16732
A	398	HIS	-	expression tag	UNP P16732
A	399	HIS	-	expression tag	UNP P16732
A	400	HIS	-	expression tag	UNP P16732
A	401	HIS	-	expression tag	UNP P16732
A	402	HIS	-	expression tag	UNP P16732
A	403	HIS	-	expression tag	UNP P16732
A	404	ASP	-	expression tag	UNP P16732
A	405	TYR	-	expression tag	UNP P16732
A	406	ASP	-	expression tag	UNP P16732
A	407	ILE	-	expression tag	UNP P16732
A	408	PRO	-	expression tag	UNP P16732
A	409	THR	-	expression tag	UNP P16732
A	410	THR	-	expression tag	UNP P16732
A	411	GLU	-	expression tag	UNP P16732
A	412	ASN	-	expression tag	UNP P16732
A	413	LEU	-	expression tag	UNP P16732
A	414	TYR	-	expression tag	UNP P16732
A	415	PHE	-	expression tag	UNP P16732
A	416	GLN	-	expression tag	UNP P16732

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Chain	Residue	Modelled	Actual	Comment	Reference
A	417	GLY	-	expression tag	UNP P16732
B	396	MET	-	expression tag	UNP P16732
B	397	GLY	-	expression tag	UNP P16732
B	398	HIS	-	expression tag	UNP P16732
B	399	HIS	-	expression tag	UNP P16732
B	400	HIS	-	expression tag	UNP P16732
B	401	HIS	-	expression tag	UNP P16732
B	402	HIS	-	expression tag	UNP P16732
B	403	HIS	-	expression tag	UNP P16732
B	404	ASP	-	expression tag	UNP P16732
B	405	TYR	-	expression tag	UNP P16732
B	406	ASP	-	expression tag	UNP P16732
B	407	ILE	-	expression tag	UNP P16732
B	408	PRO	-	expression tag	UNP P16732
B	409	THR	-	expression tag	UNP P16732
B	410	THR	-	expression tag	UNP P16732
B	411	GLU	-	expression tag	UNP P16732
B	412	ASN	-	expression tag	UNP P16732
B	413	LEU	-	expression tag	UNP P16732
B	414	TYR	-	expression tag	UNP P16732
B	415	PHE	-	expression tag	UNP P16732
B	416	GLN	-	expression tag	UNP P16732
B	417	GLY	-	expression tag	UNP P16732
C	396	MET	-	expression tag	UNP P16732
C	397	GLY	-	expression tag	UNP P16732
C	398	HIS	-	expression tag	UNP P16732
C	399	HIS	-	expression tag	UNP P16732
C	400	HIS	-	expression tag	UNP P16732
C	401	HIS	-	expression tag	UNP P16732
C	402	HIS	-	expression tag	UNP P16732
C	403	HIS	-	expression tag	UNP P16732
C	404	ASP	-	expression tag	UNP P16732
C	405	TYR	-	expression tag	UNP P16732
C	406	ASP	-	expression tag	UNP P16732
C	407	ILE	-	expression tag	UNP P16732
C	408	PRO	-	expression tag	UNP P16732
C	409	THR	-	expression tag	UNP P16732
C	410	THR	-	expression tag	UNP P16732
C	411	GLU	-	expression tag	UNP P16732
C	412	ASN	-	expression tag	UNP P16732
C	413	LEU	-	expression tag	UNP P16732
C	414	TYR	-	expression tag	UNP P16732

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Chain	Residue	Modelled	Actual	Comment	Reference
C	415	PHE	-	expression tag	UNP P16732
C	416	GLN	-	expression tag	UNP P16732
C	417	GLY	-	expression tag	UNP P16732
D	396	MET	-	expression tag	UNP P16732
D	397	GLY	-	expression tag	UNP P16732
D	398	HIS	-	expression tag	UNP P16732
D	399	HIS	-	expression tag	UNP P16732
D	400	HIS	-	expression tag	UNP P16732
D	401	HIS	-	expression tag	UNP P16732
D	402	HIS	-	expression tag	UNP P16732
D	403	HIS	-	expression tag	UNP P16732
D	404	ASP	-	expression tag	UNP P16732
D	405	TYR	-	expression tag	UNP P16732
D	406	ASP	-	expression tag	UNP P16732
D	407	ILE	-	expression tag	UNP P16732
D	408	PRO	-	expression tag	UNP P16732
D	409	THR	-	expression tag	UNP P16732
D	410	THR	-	expression tag	UNP P16732
D	411	GLU	-	expression tag	UNP P16732
D	412	ASN	-	expression tag	UNP P16732
D	413	LEU	-	expression tag	UNP P16732
D	414	TYR	-	expression tag	UNP P16732
D	415	PHE	-	expression tag	UNP P16732
D	416	GLN	-	expression tag	UNP P16732
D	417	GLY	-	expression tag	UNP P16732

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

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

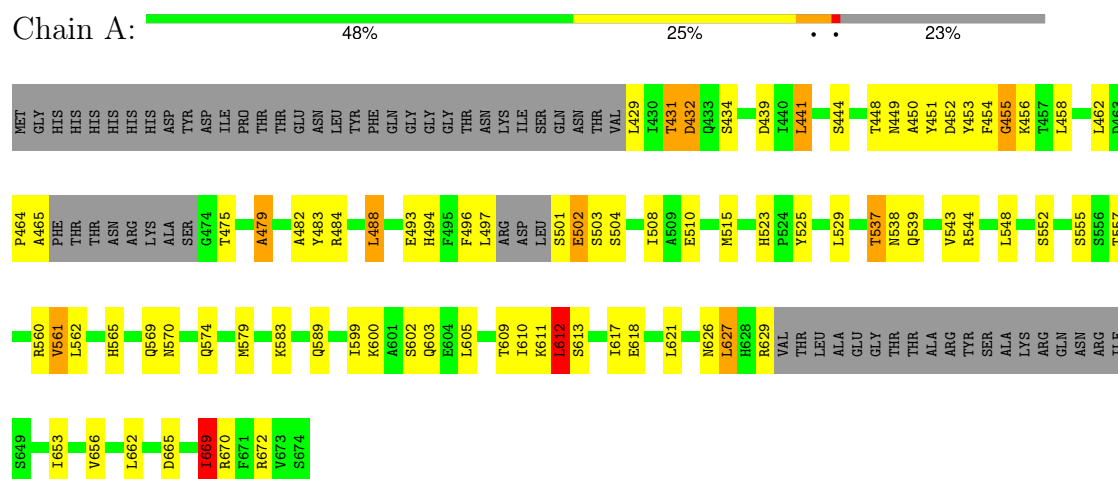
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	25	Total 25	O 25	0	0
3	C	27	Total 27	O 27	0	0
3	D	11	Total 11	O 11	0	0

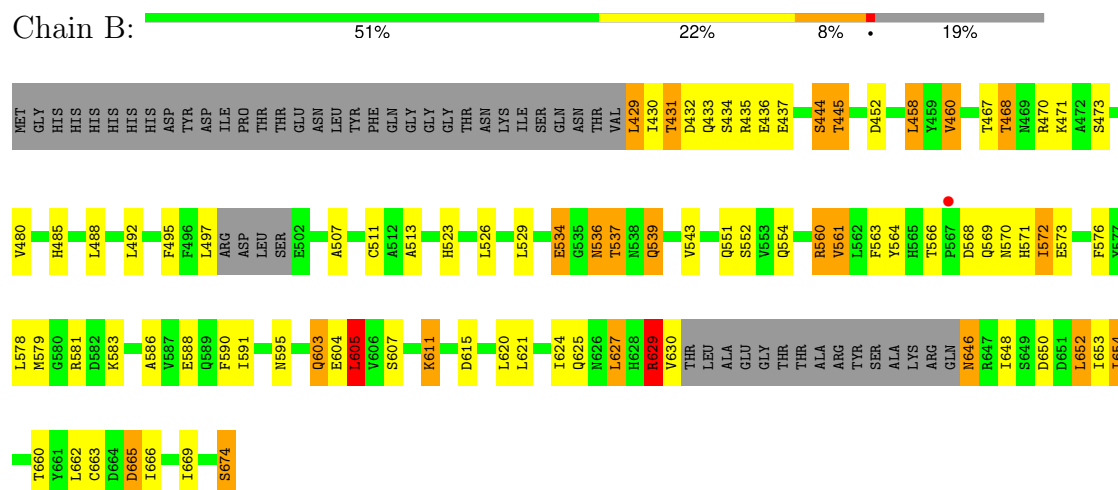
3 Residue-property plots

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: Terminase subunit UL89 protein

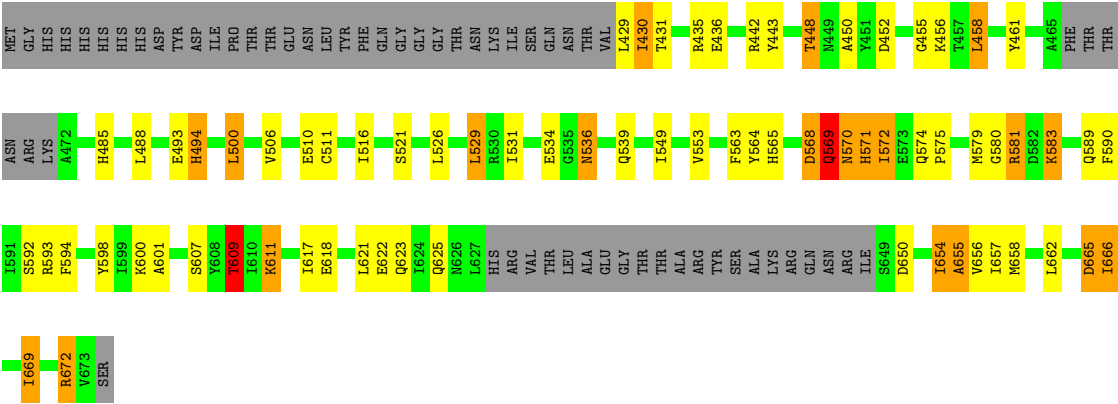


• Molecule 1: Terminase subunit UL89 protein

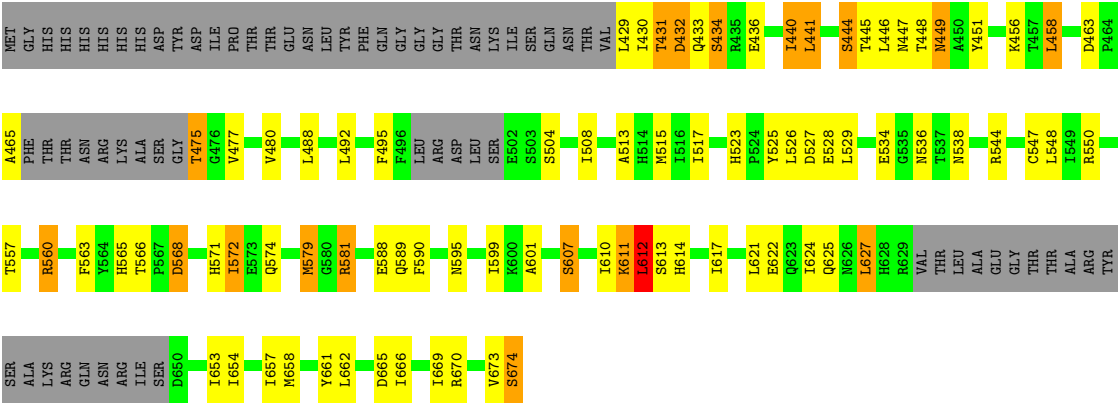


• Molecule 1: Terminase subunit UL89 protein





● Molecule 1: Terminase subunit UL89 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.86Å 87.96Å 188.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.15 19.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.99-2.15) 98.7 (19.99-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.272 0.230 , 0.275	Depositor DCC
R_{free} test set	3760 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7146	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.46	11/1770 (0.6%)	1.39	9/2399 (0.4%)
1	B	1.22	5/1875 (0.3%)	1.28	8/2542 (0.3%)
1	C	1.36	4/1781 (0.2%)	1.33	11/2416 (0.5%)
1	D	1.21	5/1754 (0.3%)	1.25	9/2378 (0.4%)
All	All	1.32	25/7180 (0.3%)	1.31	37/9735 (0.4%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	656	VAL	CA-CB	7.67	1.64	1.54
1	D	666	ILE	C-O	-7.08	1.15	1.24
1	A	479	ALA	N-CA	7.05	1.54	1.46
1	A	669	ILE	CA-CB	-7.00	1.45	1.54
1	D	441	LEU	CA-C	-6.73	1.45	1.53
1	A	561	VAL	N-CA	6.44	1.54	1.46
1	A	561	VAL	C-O	-6.31	1.17	1.24
1	B	603	GLN	CA-C	6.13	1.60	1.52
1	B	586	ALA	CA-CB	6.11	1.62	1.53
1	A	599	ILE	C-O	-6.10	1.17	1.24
1	D	588	GLU	CA-C	5.83	1.60	1.52
1	D	523	HIS	CA-CB	5.74	1.59	1.53
1	C	494	HIS	N-CA	-5.71	1.39	1.46
1	B	605	LEU	CA-C	5.55	1.59	1.52
1	A	482	ALA	CA-CB	5.52	1.62	1.53
1	C	549	ILE	CA-CB	5.40	1.60	1.54
1	C	485	HIS	N-CA	5.40	1.52	1.46
1	B	615	ASP	N-CA	5.38	1.52	1.45
1	A	453	TYR	CA-C	5.36	1.59	1.52
1	A	439	ASP	CA-C	5.17	1.59	1.52
1	B	460	VAL	CA-CB	5.15	1.63	1.55
1	A	557	THR	CA-CB	5.14	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	655	ALA	C-O	-5.10	1.18	1.24
1	D	661	TYR	CA-C	5.04	1.59	1.52
1	A	454	PHE	CA-C	-5.02	1.46	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	629	ARG	N-CA-C	10.05	122.48	111.53
1	D	523	HIS	CA-C-N	-9.20	109.91	120.12
1	D	523	HIS	C-N-CA	-9.20	109.91	120.12
1	A	613	SER	N-CA-C	-9.19	101.07	114.39
1	C	511	CYS	N-CA-C	-7.93	102.71	111.36
1	A	496	PHE	N-CA-C	7.31	120.70	108.20
1	D	599	ILE	CB-CA-C	-7.24	100.50	110.77
1	C	553	VAL	N-CA-C	6.92	117.68	110.62
1	A	455	GLY	N-CA-C	-6.92	102.68	112.37
1	A	589	GLN	CB-CA-C	-6.86	99.40	110.79
1	A	626	ASN	N-CA-C	6.86	121.82	113.17
1	A	627	LEU	N-CA-C	6.83	120.11	109.52
1	A	456	LYS	N-CA-C	-6.38	104.81	112.59
1	C	622	GLU	N-CA-C	-6.36	103.87	111.69
1	D	568	ASP	N-CA-C	6.28	118.32	108.96
1	C	569	GLN	N-CA-C	-6.28	97.44	110.80
1	B	551	GLN	N-CA-C	5.98	118.32	111.02
1	C	500	LEU	N-CA-C	-5.85	106.38	112.93
1	A	538	ASN	N-CA-C	5.82	116.74	108.54
1	B	564	TYR	N-CA-C	-5.78	101.30	109.96
1	C	623	GLN	N-CA-C	5.66	117.45	111.28
1	D	601	ALA	N-CA-C	-5.52	101.86	110.42
1	A	560	ARG	CG-CD-NE	-5.51	99.88	112.00
1	B	595	ASN	CA-C-N	-5.37	114.09	122.73
1	B	595	ASN	C-N-CA	-5.37	114.09	122.73
1	C	448	THR	CB-CA-C	-5.35	100.97	109.80
1	C	654	ILE	CB-CA-C	-5.34	104.92	112.14
1	C	455	GLY	N-CA-C	-5.33	105.72	112.54
1	B	603	GLN	N-CA-C	5.31	117.07	111.28
1	D	440	ILE	CB-CA-C	-5.29	101.36	110.94
1	C	656	VAL	CB-CA-C	-5.26	105.04	112.14
1	D	673	VAL	CA-C-N	5.10	130.88	121.70
1	D	673	VAL	C-N-CA	5.10	130.88	121.70
1	B	607	SER	CB-CA-C	-5.08	105.14	111.43
1	B	654	ILE	CB-CA-C	-5.07	105.30	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	609	THR	N-CA-C	-5.04	107.30	113.50
1	D	613	SER	N-CA-C	5.03	118.68	112.54

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	1736	0	1707	33	0
1	B	1838	0	1813	53	0
1	C	1747	0	1721	53	0
1	D	1720	0	1688	48	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	35	0	0	2	0
3	B	25	0	0	1	0
3	C	27	0	0	1	0
3	D	11	0	0	0	0
All	All	7146	0	6929	177	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 13.

All (177) 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:D:550:ARG:HD3	1:D:674:SER:HB2	1.14	1.14
1:C:430:ILE:HD11	1:C:435:ARG:HG3	1.25	1.09
1:C:669:ILE:H	1:C:669:ILE:HD12	1.18	1.07
1:A:494:HIS:H	1:A:609:THR:HG21	1.24	1.03
1:C:430:ILE:HD11	1:C:435:ARG:CG	1.91	1.01
1:D:431:THR:HG22	1:D:434:SER:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LYS:O	1:A:612:LEU:HB2	1.66	0.93
1:D:550:ARG:CD	1:D:674:SER:HB2	2.02	0.88
1:B:431:THR:HG22	1:B:434:SER:H	1.37	0.87
1:C:494:HIS:H	1:C:609:THR:CG2	1.87	0.86
1:B:588:GLU:HG2	1:C:592:SER:HA	1.57	0.85
1:C:493:GLU:OE1	1:C:609:THR:HB	1.78	0.83
1:D:440:ILE:O	1:D:440:ILE:HG22	1.80	0.82
1:D:550:ARG:HD3	1:D:674:SER:CB	2.05	0.81
1:B:539:GLN:O	1:B:543:VAL:HG23	1.80	0.81
1:D:448:THR:C	1:D:449:ASN:HD22	1.89	0.81
1:C:669:ILE:H	1:C:669:ILE:CD1	1.89	0.79
1:D:432:ASP:N	1:D:432:ASP:OD1	2.13	0.79
1:D:581:ARG:HH11	1:D:581:ARG:HG3	1.47	0.79
1:D:492:LEU:O	1:D:607:SER:HB3	1.83	0.79
1:C:494:HIS:H	1:C:609:THR:HG21	1.48	0.78
1:D:440:ILE:O	1:D:440:ILE:CG2	2.31	0.78
1:C:581:ARG:HB2	1:C:581:ARG:HH11	1.49	0.77
1:A:494:HIS:H	1:A:609:THR:CG2	1.99	0.76
1:C:581:ARG:HB2	1:C:581:ARG:NH1	2.01	0.76
1:A:494:HIS:N	1:A:609:THR:HG21	2.00	0.75
1:B:432:ASP:OD2	1:B:435:ARG:NH1	2.20	0.75
1:D:449:ASN:HD22	1:D:449:ASN:N	1.80	0.75
1:D:430:ILE:HD13	1:D:624:ILE:HG23	1.68	0.74
1:B:523:HIS:HE1	3:B:63:HOH:O	1.71	0.73
1:A:431:THR:HG22	1:A:434:SER:H	1.54	0.72
1:D:475:THR:HG23	1:D:495:PHE:O	1.90	0.71
1:C:430:ILE:CD1	1:C:435:ARG:HG3	2.16	0.70
1:C:430:ILE:HD12	1:C:431:THR:O	1.92	0.70
1:D:513:ALA:O	1:D:517:ILE:HG13	1.92	0.70
1:B:445:THR:HG21	1:B:523:HIS:CD2	2.26	0.70
1:B:566:THR:HG23	1:B:576:PHE:O	1.92	0.70
1:B:534:GLU:OE1	1:B:536:ASN:HB3	1.92	0.69
1:D:434:SER:OG	1:D:595:ASN:HA	1.92	0.69
1:A:484:ARG:NH1	1:B:436:GLU:OE1	2.26	0.69
1:C:443:TYR:HE1	1:C:600:LYS:HG3	1.58	0.68
1:C:607:SER:O	1:C:611:LYS:HB2	1.94	0.68
1:A:603:GLN:OE1	1:B:603:GLN:NE2	2.27	0.67
1:D:581:ARG:HH11	1:D:581:ARG:CG	2.08	0.67
1:B:445:THR:HB	1:B:604:GLU:OE2	1.94	0.67
1:B:536:ASN:HD22	1:B:536:ASN:C	2.02	0.66
1:B:536:ASN:C	1:B:536:ASN:ND2	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ALA:N	1:A:475:THR:HG22	2.12	0.65
1:A:609:THR:HG23	1:A:610:ILE:HG13	1.77	0.65
1:B:534:GLU:OE1	1:B:536:ASN:CB	2.45	0.64
1:C:669:ILE:O	1:C:672:ARG:NH2	2.31	0.64
1:D:544:ARG:O	1:D:547:CYS:SG	2.53	0.64
1:D:563:PHE:CD1	1:D:674:SER:HB3	2.33	0.64
1:C:443:TYR:HD2	1:D:440:ILE:CG2	2.11	0.63
1:D:432:ASP:O	1:D:436:GLU:HG3	1.98	0.63
1:D:581:ARG:HG3	1:D:581:ARG:NH1	2.11	0.63
1:B:568:ASP:CG	1:B:569:GLN:N	2.55	0.63
1:C:494:HIS:N	1:C:609:THR:HG21	2.13	0.62
1:C:506:VAL:O	1:C:510:GLU:HG2	1.99	0.62
1:C:589:GLN:O	1:C:593:ARG:HG3	2.00	0.62
1:C:583:LYS:HA	1:C:658:MET:HE1	1.83	0.59
1:A:465:ALA:H	1:A:475:THR:CG2	2.15	0.58
1:B:568:ASP:CG	1:B:569:GLN:H	2.11	0.58
1:B:444:SER:OG	1:B:603:GLN:OE1	2.22	0.58
1:B:569:GLN:C	1:B:571:HIS:H	2.10	0.58
1:D:449:ASN:N	1:D:449:ASN:ND2	2.47	0.57
1:C:443:TYR:CE1	1:C:600:LYS:HG3	2.39	0.57
1:C:601:ALA:HB1	1:C:617:ILE:HD11	1.86	0.57
1:A:493:GLU:OE1	1:A:609:THR:HG22	2.06	0.56
1:B:660:THR:O	1:B:663:CYS:HB2	2.06	0.55
1:C:590:PHE:CG	1:C:657:ILE:HG12	2.42	0.55
1:B:588:GLU:HG2	1:C:592:SER:CB	2.37	0.55
1:C:650:ASP:O	1:C:654:ILE:HG13	2.07	0.55
1:C:458:LEU:HG	1:C:526:LEU:HD13	1.89	0.54
1:B:588:GLU:HG2	1:C:592:SER:CA	2.35	0.54
1:C:461:TYR:OH	1:C:534:GLU:HG3	2.07	0.53
1:A:455:GLY:HA2	3:A:15:HOH:O	2.09	0.53
1:A:539:GLN:O	1:A:543:VAL:HG23	2.09	0.53
1:B:445:THR:HG21	1:B:523:HIS:HD2	1.74	0.53
1:C:516:ILE:HG21	1:C:529:LEU:HD11	1.91	0.52
1:D:477:VAL:CG1	1:D:515:MET:HE1	2.40	0.52
1:A:432:ASP:OD1	1:A:432:ASP:N	2.39	0.51
1:D:444:SER:HB3	1:D:447:ASN:HD22	1.74	0.51
1:D:534:GLU:OE2	1:D:536[B]:ASN:CG	2.54	0.51
1:C:618:GLU:HG3	3:C:96:HOH:O	2.11	0.50
1:D:611:LYS:HD3	1:D:612:LEU:HD12	1.93	0.50
1:B:536:ASN:HD22	1:B:537:THR:N	2.09	0.50
1:B:563:PHE:CD1	1:B:674:SER:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:TYR:HD2	1:D:440:ILE:HG22	1.76	0.50
1:C:565:HIS:HA	1:C:574:GLN:O	2.11	0.50
1:C:654:ILE:O	1:C:658:MET:HG2	2.11	0.50
1:A:465:ALA:N	1:A:475:THR:CG2	2.75	0.50
1:A:523:HIS:HB3	1:A:525:TYR:CE1	2.47	0.50
1:C:448:THR:HB	1:C:450:ALA:H	1.76	0.50
1:C:443:TYR:HD2	1:D:440:ILE:HG21	1.76	0.49
1:A:562:LEU:HD12	1:A:562:LEU:N	2.27	0.49
1:B:429:LEU:HD11	1:B:627:LEU:O	2.13	0.49
1:D:579:MET:HE1	1:D:658:MET:SD	2.53	0.49
1:C:669:ILE:HD12	1:C:669:ILE:N	2.04	0.48
1:B:588:GLU:HG2	1:C:592:SER:HB2	1.96	0.48
1:A:462:LEU:N	1:A:462:LEU:HD23	2.28	0.48
1:C:579:MET:HE2	1:C:658:MET:HE3	1.96	0.48
1:D:610:ILE:HG22	1:D:610:ILE:O	2.13	0.48
1:B:554:GLN:HE21	1:B:561:VAL:HG23	1.78	0.47
1:A:483:TYR:CZ	1:A:484:ARG:HD2	2.49	0.47
1:C:568:ASP:HB2	1:C:572:ILE:HG23	1.96	0.47
1:D:624:ILE:O	1:D:627:LEU:HB2	2.13	0.47
1:C:534:GLU:OE2	1:C:536:ASN:ND2	2.48	0.47
1:C:430:ILE:HD13	1:C:594:PHE:CE2	2.50	0.47
1:C:621:LEU:O	1:C:625:GLN:HG2	2.15	0.47
1:C:442:ARG:NH1	1:C:617:ILE:HD12	2.29	0.47
1:C:593:ARG:HB3	1:C:598:TYR:HB2	1.97	0.47
1:B:513:ALA:HB1	1:B:552:SER:HB2	1.97	0.46
1:A:464:PRO:HA	1:A:475:THR:HG22	1.96	0.46
1:D:563:PHE:HD1	1:D:674:SER:HB3	1.75	0.46
1:B:492:LEU:HB3	1:B:652:LEU:HD21	1.96	0.46
1:D:463:ASP:HA	1:D:534:GLU:HB3	1.98	0.46
1:A:488:LEU:HD12	1:A:488:LEU:H	1.81	0.45
1:A:565:HIS:O	1:A:670:ARG:NH1	2.48	0.45
1:D:477:VAL:HG12	1:D:515:MET:HE1	1.99	0.45
1:A:441:LEU:HD13	1:A:600:LYS:HE2	1.99	0.45
1:B:539:GLN:H	1:B:539:GLN:HG2	1.56	0.45
1:B:458:LEU:HB3	1:B:529:LEU:HD23	1.97	0.45
1:B:560:ARG:H	1:B:560:ARG:HG2	1.55	0.45
1:D:458:LEU:HG	1:D:526:LEU:HD13	1.99	0.45
1:D:566:THR:HA	1:D:670:ARG:HH12	1.82	0.45
1:B:430:ILE:O	1:B:430:ILE:CG2	2.65	0.45
1:D:572:ILE:HG13	1:D:574:GLN:HE21	1.82	0.44
1:B:495:PHE:CZ	1:B:507:ALA:HB1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:ASP:N	1:B:665:ASP:OD1	2.50	0.44
1:C:579:MET:HE1	1:C:583:LYS:HE2	1.99	0.44
1:C:564:TYR:O	1:C:575:PRO:HA	2.17	0.44
1:B:605:LEU:O	1:B:611:LYS:NZ	2.51	0.44
1:B:430:ILE:O	1:B:430:ILE:HG23	2.17	0.44
1:C:570:ASN:OD1	1:C:572:ILE:HG22	2.17	0.44
1:A:497:LEU:HD11	1:A:508:ILE:HD11	1.99	0.44
1:B:563:PHE:HD1	1:B:674:SER:HB3	1.82	0.44
1:C:666:ILE:HD12	1:C:666:ILE:HA	1.79	0.44
1:B:620:LEU:HD13	1:B:652:LEU:HD13	2.00	0.43
1:B:629:ARG:O	1:B:630:VAL:HB	2.18	0.43
1:D:590:PHE:CG	1:D:657:ILE:HG12	2.54	0.43
1:C:672:ARG:HE	1:C:672:ARG:HB2	1.53	0.43
1:B:433:GLN:NE2	1:B:437:GLU:OE2	2.39	0.43
1:B:569:GLN:C	1:B:571:HIS:N	2.76	0.43
1:A:450:ALA:O	1:A:451:TYR:HB2	2.19	0.43
1:C:461:TYR:CD2	1:C:655:ALA:HA	2.54	0.43
1:B:646:ASN:OD1	1:B:646:ASN:N	2.51	0.43
1:D:579:MET:CE	1:D:658:MET:HE2	2.48	0.43
1:D:444:SER:CB	1:D:447:ASN:HD22	2.32	0.42
1:B:458:LEU:HG	1:B:526:LEU:HD13	2.00	0.42
1:A:502:GLU:HB2	1:A:503:SER:H	1.45	0.42
1:B:588:GLU:HB3	1:C:592:SER:HB2	2.00	0.42
1:A:464:PRO:HA	1:A:475:THR:CG2	2.49	0.42
1:A:669:ILE:H	1:A:669:ILE:HG13	1.62	0.42
1:B:534:GLU:OE1	1:B:536:ASN:HB2	2.19	0.42
1:B:513:ALA:CB	1:B:552:SER:HB2	2.49	0.42
1:B:554:GLN:NE2	1:B:561:VAL:HG23	2.34	0.42
1:D:528:GLU:HG3	1:D:560:ARG:HB3	2.02	0.42
1:A:458:LEU:HD11	1:A:479:ALA:HB1	2.01	0.42
1:A:529:LEU:HD12	1:A:561:VAL:HG22	2.02	0.42
1:C:611:LYS:HZ2	1:C:611:LYS:HG2	1.59	0.42
1:D:451:TYR:CE2	1:D:525:TYR:CD1	3.08	0.41
1:C:531:ILE:O	1:C:563:PHE:HA	2.20	0.41
1:A:449:ASN:ND2	3:A:97:HOH:O	2.49	0.41
1:B:590:PHE:O	1:B:591:ILE:C	2.63	0.41
1:D:515:MET:HB3	1:D:515:MET:HE2	1.82	0.41
1:B:627:LEU:HD23	1:B:627:LEU:HA	1.93	0.41
1:D:572:ILE:H	1:D:572:ILE:HG12	1.68	0.41
1:D:477:VAL:HG11	1:D:515:MET:HE1	2.02	0.41
1:D:565:HIS:HA	1:D:574:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ARG:O	1:A:548:LEU:HG	2.20	0.41
1:D:465:ALA:H	1:D:475:THR:HB	1.86	0.40
1:A:488:LEU:HD12	1:A:488:LEU:N	2.36	0.40
1:B:650:ASP:OD2	1:B:654:ILE:HD11	2.20	0.40
1:D:456:LYS:HB3	1:D:527:ASP:OD1	2.21	0.40
1:B:624:ILE:HG13	1:B:653:ILE:HD13	2.04	0.40
1:B:572:ILE:HD13	1:B:573:GLU:H	1.87	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	208/279 (75%)	196 (94%)	9 (4%)	3 (1%)	9	4
1	B	222/279 (80%)	206 (93%)	13 (6%)	3 (1%)	9	4
1	C	212/279 (76%)	204 (96%)	3 (1%)	5 (2%)	4	1
1	D	205/279 (74%)	190 (93%)	13 (6%)	2 (1%)	12	8
All	All	847/1116 (76%)	796 (94%)	38 (4%)	13 (2%)	8	4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	GLN
1	A	612	LEU
1	B	467	THR
1	C	571	HIS
1	C	569	GLN
1	C	580	GLY
1	D	612	LEU
1	A	537	THR

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Mol	Chain	Res	Type
1	B	468	THR
1	C	568	ASP
1	C	665	ASP
1	D	571	HIS
1	B	570	ASN

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	188/242 (78%)	155 (82%)	33 (18%)	2	0
1	B	199/242 (82%)	158 (79%)	41 (21%)	1	0
1	C	189/242 (78%)	164 (87%)	25 (13%)	4	1
1	D	186/242 (77%)	145 (78%)	41 (22%)	1	0
All	All	762/968 (79%)	622 (82%)	140 (18%)	1	0

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	429	LEU
1	A	431	THR
1	A	432	ASP
1	A	441	LEU
1	A	444	SER
1	A	448	THR
1	A	452	ASP
1	A	488	LEU
1	A	501	SER
1	A	502	GLU
1	A	504	SER
1	A	510	GLU
1	A	515	MET
1	A	537	THR
1	A	552	SER
1	A	555	SER

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Mol	Chain	Res	Type
1	A	570	ASN
1	A	574	GLN
1	A	579	MET
1	A	583	LYS
1	A	602	SER
1	A	605	LEU
1	A	612	LEU
1	A	617	ILE
1	A	618	GLU
1	A	621	LEU
1	A	627	LEU
1	A	629	ARG
1	A	653	ILE
1	A	662	LEU
1	A	665	ASP
1	A	669	ILE
1	A	672	ARG
1	B	429	LEU
1	B	431	THR
1	B	444	SER
1	B	445	THR
1	B	452	ASP
1	B	458	LEU
1	B	460	VAL
1	B	468	THR
1	B	470	ARG
1	B	471	LYS
1	B	473	SER
1	B	480	VAL
1	B	485	HIS
1	B	488	LEU
1	B	497	LEU
1	B	511	CYS
1	B	534	GLU
1	B	536	ASN
1	B	537	THR
1	B	539	GLN
1	B	560	ARG
1	B	561	VAL
1	B	572	ILE
1	B	578	LEU
1	B	579	MET

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Mol	Chain	Res	Type
1	B	581	ARG
1	B	583	LYS
1	B	605	LEU
1	B	611	LYS
1	B	621	LEU
1	B	625	GLN
1	B	627	LEU
1	B	629	ARG
1	B	646	ASN
1	B	648	ILE
1	B	652	LEU
1	B	662	LEU
1	B	665	ASP
1	B	666	ILE
1	B	669	ILE
1	B	674	SER
1	C	429	LEU
1	C	430	ILE
1	C	436	GLU
1	C	452	ASP
1	C	456	LYS
1	C	458	LEU
1	C	488	LEU
1	C	500	LEU
1	C	521	SER
1	C	529	LEU
1	C	536	ASN
1	C	539	GLN
1	C	569	GLN
1	C	570	ASN
1	C	571	HIS
1	C	572	ILE
1	C	581	ARG
1	C	583	LYS
1	C	609	THR
1	C	611	LYS
1	C	662	LEU
1	C	665	ASP
1	C	666	ILE
1	C	669	ILE
1	C	672	ARG
1	D	429	LEU

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Mol	Chain	Res	Type
1	D	431	THR
1	D	432	ASP
1	D	433	GLN
1	D	434	SER
1	D	441	LEU
1	D	444	SER
1	D	445	THR
1	D	446	LEU
1	D	449	ASN
1	D	458	LEU
1	D	475	THR
1	D	480	VAL
1	D	488	LEU
1	D	504	SER
1	D	508	ILE
1	D	529	LEU
1	D	538	ASN
1	D	548	LEU
1	D	557	THR
1	D	560	ARG
1	D	568	ASP
1	D	572	ILE
1	D	579	MET
1	D	581	ARG
1	D	589	GLN
1	D	607	SER
1	D	611	LYS
1	D	612	LEU
1	D	614	HIS
1	D	617	ILE
1	D	621	LEU
1	D	622	GLU
1	D	625	GLN
1	D	627	LEU
1	D	653	ILE
1	D	654	ILE
1	D	662	LEU
1	D	665	ASP
1	D	669	ILE
1	D	674	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	ASN
1	A	538	ASN
1	A	539	GLN
1	A	551	GLN
1	A	570	ASN
1	A	589	GLN
1	B	469	ASN
1	B	523	HIS
1	B	536	ASN
1	B	539	GLN
1	B	554	GLN
1	B	565	HIS
1	B	574	GLN
1	B	589	GLN
1	B	646	ASN
1	C	433	GLN
1	C	447	ASN
1	C	536	ASN
1	C	539	GLN
1	C	625	GLN
1	C	667	HIS
1	D	447	ASN
1	D	449	ASN
1	D	538	ASN
1	D	554	GLN
1	D	589	GLN
1	D	625	GLN
1	D	628	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	216/279 (77%)	-0.93	0 100 100	28, 53, 91, 132	2 (0%)
1	B	227/279 (81%)	-0.60	1 (0%) 88 90	36, 62, 104, 136	3 (1%)
1	C	218/279 (78%)	-0.58	0 100 100	31, 63, 101, 138	1 (0%)
1	D	212/279 (75%)	-0.58	0 100 100	39, 71, 108, 139	7 (3%)
All	All	873/1116 (78%)	-0.67	1 (0%) 92 93	28, 62, 103, 139	13 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	567	PRO	3.0

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(Å ²)	Q<0.9
2	MG	B	1	1/1	0.92	0.09	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	C	2	1/1	0.96	0.06	130,130,130,130	0
2	MG	C	7	1/1	0.97	0.12	102,102,102,102	0
2	MG	A	4	1/1	0.98	0.07	100,100,100,100	0
2	MG	D	3	1/1	0.98	0.05	122,122,122,122	0
2	MG	D	6	1/1	0.98	0.07	130,130,130,130	0
2	MG	B	5	1/1	0.99	0.05	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.