



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2025 – 02:09 PM JST

PDB ID : 9X6Q / pdb_00009x6q
Title : Crystal structure of the Songling virus nucleoprotein
Authors : Yanshin, A.O.; Gladysheva, A.V.
Deposited on : 2025-10-15
Resolution : 2.52 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

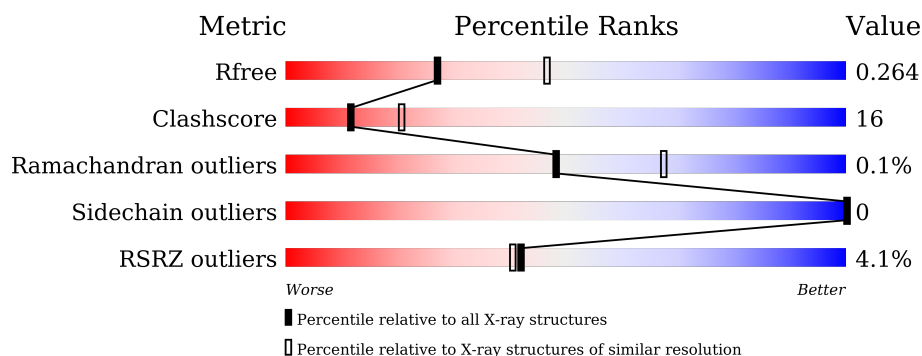
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	164625	6935 (2.54-2.50)
Clashscore	180529	7778 (2.54-2.50)
Ramachandran outliers	177936	7674 (2.54-2.50)
Sidechain outliers	177891	7676 (2.54-2.50)
RSRZ outliers	164620	6935 (2.54-2.50)

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	483	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div></div> </div> </div>
1	B	483	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>25%</div> <div></div> </div> </div>

2 Entry composition [i](#)

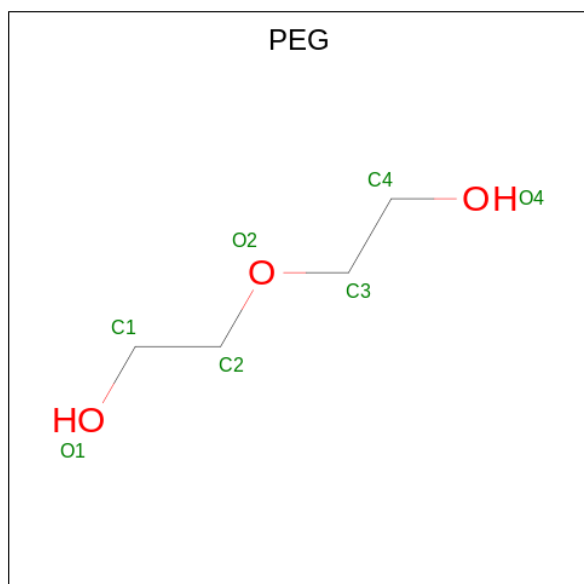
There are 5 unique types of molecules in this entry. The entry contains 7586 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3760	2394	639	707	20			
1	B	479	Total	C	N	O	S	0	0	0
			3781	2407	642	712	20			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total K 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	17	Total O 17 17	0	0
5	B	12	Total O 12 12	0	0

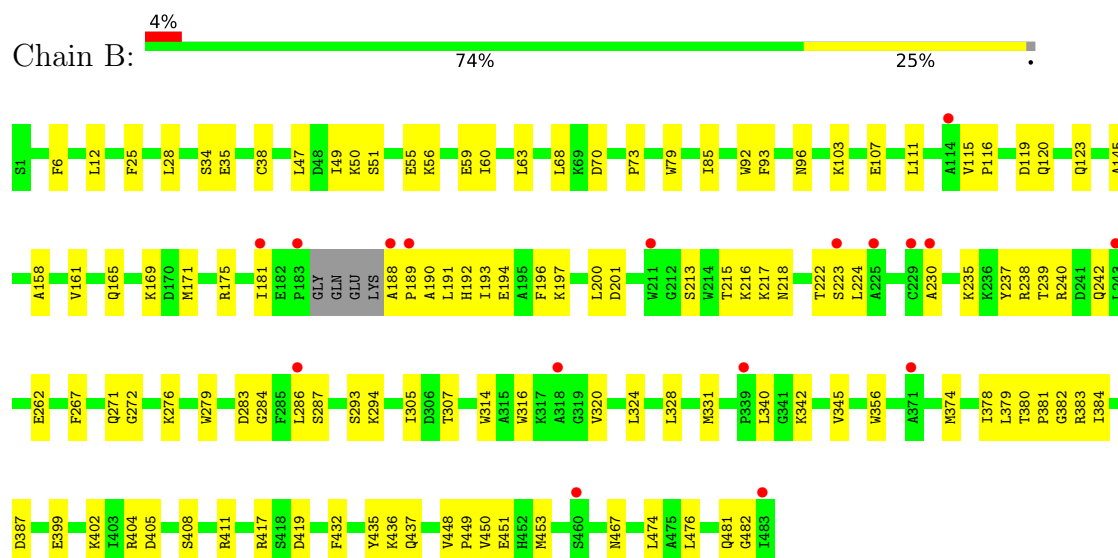
3 Residue-property plots

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: Nucleoprotein



• Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	54.49Å 113.35Å 215.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.27 – 2.52 34.27 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.27-2.52) 99.7 (34.27-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.212 , 0.257 0.218 , 0.264	Depositor DCC
R_{free} test set	2350 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, PEG, K

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	0.43	0/3849	0.65	0/5191
1	B	0.43	0/3871	0.63	0/5223
All	All	0.43	0/7720	0.64	0/10414

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3760	0	3714	123	0
1	B	3781	0	3731	114	0
2	A	7	0	10	0	0
2	B	7	0	10	1	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
5	A	17	0	0	1	0
5	B	12	0	0	1	0
All	All	7586	0	7465	236	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 16.

All (236) 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:69:LYS:CE	1:A:406:GLY:HA2	1.47	1.42
1:A:69:LYS:HE3	1:A:406:GLY:CA	1.51	1.38
1:A:233:VAL:HG21	1:A:240:ARG:HG3	1.46	0.96
1:A:56:LYS:HE3	1:A:438:GLU:O	1.65	0.95
1:A:69:LYS:HD3	1:A:407:SER:N	1.82	0.95
1:A:193:ILE:HD12	1:A:235:LYS:HD2	1.47	0.94
1:A:69:LYS:CD	1:A:406:GLY:HA2	1.98	0.92
1:B:340:LEU:HD23	1:B:340:LEU:O	1.71	0.90
1:B:239:THR:HG23	1:B:242:GLN:H	1.36	0.87
1:B:217:LYS:HA	1:B:224:LEU:CD1	2.07	0.85
1:B:47:LEU:HG	1:B:63:LEU:HD13	1.59	0.84
1:A:69:LYS:HD3	1:A:407:SER:H	1.42	0.84
1:A:233:VAL:HG11	1:A:286:LEU:HD11	1.61	0.82
1:B:374:MET:HB3	1:B:378:ILE:HD11	1.61	0.82
1:A:71:MET:HE1	1:A:413:LEU:HD12	1.63	0.81
1:B:217:LYS:NZ	1:B:218:ASN:OD1	2.14	0.80
1:A:69:LYS:HE3	1:A:406:GLY:N	1.95	0.79
1:A:193:ILE:HD12	1:A:235:LYS:CD	2.13	0.79
1:B:340:LEU:O	1:B:340:LEU:CD2	2.31	0.78
1:B:217:LYS:HA	1:B:224:LEU:HD12	1.66	0.76
1:A:161:VAL:O	1:A:165:GLN:HG3	1.86	0.75
1:B:217:LYS:HD2	1:B:218:ASN:H	1.51	0.75
1:B:107:GLU:O	1:B:111:LEU:CD2	2.34	0.74
1:A:197:LYS:HG3	1:A:237:TYR:CD2	2.22	0.74
1:A:40:GLU:HG3	1:A:42:LEU:HD13	1.69	0.74
1:A:258:GLY:O	1:A:265:LYS:HD2	1.88	0.73
1:A:69:LYS:HE3	1:A:406:GLY:HA2	0.75	0.73
1:B:107:GLU:O	1:B:111:LEU:HD22	1.88	0.73
1:B:217:LYS:HD2	1:B:224:LEU:HD12	1.71	0.72
1:A:69:LYS:CD	1:A:407:SER:H	2.02	0.71
1:A:255:GLU:OE2	1:A:276:LYS:NZ	2.24	0.71
1:A:50:LYS:O	1:A:56:LYS:NZ	2.24	0.71
1:A:31:LEU:O	1:A:417:ARG:HG3	1.94	0.68
1:B:196:PHE:CZ	1:B:200:LEU:HD11	2.29	0.68
1:A:69:LYS:CE	1:A:406:GLY:CA	2.34	0.66
1:B:107:GLU:HB2	1:B:111:LEU:HD21	1.78	0.64
1:A:168:LEU:HD12	1:A:480:ILE:HD11	1.79	0.64
1:B:217:LYS:HE3	1:B:222:THR:C	2.23	0.64
1:B:158:ALA:HA	1:B:161:VAL:HG23	1.80	0.63
1:A:218:ASN:HB3	1:A:224:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASP:OD1	1:B:238:ARG:NH2	2.32	0.63
1:B:111:LEU:HD11	1:B:120:GLN:NE2	2.14	0.62
1:A:196:PHE:CE2	1:A:200:LEU:HD11	2.34	0.62
1:A:233:VAL:CG1	1:A:286:LEU:HD11	2.29	0.62
1:B:49:ILE:HD12	1:B:49:ILE:H	1.64	0.62
1:A:230:ALA:HB2	1:A:282:VAL:HG23	1.82	0.62
1:B:293:SER:C	1:B:294:LYS:HD3	2.25	0.61
1:A:71:MET:HE3	1:A:416:LEU:HD11	1.83	0.61
1:A:168:LEU:HD11	1:A:478:VAL:HG13	1.83	0.61
1:A:217:LYS:HG2	1:A:223:SER:HA	1.83	0.61
1:B:47:LEU:H	1:B:437:GLN:HE22	1.49	0.60
1:A:193:ILE:CD1	1:A:235:LYS:HD2	2.25	0.60
1:B:283:ASP:OD1	1:B:284:GLY:N	2.35	0.60
1:B:235:LYS:HE3	1:B:237:TYR:CZ	2.36	0.60
1:B:217:LYS:HD2	1:B:224:LEU:CD1	2.31	0.60
1:B:217:LYS:HD2	1:B:218:ASN:N	2.17	0.59
1:A:152:LYS:HD3	1:A:153:ILE:H	1.67	0.59
1:B:191:LEU:HG	1:B:194:GLU:OE1	2.01	0.59
1:B:111:LEU:HD22	1:B:111:LEU:H	1.67	0.59
1:B:115:VAL:HG22	1:B:116:PRO:HD2	1.85	0.58
1:B:293:SER:O	1:B:294:LYS:HD3	2.04	0.58
1:B:103:LYS:O	1:B:107:GLU:HG3	2.03	0.58
1:A:150:VAL:HG12	1:A:459:LEU:HD23	1.84	0.58
1:A:25:PHE:HE1	1:A:404:ARG:HD2	1.68	0.58
1:B:50:LYS:HG3	1:B:55:GLU:O	2.04	0.58
1:B:218:ASN:N	1:B:224:LEU:HD11	2.19	0.57
1:A:239:THR:OG1	1:A:242:GLN:HG3	2.04	0.57
1:A:193:ILE:O	1:A:232:LEU:HD21	2.04	0.57
1:A:450:VAL:HA	1:A:453:MET:HE3	1.87	0.57
1:B:342:LYS:HD2	1:B:382:GLY:HA2	1.87	0.57
1:A:155:ARG:NH1	1:A:481:GLN:HE21	2.03	0.57
1:A:435:TYR:CE2	1:A:448:VAL:HG23	2.40	0.57
1:B:175:ARG:HD2	1:B:476:LEU:HD12	1.85	0.57
1:A:260:LEU:O	1:A:265:LYS:NZ	2.37	0.56
1:A:218:ASN:HD22	1:A:219:LYS:HG3	1.70	0.56
1:A:272:GLY:O	1:A:276:LYS:HG2	2.05	0.56
1:B:320:VAL:HG11	1:B:328:LEU:HD22	1.85	0.56
1:A:289:THR:HB	1:A:301:GLN:HG2	1.86	0.56
1:A:320:VAL:HG23	1:A:324:LEU:HB2	1.88	0.56
1:B:6:PHE:CE1	1:B:12:LEU:HD12	2.41	0.56
1:A:332:LEU:HD11	1:A:388:MET:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:VAL:HG23	1:A:461:LYS:HG2	1.88	0.55
1:A:413:LEU:HD21	1:A:428:ILE:HG22	1.88	0.55
1:A:423:PRO:HA	1:A:426:GLN:HB2	1.87	0.55
1:A:69:LYS:HD2	1:A:69:LYS:O	2.08	0.54
1:A:246:GLU:O	1:A:250:ILE:HG13	2.07	0.54
1:A:428:ILE:HG13	1:A:429:CYS:N	2.23	0.54
1:A:197:LYS:NZ	1:A:201:ASP:OD2	2.32	0.54
1:A:232:LEU:HD22	1:A:237:TYR:HD2	1.72	0.53
1:A:421:GLU:O	1:A:426:GLN:NE2	2.41	0.53
1:B:307:THR:HB	1:B:387:ASP:HB3	1.90	0.53
1:B:6:PHE:CZ	1:B:12:LEU:HD12	2.43	0.53
1:A:360:MET:HA	1:A:363:MET:HG3	1.90	0.53
1:B:171:MET:HE3	1:B:451:GLU:O	2.09	0.53
1:B:79:TRP:CZ2	1:B:85:ILE:HD11	2.44	0.53
1:A:40:GLU:HG3	1:A:42:LEU:CD1	2.38	0.53
1:A:197:LYS:HE2	1:A:238:ARG:NH1	2.24	0.53
1:B:217:LYS:HE3	1:B:222:THR:O	2.09	0.52
1:B:450:VAL:HA	1:B:453:MET:HE3	1.91	0.52
1:B:161:VAL:O	1:B:165:GLN:HG3	2.10	0.52
1:B:399:GLU:HG3	1:B:402:LYS:HG3	1.92	0.52
1:A:344:LYS:O	1:A:348:LYS:HG3	2.10	0.52
1:A:232:LEU:HD22	1:A:237:TYR:CD2	2.44	0.51
1:B:217:LYS:CE	1:B:222:THR:H	2.24	0.51
1:B:272:GLY:O	1:B:276:LYS:HG2	2.10	0.51
1:B:267:PHE:CE2	1:B:271:GLN:HG3	2.45	0.51
1:A:69:LYS:HD3	1:A:406:GLY:C	2.34	0.51
1:B:194:GLU:HA	1:B:197:LYS:CB	2.41	0.51
1:B:287:SER:HB3	1:B:474:LEU:HB2	1.93	0.51
1:A:150:VAL:CG1	1:A:459:LEU:HD23	2.41	0.50
1:A:374:MET:HE2	1:A:374:MET:HA	1.93	0.50
1:A:259:GLU:C	1:A:265:LYS:NZ	2.69	0.50
1:B:191:LEU:HA	1:B:193:ILE:HD12	1.92	0.50
1:B:314:TRP:CD2	1:B:379:LEU:HD13	2.47	0.50
1:A:401:ALA:O	1:A:404:ARG:HG3	2.11	0.50
1:B:25:PHE:CE2	1:B:404:ARG:HG3	2.46	0.50
1:B:217:LYS:HE3	1:B:222:THR:H	1.76	0.50
1:B:217:LYS:CD	1:B:224:LEU:HD12	2.38	0.50
1:A:259:GLU:O	1:A:265:LYS:NZ	2.45	0.50
1:B:107:GLU:C	1:B:111:LEU:CD2	2.85	0.50
1:B:305:ILE:HD11	1:B:383:ARG:HE	1.76	0.50
1:A:200:LEU:HD12	1:A:200:LEU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ASP:O	1:B:123:GLN:HG3	2.11	0.49
1:A:7:SER:CB	1:A:84:GLY:HA3	2.42	0.49
1:A:196:PHE:O	1:A:200:LEU:HD12	2.11	0.49
1:A:251:GLY:O	1:A:255:GLU:HG3	2.12	0.49
1:A:417:ARG:NH1	1:A:419:ASP:OD1	2.45	0.49
1:A:259:GLU:C	1:A:265:LYS:HZ3	2.20	0.48
1:B:107:GLU:C	1:B:111:LEU:HD23	2.38	0.48
1:B:190:ALA:HB1	1:B:192:HIS:CD2	2.48	0.48
1:B:218:ASN:H	1:B:224:LEU:HD11	1.77	0.48
1:A:178:ALA:HB1	1:A:294:LYS:HZ2	1.78	0.48
1:B:402:LYS:O	1:B:405:ASP:HB2	2.14	0.48
1:B:432:PHE:CE2	1:B:436:LYS:HE2	2.49	0.47
1:B:145:ALA:HA	1:B:467:ASN:HB3	1.96	0.47
1:A:247:LEU:HD12	1:A:279:TRP:HE3	1.80	0.47
1:B:196:PHE:O	1:B:200:LEU:HD13	2.15	0.47
1:B:380:THR:HG23	1:B:383:ARG:HD2	1.97	0.47
1:A:25:PHE:CE1	1:A:404:ARG:HD2	2.48	0.46
1:B:107:GLU:O	1:B:111:LEU:HD23	2.15	0.46
1:B:188:ALA:N	1:B:189:PRO:HD2	2.29	0.46
1:B:196:PHE:CE1	1:B:200:LEU:HD11	2.50	0.46
1:B:240:ARG:HG3	1:B:279:TRP:CZ2	2.51	0.46
1:B:217:LYS:HE3	1:B:222:THR:CA	2.45	0.46
1:A:226:VAL:HG12	1:A:278:LEU:HD11	1.97	0.46
1:A:269:LYS:HE3	1:A:273:THR:HB	1.98	0.46
1:A:69:LYS:CD	1:A:406:GLY:CA	2.82	0.45
1:A:196:PHE:HB2	1:A:211:TRP:CZ3	2.51	0.45
1:A:100:LYS:O	1:A:103:LYS:HE2	2.16	0.45
1:A:418:SER:HA	1:A:422:ASN:OD1	2.16	0.45
1:B:111:LEU:HD22	1:B:111:LEU:N	2.30	0.45
1:A:279:TRP:CE3	1:A:282:VAL:HG11	2.52	0.45
1:B:34:SER:HB3	1:B:73:PRO:HB3	1.98	0.45
1:B:194:GLU:HA	1:B:197:LYS:HB2	1.99	0.45
1:A:47:LEU:HD22	1:A:63:LEU:CD1	2.46	0.45
1:B:381:PRO:O	1:B:384:ILE:HG22	2.17	0.45
1:A:300:GLN:NE2	5:A:603:HOH:O	2.48	0.45
1:A:450:VAL:HA	1:A:453:MET:CE	2.46	0.45
1:B:196:PHE:CE2	1:B:200:LEU:HD11	2.51	0.45
1:A:84:GLY:O	1:A:88:ARG:HG3	2.15	0.45
1:B:47:LEU:H	1:B:437:GLN:NE2	2.13	0.45
1:B:320:VAL:HG23	1:B:324:LEU:HB2	1.98	0.45
1:B:93:PHE:HB3	1:B:316:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:H	1:A:152:LYS:CD	2.30	0.44
1:A:176:ASN:O	1:A:180:LYS:HG3	2.15	0.44
1:B:217:LYS:NZ	1:B:218:ASN:CG	2.76	0.44
1:A:69:LYS:CE	1:A:407:SER:H	2.30	0.44
1:A:197:LYS:HE2	1:A:238:ARG:HH12	1.82	0.44
1:B:481:GLN:HG2	1:B:482:GLY:N	2.32	0.44
1:B:51:SER:O	1:B:56:LYS:HE2	2.17	0.44
1:A:315:ALA:O	1:A:320:VAL:HG12	2.18	0.44
1:A:331:MET:HE3	1:A:331:MET:HB3	1.77	0.44
1:B:342:LYS:O	1:B:345:VAL:HG12	2.18	0.44
1:A:71:MET:HE3	1:A:416:LEU:CD1	2.47	0.44
1:A:216:LYS:HA	1:A:216:LYS:HD3	1.46	0.44
1:B:215:THR:OG1	1:B:216:LYS:HE2	2.18	0.44
1:A:355:VAL:HG23	1:B:262:GLU:O	2.18	0.43
1:A:243:LEU:O	1:A:247:LEU:HB2	2.18	0.43
1:B:169:LYS:HE3	1:B:169:LYS:HB2	1.62	0.43
1:B:402:LYS:HB3	1:B:402:LYS:HE2	1.61	0.43
1:A:197:LYS:HA	1:A:232:LEU:HD11	2.00	0.43
1:B:191:LEU:C	1:B:193:ILE:N	2.76	0.43
1:B:331:MET:HG2	1:B:356:TRP:HH2	1.83	0.43
1:A:233:VAL:HA	1:A:238:ARG:O	2.18	0.43
1:A:238:ARG:HB2	1:A:243:LEU:HD11	2.00	0.42
1:A:320:VAL:HG11	1:A:328:LEU:HD22	2.00	0.42
1:B:239:THR:OG1	1:B:240:ARG:N	2.52	0.42
1:B:194:GLU:OE1	1:B:194:GLU:N	2.52	0.42
1:A:196:PHE:CZ	1:A:200:LEU:HD11	2.53	0.42
1:A:339:PRO:O	1:A:340:LEU:HD23	2.19	0.42
1:A:411:ARG:NH1	1:A:456:GLN:HG2	2.35	0.42
1:B:283:ASP:OD1	1:B:283:ASP:C	2.62	0.42
1:A:279:TRP:HA	1:A:282:VAL:HG12	2.00	0.42
1:B:217:LYS:HA	1:B:217:LYS:HD2	1.66	0.42
1:A:209:CYS:HB3	1:A:212:GLY:O	2.20	0.42
1:A:254:VAL:HG12	1:A:268:CYS:O	2.19	0.42
1:B:240:ARG:HG3	1:B:279:TRP:CH2	2.55	0.42
1:A:337:LYS:HG2	1:A:406:GLY:O	2.19	0.42
1:A:347:LYS:HE3	1:A:351:GLU:OE2	2.20	0.42
1:B:194:GLU:HA	1:B:197:LYS:HB3	2.00	0.42
1:A:190:ALA:C	1:A:192:HIS:H	2.28	0.41
1:A:327:THR:HG21	1:A:354:PHE:CZ	2.55	0.41
1:A:155:ARG:HA	1:A:481:GLN:O	2.19	0.41
1:A:482:GLY:O	1:A:483:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:HE3	1:A:405:ASP:HB3	2.01	0.41
1:A:428:ILE:HD13	1:A:454:LEU:HD13	2.03	0.41
1:B:38:CYS:N	1:B:70:ASP:O	2.54	0.41
1:B:56:LYS:O	1:B:60:ILE:HG13	2.20	0.41
1:B:217:LYS:HZ1	1:B:218:ASN:CG	2.23	0.41
1:A:193:ILE:HG13	1:A:194:GLU:CD	2.46	0.41
1:B:35:GLU:HG3	2:B:501:PEG:H41	2.03	0.41
1:B:49:ILE:HD12	1:B:49:ILE:N	2.33	0.41
1:B:92:TRP:O	1:B:96:ASN:ND2	2.43	0.41
1:A:348:LYS:HE3	1:A:348:LYS:HB3	1.95	0.41
1:B:435:TYR:CE2	1:B:448:VAL:HG23	2.56	0.41
1:A:7:SER:HB3	1:A:84:GLY:HA3	2.02	0.41
1:A:89:SER:OG	1:A:312:HIS:HB3	2.21	0.41
1:A:196:PHE:CD2	1:A:200:LEU:HD11	2.56	0.41
1:B:181:ILE:HD13	1:B:181:ILE:HA	1.93	0.41
1:B:213:SER:HB3	1:B:216:LYS:HG2	2.01	0.41
1:A:68:LEU:N	1:A:68:LEU:HD23	2.36	0.41
1:B:222:THR:O	1:B:223:SER:C	2.64	0.41
1:B:417:ARG:HB3	1:B:419:ASP:OD1	2.21	0.41
1:A:69:LYS:CD	1:A:407:SER:N	2.62	0.40
1:B:59:GLU:O	1:B:63:LEU:HD12	2.21	0.40
1:B:374:MET:HE3	1:B:378:ILE:HD11	2.03	0.40
1:A:294:LYS:HD3	1:A:295:ASN:N	2.35	0.40
1:B:68:LEU:HB2	1:B:408:SER:HB2	2.04	0.40
1:B:158:ALA:HA	1:B:161:VAL:CG2	2.49	0.40
1:B:230:ALA:HB1	1:B:286:LEU:HD21	2.03	0.40
1:A:379:LEU:HD11	1:A:384:ILE:HB	2.04	0.40
1:B:28:LEU:O	1:B:35:GLU:HA	2.21	0.40
1:B:449:PRO:O	1:B:453:MET:HG3	2.21	0.40
1:B:217:LYS:CD	1:B:218:ASN:H	2.29	0.40
1:A:41:VAL:HG21	1:A:426:GLN:HB3	2.03	0.40
1:B:411:ARG:HD2	5:B:601:HOH:O	2.21	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	472/483 (98%)	450 (95%)	21 (4%)	1 (0%)	44	62
1	B	475/483 (98%)	454 (96%)	21 (4%)	0	100	100
All	All	947/966 (98%)	904 (96%)	42 (4%)	1 (0%)	48	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	GLY

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	406/411 (99%)	406 (100%)	0	100	100
1	B	408/411 (99%)	408 (100%)	0	100	100
All	All	814/822 (99%)	814 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	234	ASN
1	A	300	GLN
1	A	366	GLN
1	A	481	GLN
1	B	192	HIS
1	B	437	GLN
1	B	445	GLN

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Mol	Chain	Res	Type
1	B	455	HIS
1	B	470	GLN
1	B	472	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	PEG	B	501	-	6,6,6	0.48	0	5,5,5	0.61	0
2	PEG	A	501	-	6,6,6	0.23	0	5,5,5	0.40	0

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
2	PEG	B	501	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	501	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PEG	O1-C1-C2-O2
2	A	501	PEG	O2-C3-C4-O4
2	B	501	PEG	O2-C3-C4-O4
2	B	501	PEG	O1-C1-C2-O2
2	A	501	PEG	C4-C3-O2-C2
2	A	501	PEG	C1-C2-O2-C3
2	B	501	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PEG	1	0

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	476/483 (98%)	0.22	22 (4%) 38 37	64, 81, 153, 175	0
1	B	479/483 (99%)	0.25	17 (3%) 47 46	68, 87, 124, 150	0
All	All	955/966 (98%)	0.24	39 (4%) 42 40	64, 84, 141, 175	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	PHE	4.2
1	A	189	PRO	3.6
1	B	114	ALA	3.5
1	A	192	HIS	3.2
1	A	205	TYR	3.2
1	A	191	LEU	2.9
1	A	274	PHE	2.8
1	B	181	ILE	2.7
1	B	229	CYS	2.7
1	B	230	ALA	2.7
1	A	229	CYS	2.6
1	A	199	TRP	2.6
1	A	190	ALA	2.6
1	B	460	SER	2.6
1	B	286	LEU	2.5
1	A	254	VAL	2.5
1	B	183	PRO	2.5
1	A	208	PRO	2.4
1	A	195	ALA	2.4
1	A	247	LEU	2.4
1	A	373	HIS	2.4
1	A	181	ILE	2.4
1	B	483	ILE	2.3
1	A	244	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	225	ALA	2.3
1	A	275	PHE	2.3
1	B	189	PRO	2.3
1	A	243	LEU	2.2
1	A	250	ILE	2.2
1	B	243	LEU	2.1
1	A	268	CYS	2.1
1	B	371	ALA	2.1
1	B	318	ALA	2.1
1	A	227	THR	2.1
1	A	203	LYS	2.1
1	B	188	ALA	2.1
1	B	223	SER	2.1
1	B	211	TRP	2.0
1	B	339	PRO	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(Å ²)	Q<0.9
2	PEG	B	501	7/7	0.84	0.12	86,86,91,94	0
4	K	B	503	1/1	0.84	0.12	120,120,120,120	0
3	CL	B	502	1/1	0.88	0.19	106,106,106,106	0
2	PEG	A	501	7/7	0.92	0.15	70,72,76,83	7

6.5 Other polymers [i](#)

There are no such residues in this entry.