



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:32 am BST

PDB ID : 6EB8
Title : Crystal Structure of the Nipah Virus Phosphoprotein Multimerization Domain G519N
Authors : Bruhn, J.F.; Saphire, E.O.
Deposited on : 2018-08-06
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

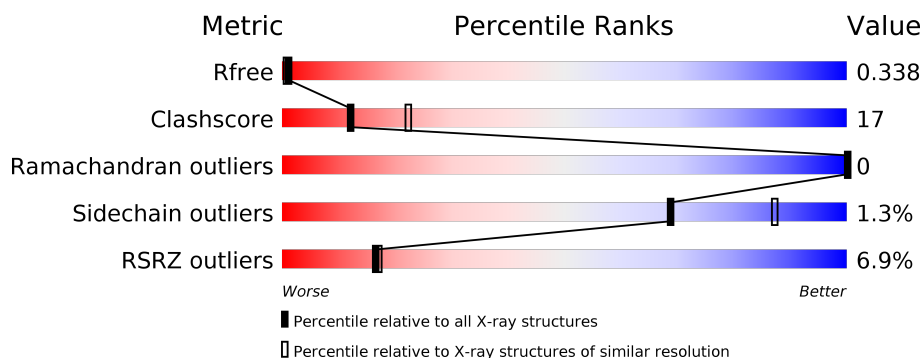
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	110	<div> <div>7%</div> <div> <div></div> <div>57%</div> <div>37%</div> <div>5%</div> </div> </div>
1	B	110	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>26%</div> <div>9%</div> </div> </div>
1	C	110	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>9%</div> </div> </div>
1	D	110	<div> <div>11%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>8%</div> </div> </div>
1	E	110	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>6%</div> </div> </div>
1	F	110	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>26%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	110	<div><div></div><div>9%</div><div>59%</div><div>33%</div><div>8%</div></div>
1	H	110	<div><div></div><div>8%</div><div>51%</div><div>40%</div><div>8%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6673 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			840	530	138	165	7			
1	E	103	Total	C	N	O	S	0	1	0
			838	529	138	164	7			
1	D	101	Total	C	N	O	S	0	0	0
			816	515	135	160	6			
1	C	100	Total	C	N	O	S	0	0	0
			807	509	133	159	6			
1	H	101	Total	C	N	O	S	0	0	0
			816	515	135	160	6			
1	F	101	Total	C	N	O	S	0	0	0
			816	515	135	160	6			
1	B	100	Total	C	N	O	S	0	0	0
			808	509	134	159	6			
1	G	101	Total	C	N	O	S	0	0	0
			816	515	135	160	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	SER	-	expression tag	UNP Q9IK91
A	519	ASN	GLY	engineered mutation	UNP Q9IK91
E	469	SER	-	expression tag	UNP Q9IK91
E	519	ASN	GLY	engineered mutation	UNP Q9IK91
D	469	SER	-	expression tag	UNP Q9IK91
D	519	ASN	GLY	engineered mutation	UNP Q9IK91
C	469	SER	-	expression tag	UNP Q9IK91
C	519	ASN	GLY	engineered mutation	UNP Q9IK91
H	469	SER	-	expression tag	UNP Q9IK91
H	519	ASN	GLY	engineered mutation	UNP Q9IK91
F	469	SER	-	expression tag	UNP Q9IK91
F	519	ASN	GLY	engineered mutation	UNP Q9IK91
B	469	SER	-	expression tag	UNP Q9IK91

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Chain	Residue	Modelled	Actual	Comment	Reference
B	519	ASN	GLY	engineered mutation	UNP Q9IK91
G	469	SER	-	expression tag	UNP Q9IK91
G	519	ASN	GLY	engineered mutation	UNP Q9IK91

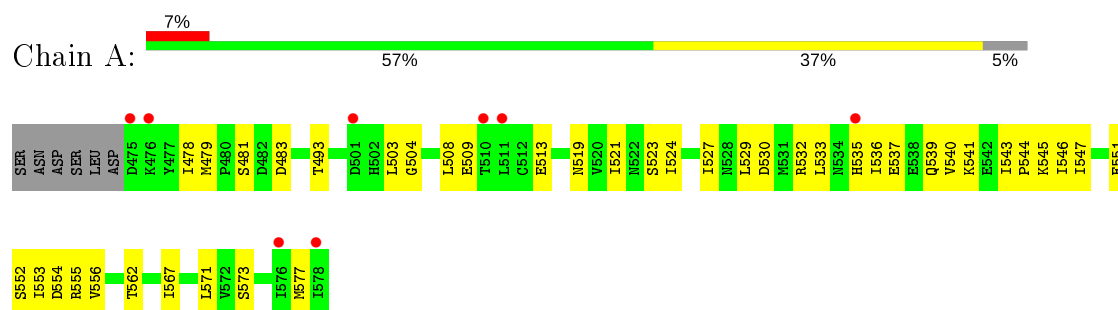
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	E	20	Total O 20 20	0	0
2	D	12	Total O 12 12	0	0
2	C	22	Total O 22 22	0	0
2	H	5	Total O 5 5	0	0
2	F	22	Total O 22 22	0	0
2	B	10	Total O 10 10	0	0
2	G	16	Total O 16 16	0	0

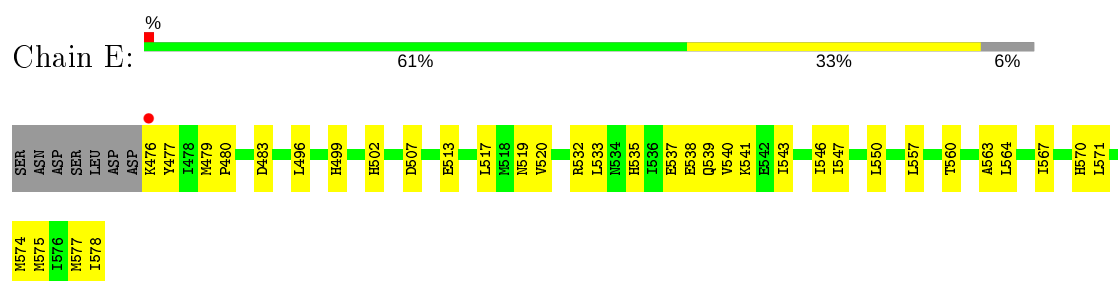
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

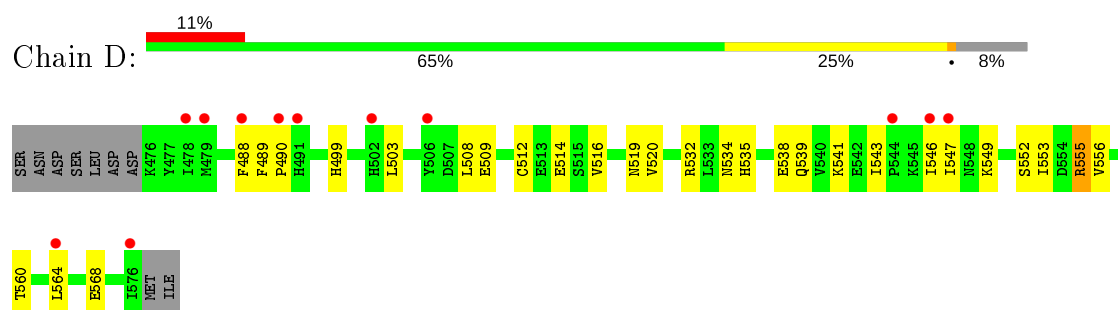
• Molecule 1: Phosphoprotein



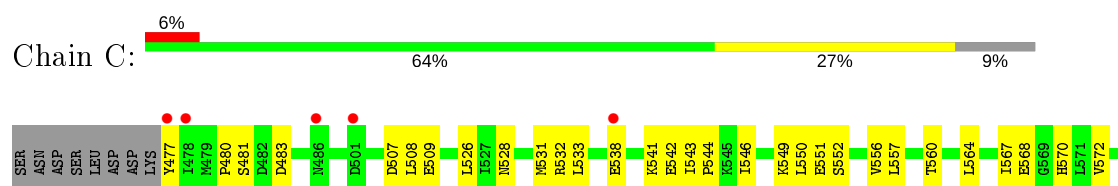
• Molecule 1: Phosphoprotein



• Molecule 1: Phosphoprotein

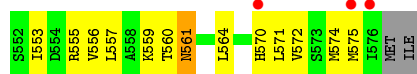


• Molecule 1: Phosphoprotein

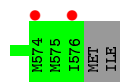




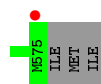
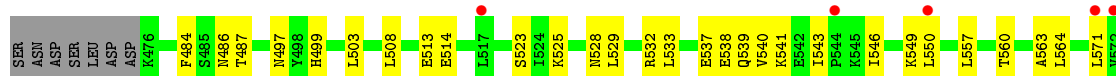
- Molecule 1: Phosphoprotein



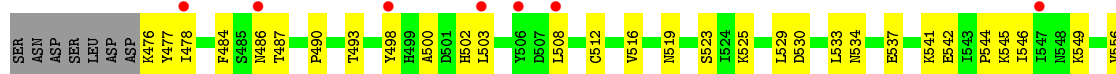
- Molecule 1: Phosphoprotein



- Molecule 1: Phosphoprotein



- Molecule 1: Phosphoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.00Å 76.62Å 80.54Å 100.46° 100.94° 108.05°	Depositor
Resolution (Å)	38.20 – 2.50 38.20 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.20-2.50) 86.8 (38.20-2.50)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.276 , 0.338 0.276 , 0.338	Depositor DCC
R_{free} test set	1771 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 70.4	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	0.86	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.34% 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](#)

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	0.45	0/853	0.69	0/1153
1	B	0.45	0/821	0.66	0/1110
1	C	0.45	0/820	0.67	0/1110
1	D	0.52	0/829	0.72	0/1121
1	E	0.49	0/851	0.73	0/1150
1	F	0.48	0/829	0.71	0/1121
1	G	0.66	0/829	0.73	1/1121 (0.1%)
1	H	0.52	0/829	0.67	0/1121
All	All	0.51	0/6661	0.70	1/9007 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	525	LYS	CD-CE-NZ	-6.58	96.56	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	840	0	836	39	0
1	B	808	0	801	28	0
1	C	807	0	799	33	0
1	D	816	0	812	36	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	838	0	836	51	1
1	F	816	0	812	40	0
1	G	816	0	812	51	0
1	H	816	0	812	57	0
2	A	9	0	0	1	0
2	B	10	0	0	1	0
2	C	22	0	0	1	0
2	D	12	0	0	0	0
2	E	20	0	0	0	0
2	F	22	0	0	2	0
2	G	16	0	0	1	0
2	H	5	0	0	1	0
All	All	6673	0	6520	224	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 17.

All (224) 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:H:508:LEU:HD22	1:G:508:LEU:CD1	1.56	1.34
1:H:508:LEU:CD2	1:G:508:LEU:HD13	1.71	1.20
1:H:508:LEU:HD22	1:G:508:LEU:HD13	1.14	1.08
1:F:525:LYS:NZ	1:G:523:SER:OG	1.87	1.08
1:H:508:LEU:CD2	1:G:508:LEU:CD1	2.35	1.02
1:H:508:LEU:HD22	1:G:508:LEU:HD11	1.42	1.00
1:E:560:THR:OG1	1:F:561:ASN:ND2	1.96	0.98
1:E:560:THR:HG1	1:F:561:ASN:ND2	1.68	0.91
1:E:541:LYS:HA	1:H:539:GLN:HE22	1.34	0.90
1:H:533:LEU:HD21	1:G:533:LEU:CD1	2.01	0.90
1:H:533:LEU:HD21	1:G:533:LEU:HD12	1.53	0.89
1:D:489:PHE:HB3	1:D:490:PRO:HD2	1.63	0.81
1:E:479:MET:CE	1:F:514:GLU:HG3	2.12	0.80
1:C:543:ILE:HD11	1:B:539:GLN:O	1.82	0.80
1:E:533:LEU:HD12	1:H:529:LEU:HD22	1.63	0.78
1:E:532:ARG:NH2	1:F:534:ASN:OD1	2.16	0.77
1:F:560:THR:HG23	1:G:564:LEU:HD11	1.65	0.76
1:F:545:LYS:HG2	1:F:549:LYS:HE2	1.67	0.76
1:E:479:MET:HE1	1:F:514:GLU:HG3	1.66	0.76
1:E:483:ASP:OD2	1:F:499:HIS:NE2	2.17	0.75
1:E:578:ILE:O	1:E:578:ILE:HG13	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:561:ASN:ND2	1:G:560:THR:OG1	2.14	0.74
1:G:476:LYS:HG3	1:G:477:TYR:H	1.53	0.74
1:G:498:TYR:O	1:G:502:HIS:ND1	2.21	0.72
1:H:533:LEU:CD2	1:G:533:LEU:HD12	2.20	0.72
1:C:549:LYS:NZ	2:C:601:HOH:O	2.23	0.71
1:E:476:LYS:HG3	1:E:477:TYR:H	1.55	0.71
1:H:498:TYR:O	1:H:502:HIS:ND1	2.24	0.70
1:D:489:PHE:HB3	1:D:490:PRO:CD	2.22	0.69
1:E:541:LYS:HA	1:H:539:GLN:NE2	2.06	0.69
1:E:479:MET:HE3	1:E:480:PRO:CD	2.23	0.68
1:H:559:LYS:NZ	2:H:602:HOH:O	2.26	0.68
1:D:499:HIS:O	1:D:503:LEU:HD22	1.92	0.67
1:E:479:MET:CE	1:E:480:PRO:HD2	2.23	0.67
1:H:551:GLU:OE1	1:H:555:ARG:NH1	2.27	0.67
1:F:545:LYS:NZ	2:F:601:HOH:O	2.28	0.66
1:F:532:ARG:NH1	1:G:537:GLU:OE1	2.27	0.66
1:H:509:GLU:HA	1:G:508:LEU:HD21	1.78	0.65
1:H:542:GLU:OE1	1:H:545:LYS:HD2	1.96	0.65
1:A:508:LEU:H	1:A:508:LEU:HD12	1.61	0.64
1:H:533:LEU:HD21	1:G:533:LEU:HD11	1.80	0.64
1:H:556:VAL:O	1:H:560:THR:HG23	1.98	0.63
1:H:571:LEU:HD13	1:G:570:HIS:HB2	1.80	0.63
1:A:552:SER:HA	1:A:555:ARG:HE	1.63	0.63
1:E:479:MET:HE3	1:E:480:PRO:HD2	1.80	0.62
1:B:537:GLU:HA	1:B:540:VAL:HG22	1.80	0.62
1:C:564:LEU:HD11	1:B:560:THR:HG23	1.82	0.62
1:A:554:ASP:OD2	1:D:549:LYS:NZ	2.34	0.61
1:F:519:ASN:OD1	1:G:519:ASN:ND2	2.33	0.61
1:D:568:GLU:HG2	1:C:567:ILE:HG12	1.83	0.60
1:H:508:LEU:HD21	1:G:508:LEU:HD13	1.79	0.60
1:A:547:ILE:O	1:A:551:GLU:HG3	2.01	0.60
1:A:567:ILE:HD11	1:B:564:LEU:O	2.02	0.60
1:D:499:HIS:O	1:D:503:LEU:CD2	2.50	0.60
1:A:533:LEU:HD23	1:A:536:ILE:HB	1.85	0.59
1:C:509:GLU:HG3	1:B:508:LEU:HD21	1.83	0.59
1:D:509:GLU:HA	1:C:508:LEU:HD21	1.84	0.59
1:E:479:MET:HE2	1:F:514:GLU:HG3	1.84	0.59
1:H:529:LEU:O	1:H:533:LEU:HD12	2.03	0.59
1:A:519:ASN:ND2	1:D:519:ASN:OD1	2.35	0.59
1:C:533:LEU:HD12	1:B:529:LEU:HD22	1.85	0.58
1:H:484:PHE:CZ	1:F:520:VAL:HG13	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:GLU:OE1	1:C:570:HIS:CD2	2.57	0.57
1:A:571:LEU:HG	1:B:571:LEU:HD11	1.86	0.57
1:A:554:ASP:CG	1:D:549:LYS:HZ1	2.07	0.57
1:A:529:LEU:HD22	1:B:533:LEU:HD12	1.86	0.57
1:D:512:CYS:O	1:D:516:VAL:HG23	2.06	0.56
1:A:544:PRO:HD3	1:D:539:GLN:OE1	2.05	0.56
1:C:557:LEU:HD21	1:B:557:LEU:HD21	1.86	0.56
1:D:503:LEU:HD22	1:D:503:LEU:N	2.21	0.56
1:A:537:GLU:O	1:A:541:LYS:HD3	2.05	0.55
1:F:507:ASP:HB2	2:F:605:HOH:O	2.07	0.55
1:A:481:SER:OG	1:B:514:GLU:OE2	2.24	0.55
1:E:479:MET:HE3	1:E:480:PRO:HD3	1.87	0.54
1:E:537:GLU:HB2	1:H:536:ILE:HD11	1.89	0.54
1:B:538:GLU:O	1:B:541:LYS:HG2	2.08	0.54
1:D:499:HIS:NE2	1:C:483:ASP:OD2	2.41	0.54
1:G:512:CYS:O	1:G:516:VAL:HG23	2.08	0.53
1:C:552:SER:O	1:C:556:VAL:HG23	2.09	0.53
1:A:573:SER:O	1:A:577:MET:HG3	2.09	0.53
1:B:540:VAL:O	1:B:543:ILE:HD12	2.09	0.53
1:F:532:ARG:HD2	1:G:530:ASP:OD2	2.09	0.52
1:A:546:ILE:HG23	1:B:550:LEU:HD11	1.92	0.52
1:B:528:ASN:O	1:B:532:ARG:HD2	2.08	0.52
1:D:543:ILE:HG23	1:C:546:ILE:HD11	1.92	0.52
1:E:538:GLU:O	1:E:541:LYS:HG2	2.10	0.52
1:A:539:GLN:N	1:A:539:GLN:OE1	2.41	0.52
1:F:535:HIS:HA	1:F:538:GLU:HG3	1.91	0.52
1:E:520:VAL:HG13	1:G:484:PHE:CZ	2.45	0.51
1:A:521:ILE:HG23	1:D:488:PHE:CZ	2.45	0.51
1:B:497:ASN:HB2	2:B:602:HOH:O	2.09	0.51
1:B:486:ASN:OD1	1:B:487:THR:HG23	2.10	0.51
1:D:503:LEU:HD22	1:D:503:LEU:H	1.75	0.51
1:F:545:LYS:O	1:F:549:LYS:HG2	2.10	0.51
1:G:476:LYS:HG3	1:G:477:TYR:N	2.25	0.51
1:E:546:ILE:HD11	1:F:543:ILE:HG23	1.92	0.51
1:G:529:LEU:O	1:G:533:LEU:HD13	2.11	0.51
1:D:514:GLU:OE1	1:C:481:SER:N	2.36	0.51
1:E:575:MET:HG2	1:H:574:MET:HG3	1.93	0.50
1:A:546:ILE:HG23	1:B:550:LEU:CD1	2.41	0.50
1:D:520:VAL:HG13	1:B:484:PHE:CZ	2.47	0.50
1:F:545:LYS:HG2	1:F:549:LYS:CE	2.40	0.50
1:F:545:LYS:HE3	1:F:549:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:551:GLU:OE1	1:H:555:ARG:CZ	2.59	0.50
1:A:530:ASP:OD1	1:D:532:ARG:NE	2.44	0.50
1:A:540:VAL:HG12	1:D:539:GLN:HB2	1.94	0.50
1:E:537:GLU:OE1	1:H:535:HIS:ND1	2.45	0.50
1:D:534:ASN:OD1	1:C:532:ARG:NH2	2.35	0.49
1:A:536:ILE:HD11	1:B:537:GLU:HG3	1.94	0.49
1:E:563:ALA:HB1	1:F:564:LEU:HB3	1.94	0.49
1:C:543:ILE:CD1	1:B:539:GLN:O	2.59	0.49
1:E:499:HIS:CE1	1:H:480:PRO:HA	2.48	0.49
1:C:550:LEU:HD11	1:B:546:ILE:HG23	1.95	0.48
1:G:545:LYS:O	1:G:549:LYS:HG2	2.13	0.48
1:F:561:ASN:N	1:F:561:ASN:HD22	2.11	0.48
1:A:543:ILE:HG23	1:D:546:ILE:HD11	1.95	0.48
1:G:549:LYS:HA	1:G:549:LYS:HD3	1.62	0.48
1:A:533:LEU:HA	1:A:533:LEU:HD23	1.69	0.48
1:G:557:LEU:HA	1:G:560:THR:HB	1.95	0.47
1:H:493:THR:HG22	1:H:494:ASP:OD1	2.15	0.47
1:D:568:GLU:OE1	1:C:570:HIS:HD2	1.96	0.47
1:E:479:MET:HE2	1:E:480:PRO:HD2	1.95	0.47
1:A:553:ILE:HA	1:A:556:VAL:HG12	1.95	0.47
1:H:555:ARG:O	1:H:559:LYS:HG3	2.15	0.47
1:A:509:GLU:HA	1:D:508:LEU:HD21	1.97	0.46
1:E:520:VAL:HG13	1:G:484:PHE:CE2	2.50	0.46
1:E:543:ILE:O	1:E:547:ILE:HD12	2.15	0.46
1:G:570:HIS:O	1:G:574:MET:HG2	2.15	0.46
1:C:551:GLU:HG3	1:B:549:LYS:NZ	2.31	0.46
1:H:517:LEU:HD21	1:G:500:ALA:HA	1.97	0.46
1:E:571:LEU:HD21	1:H:570:HIS:HB2	1.97	0.46
1:G:541:LYS:HG2	1:G:541:LYS:O	2.15	0.46
1:H:549:LYS:HA	1:H:549:LYS:HD3	1.63	0.46
1:B:499:HIS:O	1:B:503:LEU:HG	2.16	0.45
1:C:528:ASN:HA	1:C:531:MET:HE2	1.98	0.45
1:D:549:LYS:HE2	1:D:553:ILE:HG13	1.98	0.45
1:C:541:LYS:HG2	1:C:541:LYS:O	2.16	0.45
1:F:570:HIS:HB2	1:G:571:LEU:HD13	1.97	0.45
1:C:477:TYR:OH	1:C:480:PRO:HD3	2.16	0.45
1:H:551:GLU:OE2	1:G:549:LYS:NZ	2.43	0.45
1:H:572:VAL:HA	1:H:575:MET:HE2	1.99	0.45
1:D:535:HIS:O	1:D:538:GLU:HG2	2.16	0.45
1:A:535:HIS:O	1:A:539:GLN:OE1	2.35	0.44
1:E:479:MET:HE2	1:F:514:GLU:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:557:LEU:HB3	1:G:556:VAL:HG11	1.99	0.44
1:G:560:THR:O	1:G:564:LEU:HG	2.17	0.44
1:A:552:SER:OG	1:A:555:ARG:NH2	2.50	0.44
1:D:499:HIS:ND1	1:C:480:PRO:HG3	2.33	0.44
1:E:517:LEU:HD21	1:H:500:ALA:HA	1.98	0.44
1:H:549:LYS:O	1:H:553:ILE:HD12	2.18	0.44
1:H:540:VAL:HG13	1:H:543:ILE:HD12	2.00	0.44
1:E:499:HIS:ND1	1:H:480:PRO:HG3	2.32	0.44
1:A:478:ILE:HG22	1:A:483:ASP:HB2	1.99	0.43
1:A:521:ILE:HG23	1:D:488:PHE:HZ	1.82	0.43
1:E:574:MET:HE1	1:F:571:LEU:HD12	2.00	0.43
1:E:575:MET:HG2	1:H:574:MET:CG	2.48	0.43
1:D:489:PHE:CB	1:D:490:PRO:CD	2.92	0.43
1:D:556:VAL:O	1:D:560:THR:OG1	2.28	0.43
1:E:535:HIS:O	1:E:539:GLN:HG3	2.18	0.43
1:F:532:ARG:NH2	1:G:534:ASN:OD1	2.51	0.43
1:E:507:ASP:OD1	1:E:507:ASP:N	2.50	0.43
1:F:567:ILE:HG23	1:G:571:LEU:HD11	1.99	0.43
1:E:496:LEU:HD13	1:F:521:ILE:HG13	2.01	0.43
1:E:550:LEU:HD11	1:H:546:ILE:HG23	2.00	0.43
1:E:502:HIS:HB2	1:H:477:TYR:CE1	2.53	0.43
1:A:532:ARG:O	1:A:536:ILE:N	2.39	0.43
1:H:490:PRO:HA	1:H:493:THR:HB	2.00	0.43
1:E:537:GLU:OE2	1:H:532:ARG:HD3	2.19	0.42
1:D:547:ILE:CD1	1:C:542:GLU:HB3	2.49	0.42
1:F:529:LEU:HD22	1:G:533:LEU:HD22	2.01	0.42
1:H:498:TYR:CE2	1:G:478:ILE:HG12	2.53	0.42
1:C:564:LEU:HD13	1:B:563:ALA:HB3	2.00	0.42
1:F:477:TYR:OH	1:F:480:PRO:HD3	2.18	0.42
1:F:550:LEU:HD23	1:F:550:LEU:HA	1.83	0.42
1:A:493:THR:HG22	2:A:606:HOH:O	2.18	0.42
1:G:541:LYS:O	1:G:544:PRO:HD2	2.19	0.42
1:D:564:LEU:HD11	1:C:560:THR:HG23	2.02	0.42
1:E:479:MET:HE2	1:F:514:GLU:CD	2.40	0.42
1:H:513:GLU:HA	1:H:516:VAL:HG12	2.02	0.42
1:H:519:ASN:ND2	1:G:519:ASN:OD1	2.53	0.42
1:C:543:ILE:HG13	1:C:544:PRO:HD3	2.02	0.42
1:E:537:GLU:HA	1:H:536:ILE:HG12	2.02	0.42
1:F:537:GLU:HA	1:F:540:VAL:HG22	2.01	0.42
1:A:513:GLU:HG3	1:D:503:LEU:HB2	2.01	0.41
1:E:567:ILE:HD11	1:F:564:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:ASP:N	1:C:507:ASP:OD1	2.53	0.41
1:A:532:ARG:HA	1:A:535:HIS:HB3	2.02	0.41
1:A:545:LYS:HE2	1:A:545:LYS:HB2	1.89	0.41
1:C:526:LEU:HD13	1:B:525:LYS:HB2	2.02	0.41
1:C:480:PRO:HA	1:C:483:ASP:HB3	2.01	0.41
1:C:568:GLU:O	1:C:572:VAL:HG23	2.20	0.41
1:F:532:ARG:HH12	1:G:537:GLU:CD	2.23	0.41
1:C:557:LEU:CD2	1:B:557:LEU:HD21	2.51	0.41
1:F:509:GLU:O	1:F:513:GLU:HB2	2.21	0.41
1:G:490:PRO:HA	1:G:493:THR:HB	2.01	0.41
1:G:542:GLU:HA	1:G:545:LYS:HD2	2.01	0.41
1:H:516:VAL:CG1	1:G:503:LEU:HD13	2.51	0.41
1:E:543:ILE:HG22	1:E:547:ILE:CD1	2.51	0.41
1:H:497:ASN:HA	1:H:500:ALA:HB3	2.02	0.41
1:E:540:VAL:O	1:H:539:GLN:NE2	2.54	0.41
1:E:564:LEU:HD21	1:H:564:LEU:CD2	2.50	0.41
1:E:513:GLU:O	1:E:517:LEU:HD12	2.21	0.41
1:E:557:LEU:CD1	1:H:553:ILE:HG23	2.51	0.41
1:A:504:GLY:HA2	1:B:513:GLU:OE2	2.21	0.41
1:G:477:TYR:HE2	2:G:615:HOH:O	2.04	0.41
1:E:476:LYS:CG	1:E:477:TYR:H	2.31	0.41
1:D:552:SER:HA	1:D:555:ARG:HD2	2.03	0.41
1:D:568:GLU:HG2	1:C:567:ILE:CG1	2.49	0.41
1:E:546:ILE:HG23	1:F:550:LEU:CD1	2.51	0.41
1:C:538:GLU:HA	1:C:541:LYS:CB	2.51	0.40
1:G:486:ASN:OD1	1:G:487:THR:HG23	2.21	0.40
1:G:508:LEU:HD23	1:G:508:LEU:HA	1.87	0.40
1:A:552:SER:HA	1:A:555:ARG:NE	2.34	0.40
1:B:557:LEU:HA	1:B:557:LEU:HD23	1.89	0.40
1:F:551:GLU:HB3	1:F:555:ARG:HH21	1.86	0.40
1:H:508:LEU:HD23	1:G:508:LEU:CD2	2.50	0.40
1:E:557:LEU:HD23	1:E:557:LEU:HA	1.88	0.40
1:G:542:GLU:O	1:G:545:LYS:HB2	2.22	0.40
1:H:550:LEU:HD11	1:G:546:ILE:HG23	2.03	0.40
1:A:553:ILE:O	1:A:556:VAL:HG12	2.22	0.40
1:A:503:LEU:HA	1:A:503:LEU:HD23	1.67	0.40
1:A:524:ILE:HA	1:A:527:ILE:HD12	2.04	0.40
1:F:564:LEU:HD23	1:F:564:LEU:HA	1.94	0.40
1:E:519:ASN:HB3	1:H:518:MET:HB3	2.02	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:E:577:MET:O	1:D:555:ARG:NH1[1_446]	1.68	0.52

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	102/110 (93%)	101 (99%)	1 (1%)	0	100	100
1	B	98/110 (89%)	98 (100%)	0	0	100	100
1	C	98/110 (89%)	96 (98%)	2 (2%)	0	100	100
1	D	99/110 (90%)	97 (98%)	2 (2%)	0	100	100
1	E	102/110 (93%)	100 (98%)	2 (2%)	0	100	100
1	F	99/110 (90%)	99 (100%)	0	0	100	100
1	G	99/110 (90%)	99 (100%)	0	0	100	100
1	H	99/110 (90%)	96 (97%)	3 (3%)	0	100	100
All	All	796/880 (90%)	786 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	99/105 (94%)	96 (97%)	3 (3%)	41	68
1	B	95/105 (90%)	94 (99%)	1 (1%)	73	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	95/105 (90%)	95 (100%)	0	100	100
1	D	96/105 (91%)	94 (98%)	2 (2%)	53	78
1	E	99/105 (94%)	98 (99%)	1 (1%)	76	90
1	F	96/105 (91%)	95 (99%)	1 (1%)	76	90
1	G	96/105 (91%)	96 (100%)	0	100	100
1	H	96/105 (91%)	94 (98%)	2 (2%)	53	78
All	All	772/840 (92%)	762 (99%)	10 (1%)	69	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	MET
1	A	523	SER
1	A	562	THR
1	E	570	HIS
1	D	541	LYS
1	D	555	ARG
1	H	523	SER
1	H	561	ASN
1	F	561	ASN
1	B	523	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	570	HIS
1	H	539	GLN
1	H	561	ASN
1	F	561	ASN
1	G	570	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	104/110 (94%)	0.67	8 (7%)	13 13	21, 45, 56, 65	0
1	B	100/110 (90%)	0.64	6 (6%)	21 22	26, 42, 56, 68	0
1	C	100/110 (90%)	0.65	7 (7%)	16 16	24, 41, 56, 60	0
1	D	101/110 (91%)	0.77	12 (11%)	4 4	19, 46, 59, 65	0
1	E	103/110 (93%)	0.47	1 (0%)	82 84	28, 40, 54, 63	0
1	F	101/110 (91%)	0.62	3 (2%)	50 53	26, 39, 51, 59	0
1	G	101/110 (91%)	0.72	10 (9%)	7 7	23, 47, 58, 73	0
1	H	101/110 (91%)	0.75	9 (8%)	9 9	29, 43, 56, 75	0
All	All	811/880 (92%)	0.66	56 (6%)	16 17	19, 43, 57, 75	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	576	ILE	6.4
1	H	496	LEU	5.5
1	A	578	ILE	5.0
1	A	501	ASP	4.7
1	B	572	VAL	4.4
1	G	478	ILE	4.2
1	A	475	ASP	3.4
1	D	506	TYR	3.2
1	D	479	MET	3.2
1	E	476	LYS	3.2
1	G	573	SER	3.2
1	D	488	PHE	3.2
1	G	569	GLY	3.1
1	D	564	LEU	3.1
1	G	506	TYR	3.0
1	F	485	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	476	LYS	2.9
1	G	572	VAL	2.9
1	D	502	HIS	2.8
1	D	478	ILE	2.8
1	C	486	ASN	2.8
1	G	503	LEU	2.8
1	G	486	ASN	2.7
1	A	576	ILE	2.7
1	C	477	TYR	2.7
1	D	576	ILE	2.6
1	G	498	TYR	2.6
1	H	548	ASN	2.5
1	B	571	LEU	2.4
1	C	575	MET	2.4
1	F	576	ILE	2.4
1	F	574	MET	2.3
1	G	547	ILE	2.3
1	H	544	PRO	2.3
1	H	476	LYS	2.3
1	D	546	ILE	2.3
1	A	510	THR	2.3
1	D	491	HIS	2.3
1	C	478	ILE	2.2
1	B	517	LEU	2.2
1	G	508	LEU	2.2
1	B	544	PRO	2.2
1	H	502	HIS	2.1
1	B	550	LEU	2.1
1	C	538	GLU	2.1
1	D	490	PRO	2.1
1	C	501	ASP	2.1
1	D	544	PRO	2.1
1	D	547	ILE	2.1
1	A	535	HIS	2.1
1	C	576	ILE	2.0
1	A	511	LEU	2.0
1	H	575	MET	2.0
1	H	570	HIS	2.0
1	H	501	ASP	2.0
1	B	575	MET	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.