



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:28 am BST

PDB ID : 5U0C
Title : Structure of Zika virus NS5 RNA polymerase domain
Authors : Zhao, B.; Du, F.
Deposited on : 2016-11-23
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

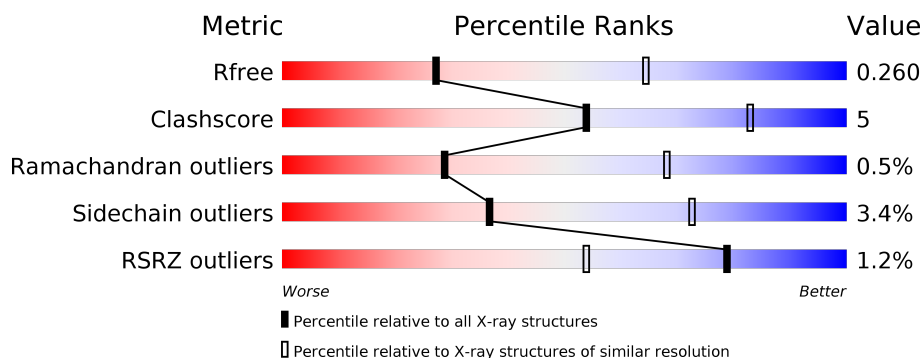
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	639	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	639	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
1	C	639	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>
1	D	639	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
1	E	639	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div> </div>
1	F	639	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	639	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>87%</div><div>10%</div><div>••</div></div></div>
1	H	639	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>84%</div><div>12%</div><div>••</div></div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 40565 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 NS5 RNA polymerase domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	0	0
			5085	3203	924	925	33			
1	B	621	Total	C	N	O	S	0	0	0
			5058	3187	917	921	33			
1	C	621	Total	C	N	O	S	0	0	0
			5058	3187	917	921	33			
1	D	623	Total	C	N	O	S	0	0	0
			5070	3195	919	923	33			
1	E	622	Total	C	N	O	S	0	0	0
			5067	3192	919	923	33			
1	F	622	Total	C	N	O	S	0	0	0
			5068	3194	919	922	33			
1	G	624	Total	C	N	O	S	0	0	0
			5075	3198	920	924	33			
1	H	623	Total	C	N	O	S	0	0	0
			5068	3194	919	922	33			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	H	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

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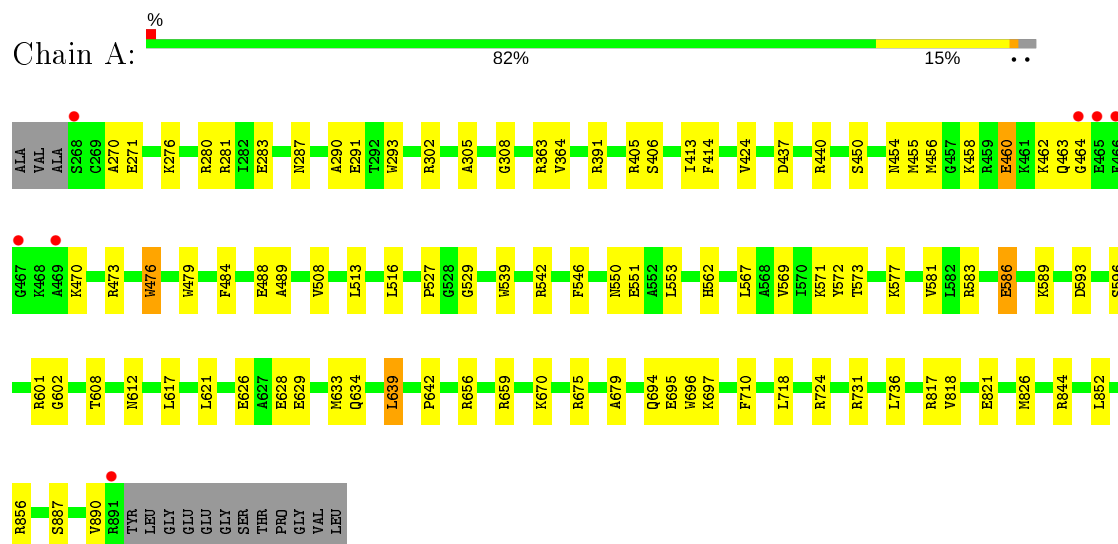
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

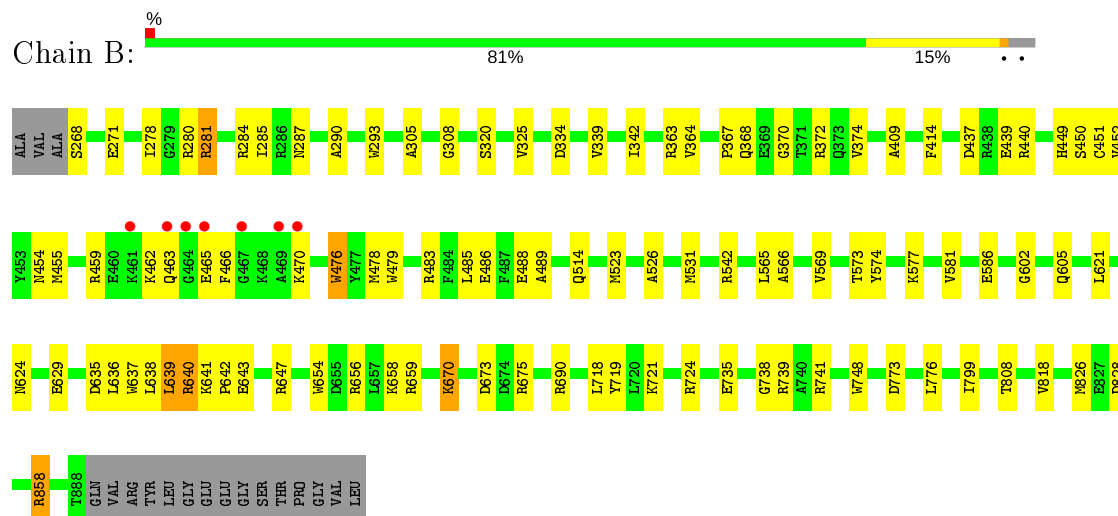
3 Residue-property plots

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 ($RSRZ > 2$). 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.

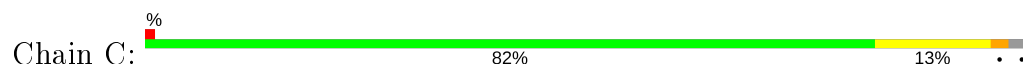
• Molecule 1: NS5 RNA polymerase domain

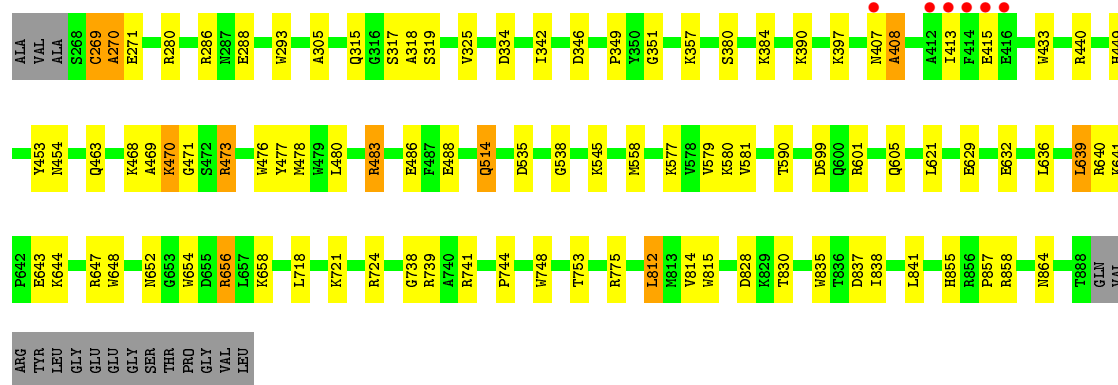


• Molecule 1: NS5 RNA polymerase domain

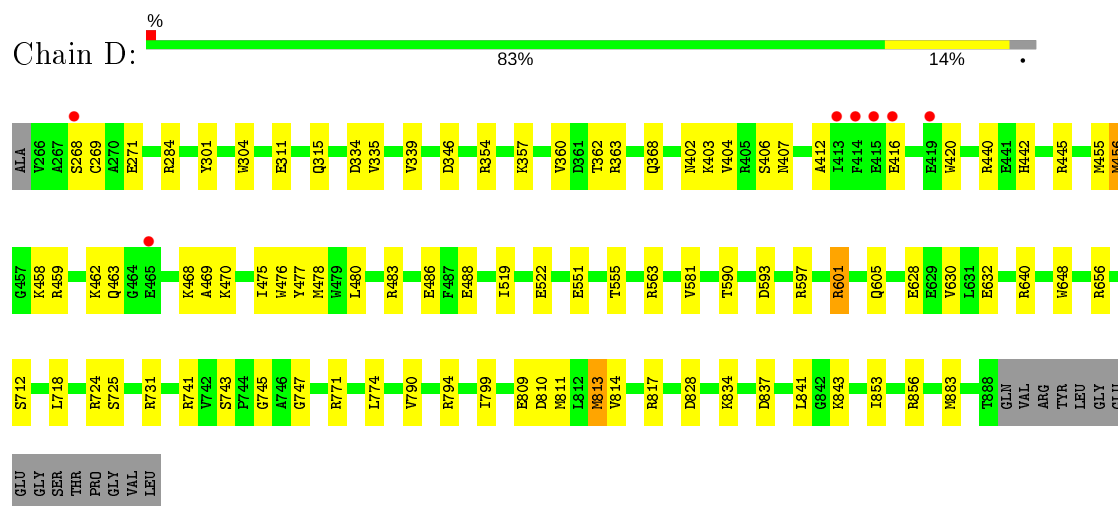


• Molecule 1: NS5 RNA polymerase domain

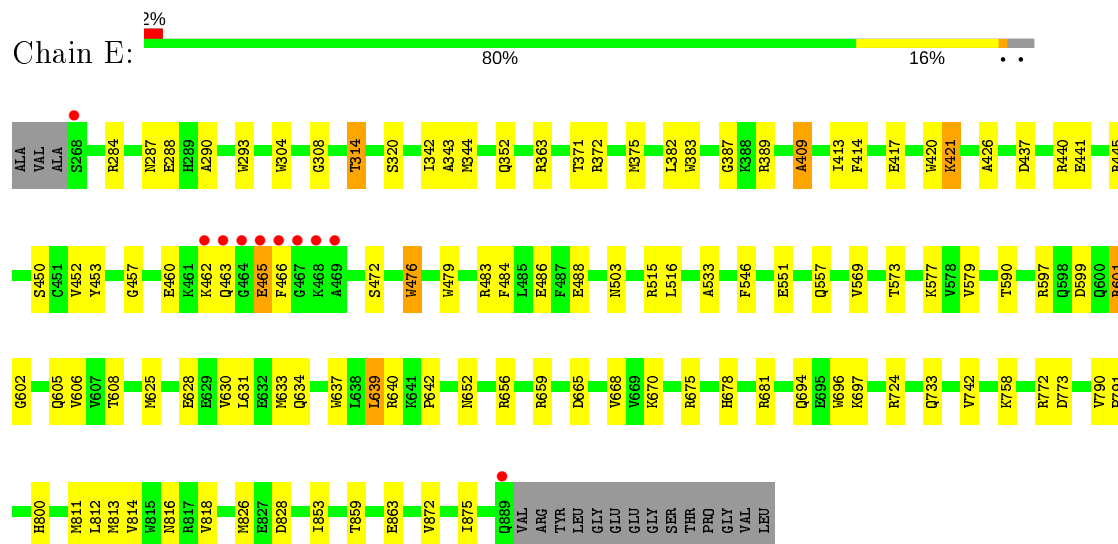




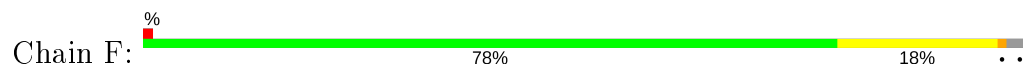
• Molecule 1: NS5 RNA polymerase domain

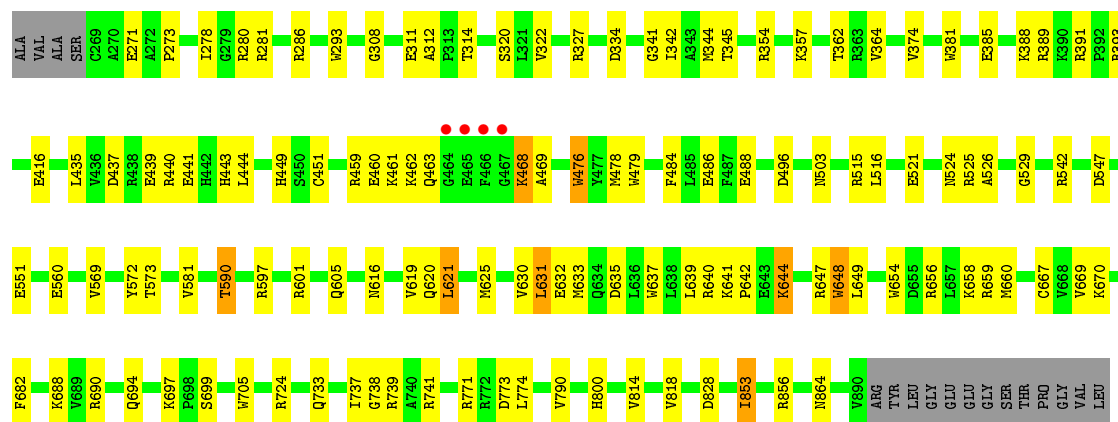


• Molecule 1: NS5 RNA polymerase domain

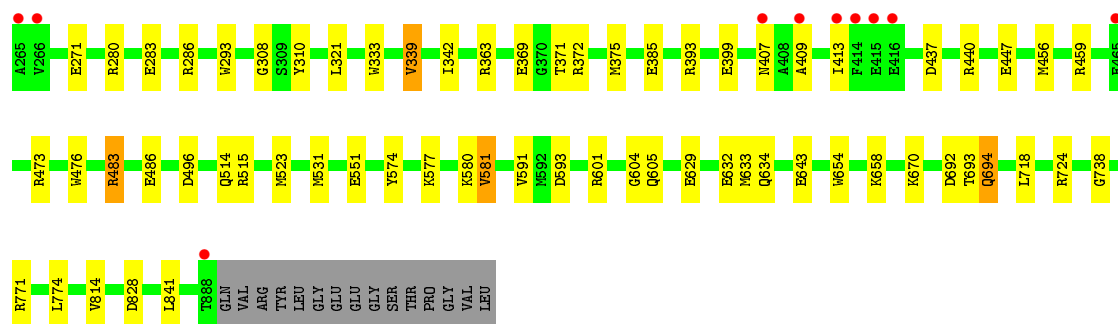
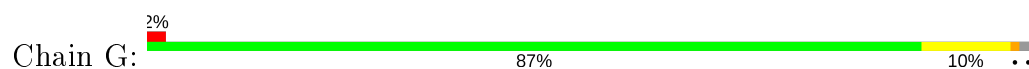


• Molecule 1: NS5 RNA polymerase domain

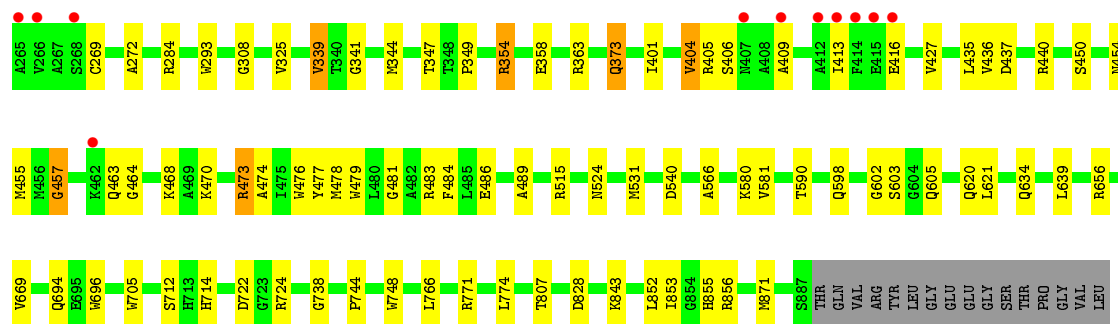
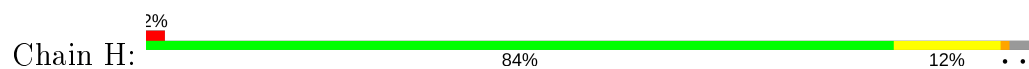




• Molecule 1: NS5 RNA polymerase domain



• Molecule 1: NS5 RNA polymerase domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.52Å 188.71Å 192.54Å 90.00° 91.99° 90.00°	Depositor
Resolution (Å)	89.14 – 3.00 96.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (89.14-3.00) 89.5 (96.21-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.226 , 0.260 0.226 , 0.260	Depositor DCC
R_{free} test set	8552 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 3.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.069 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	40565	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0502e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN

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	0.23	0/5209	0.41	0/7044
1	B	0.23	0/5182	0.42	0/7008
1	C	0.23	0/5182	0.41	0/7008
1	D	0.24	0/5194	0.42	0/7025
1	E	0.23	0/5191	0.42	0/7020
1	F	0.23	0/5192	0.43	0/7022
1	G	0.23	0/5199	0.41	0/7032
1	H	0.23	0/5192	0.41	0/7022
All	All	0.23	0/41541	0.42	0/56181

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 [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	5085	0	4983	63	0
1	B	5058	0	4953	57	0
1	C	5058	0	4953	53	1
1	D	5070	0	4967	44	0
1	E	5067	0	4961	64	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5068	0	4965	76	0
1	G	5075	0	4972	35	0
1	H	5068	0	4965	43	0
2	A	2	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
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
All	All	40565	0	39719	423	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 5.

All (423) 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:745:GLY:HA3	1:D:747:GLY:H	1.29	0.95
1:B:773:ASP:OD1	1:B:858:ARG:NH1	2.06	0.88
1:A:529:GLY:O	1:A:670:LYS:NZ	2.06	0.88
1:A:628:GLU:OE2	1:A:656:ARG:NH1	2.06	0.88
1:D:632:GLU:OE1	1:D:640:ARG:NH1	2.13	0.81
1:A:458:LYS:HD3	1:A:473:ARG:HH12	1.45	0.79
1:G:551:GLU:OE2	1:G:601:ARG:NH2	2.17	0.77
1:F:529:GLY:O	1:F:670:LYS:NZ	2.17	0.77
1:E:460:GLU:OE1	1:E:462:LYS:NZ	2.18	0.75
1:A:462:LYS:HB3	1:A:463:GLN:HB2	1.70	0.74
1:D:462:LYS:HB3	1:D:463:GLN:HB2	1.71	0.73
1:C:643:GLU:HB2	1:C:647:ARG:HH11	1.54	0.72
1:H:455:MET:HB2	1:H:581:VAL:HG12	1.72	0.72
1:C:632:GLU:OE2	1:C:640:ARG:NH1	2.24	0.71
1:A:437:ASP:OD1	1:A:440:ARG:NH1	2.25	0.70
1:E:417:GLU:OE2	1:E:450:SER:OG	2.09	0.70
1:F:690:ARG:NH1	1:F:699:SER:OG	2.25	0.69
1:D:486:GLU:OE2	1:D:605:GLN:HB3	1.92	0.69
1:F:342:ILE:HA	1:F:462:LYS:HE3	1.75	0.68
1:H:486:GLU:OE2	1:H:605:GLN:HB3	1.93	0.68
1:D:745:GLY:HA3	1:D:747:GLY:N	2.07	0.68
1:D:440:ARG:NH2	1:D:488:GLU:OE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:393:ARG:NH1	1:G:496:ASP:OD1	2.27	0.68
1:D:628:GLU:OE2	1:D:656:ARG:NH1	2.27	0.67
1:H:341:GLY:HA2	1:H:344:MET:HE2	1.76	0.67
1:E:460:GLU:HB3	1:E:462:LYS:HE3	1.76	0.67
1:C:271:GLU:HG2	1:C:305:ALA:HB2	1.76	0.67
1:G:342:ILE:HD12	1:G:738:GLY:HA3	1.76	0.67
1:E:437:ASP:OD1	1:E:440:ARG:NH1	2.23	0.67
1:F:334:ASP:OD1	1:F:741:ARG:NH2	2.29	0.66
1:G:280:ARG:NH1	1:G:447:GLU:OE2	2.29	0.65
1:C:454:ASN:HB2	1:C:477:TYR:HB2	1.77	0.65
1:C:334:ASP:OD1	1:C:741:ARG:NH2	2.30	0.65
1:B:465:GLU:H	1:B:466:PHE:HB2	1.61	0.65
1:C:318:ALA:H	1:C:319:SER:HA	1.62	0.65
1:E:551:GLU:OE2	1:E:601:ARG:NH2	2.26	0.65
1:F:694:GLN:HB3	1:F:697:LYS:HB2	1.77	0.65
1:E:694:GLN:HB3	1:E:697:LYS:HB2	1.77	0.64
1:A:462:LYS:HD2	1:A:463:GLN:HG3	1.78	0.64
1:G:632:GLU:O	1:G:634:GLN:N	2.31	0.64
1:H:401:ILE:HD13	1:H:427:VAL:HB	1.79	0.64
1:C:724:ARG:NH1	1:C:830:THR:O	2.29	0.64
1:A:364:VAL:HB	1:A:542:ARG:HH11	1.64	0.63
1:B:409:ALA:O	1:B:483:ARG:NH2	2.31	0.63
1:F:484:PHE:O	1:F:488:GLU:N	2.30	0.63
1:G:385:GLU:HB3	1:G:654:TRP:HZ3	1.62	0.63
1:E:342:ILE:HA	1:E:462:LYS:HD3	1.79	0.62
1:E:387:GLY:HA3	1:E:557:GLN:HE22	1.64	0.62
1:C:721:LYS:HE2	1:C:837:ASP:HA	1.82	0.62
1:C:514:GLN:HE21	1:C:514:GLN:H	1.45	0.62
1:A:527:PRO:O	1:A:659:ARG:NH2	2.32	0.62
1:G:486:GLU:OE2	1:G:605:GLN:HB3	1.99	0.62
1:A:440:ARG:NH2	1:A:488:GLU:OE1	2.32	0.62
1:A:270:ALA:HB1	1:A:271:GLU:HA	1.81	0.62
1:B:526:ALA:HB1	1:B:659:ARG:NH1	2.15	0.62
1:E:414:PHE:HE2	1:E:450:SER:HA	1.64	0.62
1:B:654:TRP:HE1	1:B:658:LYS:HE3	1.65	0.61
1:H:724:ARG:HD3	1:H:828:ASP:HB3	1.82	0.61
1:D:271:GLU:HB2	1:D:363:ARG:NH1	2.14	0.61
1:C:545:LYS:HG2	1:C:599:ASP:HB3	1.82	0.61
1:C:288:GLU:OE2	1:C:415:GLU:HG2	1.99	0.61
1:F:437:ASP:OD1	1:F:440:ARG:NH1	2.34	0.61
1:G:310:TYR:OH	1:G:580:LYS:NZ	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:GLU:H	1:E:466:PHE:HB2	1.64	0.61
1:C:486:GLU:OE2	1:C:605:GLN:HB3	2.00	0.60
1:G:333:TRP:HB3	1:G:339:VAL:HG11	1.83	0.60
1:D:346:ASP:HB3	1:D:459:ARG:HB3	1.83	0.60
1:D:551:GLU:OE2	1:D:601:ARG:NH2	2.34	0.60
1:A:271:GLU:HG2	1:A:363:ARG:HH22	1.64	0.60
1:B:470:LYS:NZ	1:B:739:ARG:HD2	2.16	0.60
1:E:409:ALA:O	1:E:483:ARG:NH2	2.35	0.60
1:A:608:THR:O	1:A:612:ASN:ND2	2.34	0.59
1:G:724:ARG:HD3	1:G:828:ASP:HB3	1.84	0.59
1:G:483:ARG:NH1	1:G:605:GLN:HA	2.18	0.59
1:G:339:VAL:HG23	1:G:738:GLY:HA2	1.85	0.59
1:G:409:ALA:HB3	1:G:483:ARG:HD3	1.83	0.59
1:H:437:ASP:OD1	1:H:440:ARG:NH1	2.36	0.59
1:B:342:ILE:HD12	1:B:738:GLY:HA3	1.85	0.58
1:B:455:MET:HB3	1:B:581:VAL:HG12	1.84	0.58
1:F:354:ARG:NH1	1:F:459:ARG:HH11	2.01	0.58
1:A:484:PHE:O	1:A:488:GLU:N	2.37	0.58
1:F:551:GLU:OE2	1:F:601:ARG:NH2	2.22	0.58
1:A:633:MET:HE1	1:E:681:ARG:HH11	1.67	0.58
1:D:810:ASP:HB3	1:D:813:MET:HB2	1.86	0.58
1:G:654:TRP:CD1	1:G:658:LYS:HE2	2.38	0.58
1:A:460:GLU:HB3	1:A:462:LYS:HG2	1.86	0.58
1:F:462:LYS:HB3	1:F:463:GLN:HB2	1.84	0.58
1:F:641:LYS:HD2	1:F:644:LYS:NZ	2.19	0.58
1:A:458:LYS:HD3	1:A:473:ARG:NH1	2.17	0.57
1:A:406:SER:HA	1:A:424:VAL:HB	1.86	0.57
1:A:546:PHE:O	1:A:550:ASN:ND2	2.37	0.57
1:A:694:GLN:HB3	1:A:697:LYS:HB2	1.85	0.57
1:A:856:ARG:NH2	1:G:459:ARG:HH12	2.03	0.57
1:H:457:GLY:HA2	1:H:474:ALA:HA	1.87	0.57
1:H:468:LYS:NZ	1:H:714:HIS:HD1	2.02	0.57
1:E:453:TYR:HB2	1:E:579:VAL:HG22	1.87	0.57
1:F:625:MET:HG2	1:F:630:VAL:HB	1.86	0.56
1:B:271:GLU:HB3	1:B:305:ALA:HB2	1.85	0.56
1:F:476:TRP:N	1:F:476:TRP:CD1	2.74	0.56
1:H:416:GLU:HG3	1:H:435:LEU:HD11	1.88	0.56
1:A:551:GLU:OE2	1:A:601:ARG:NH1	2.35	0.56
1:C:453:TYR:HB2	1:C:579:VAL:HG22	1.88	0.56
1:A:305:ALA:HB3	1:A:596:SER:HB3	1.88	0.55
1:G:283:GLU:OE1	1:G:286:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:437:ASP:OD1	1:G:440:ARG:NH1	2.40	0.55
1:E:724:ARG:HD3	1:E:828:ASP:HB3	1.88	0.55
1:H:413:ILE:CG1	1:H:580:LYS:HZ3	2.19	0.55
1:D:462:LYS:HB3	1:D:463:GLN:CB	2.37	0.55
1:F:385:GLU:HA	1:F:388:LYS:HE3	1.88	0.55
1:F:486:GLU:OE2	1:F:605:GLN:HB3	2.07	0.55
1:F:547:ASP:OD2	1:F:688:LYS:NZ	2.33	0.55
1:E:484:PHE:O	1:E:488:GLU:N	2.32	0.55
1:B:470:LYS:HZ3	1:B:739:ARG:HD2	1.72	0.55
1:A:633:MET:CE	1:E:681:ARG:HH11	2.20	0.55
1:D:458:LYS:HE2	1:D:475:ILE:HD12	1.89	0.54
1:C:470:LYS:HE3	1:C:739:ARG:NH1	2.22	0.54
1:B:718:LEU:HA	1:H:694:GLN:HE22	1.72	0.54
1:F:354:ARG:HH11	1:F:459:ARG:HH11	1.54	0.54
1:A:844:ARG:HH12	1:G:692:ASP:HB3	1.73	0.54
1:F:660:MET:HG2	1:F:669:VAL:HG22	1.89	0.54
1:A:639:LEU:HB3	1:A:642:PRO:HG3	1.88	0.54
1:E:665:ASP:N	1:E:665:ASP:OD1	2.41	0.54
1:H:272:ALA:O	1:H:598:GLN:NE2	2.41	0.54
1:B:364:VAL:HG22	1:B:542:ARG:NH1	2.23	0.54
1:E:515:ARG:NH1	1:E:818:VAL:O	2.38	0.53
1:B:719:TYR:H	1:H:694:GLN:NE2	2.06	0.53
1:F:362:THR:O	1:F:597:ARG:NH2	2.41	0.53
1:F:460:GLU:HB3	1:F:462:LYS:HD2	1.91	0.53
1:E:476:TRP:N	1:E:476:TRP:CD1	2.76	0.53
1:E:460:GLU:H	1:E:472:SER:HB3	1.73	0.53
1:A:280:ARG:NH2	1:A:283:GLU:OE2	2.41	0.53
1:A:516:LEU:HD22	1:A:710:PHE:HE2	1.74	0.53
1:H:269:CYS:HB3	1:H:363:ARG:HE	1.74	0.53
1:B:334:ASP:OD1	1:B:741:ARG:NH2	2.37	0.53
1:B:437:ASP:OD1	1:B:440:ARG:NH1	2.41	0.53
1:B:364:VAL:HG22	1:B:542:ARG:HH11	1.74	0.53
1:C:440:ARG:NH2	1:C:488:GLU:OE1	2.42	0.53
1:D:455:MET:HB3	1:D:581:VAL:HG12	1.91	0.53
1:E:872:VAL:HA	1:E:875:ILE:HD12	1.91	0.53
1:B:569:VAL:O	1:B:573:THR:HB	2.09	0.52
1:G:271:GLU:HB2	1:G:363:ARG:NH1	2.23	0.52
1:C:380:SER:O	1:C:384:LYS:HG2	2.08	0.52
1:B:486:GLU:OE2	1:B:605:GLN:HB3	2.09	0.52
1:G:574:TYR:O	1:G:577:LYS:NZ	2.40	0.52
1:F:439:GLU:OE1	1:F:443:HIS:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:PRO:O	1:B:372:ARG:NH2	2.43	0.52
1:D:771:ARG:HB2	1:D:774:LEU:HB2	1.92	0.52
1:H:470:LYS:HD3	1:H:473:ARG:NH2	2.25	0.52
1:B:654:TRP:NE1	1:B:658:LYS:HE3	2.26	0.51
1:B:476:TRP:N	1:B:476:TRP:CD1	2.79	0.51
1:C:724:ARG:HD3	1:C:828:ASP:HB3	1.93	0.51
1:B:268:SER:HB3	1:B:363:ARG:HB3	1.92	0.51
1:D:334:ASP:OD1	1:D:741:ARG:NH2	2.36	0.51
1:E:811:MET:HA	1:E:814:VAL:HG12	1.91	0.51
1:H:478:MET:HB2	1:H:483:ARG:CZ	2.39	0.51
1:H:476:TRP:CD2	1:H:602:GLY:HA2	2.46	0.51
1:D:724:ARG:HD3	1:D:828:ASP:HB3	1.91	0.51
1:H:843:LYS:HE2	1:H:853:ILE:HD12	1.93	0.51
1:E:389:ARG:HH22	1:E:503:ASN:HA	1.76	0.50
1:B:635:ASP:HB3	1:B:639:LEU:HD22	1.93	0.50
1:E:758:LYS:HD3	1:E:791:PRO:HG3	1.93	0.50
1:H:531:MET:HE1	1:H:705:TRP:HB3	1.92	0.50
1:F:569:VAL:O	1:F:573:THR:HB	2.10	0.50
1:H:349:PRO:HG2	1:H:590:THR:HG21	1.93	0.50
1:D:456:MET:HB2	1:D:477:TYR:HE2	1.77	0.50
1:G:514:GLN:HG2	1:G:515:ARG:HG2	1.93	0.50
1:G:483:ARG:NH2	1:G:604:GLY:O	2.44	0.50
1:D:468:LYS:HG3	1:D:712:SER:HA	1.93	0.50
1:A:539:TRP:NE1	1:A:612:ASN:OD1	2.42	0.50
1:E:413:ILE:HD12	1:E:452:VAL:HB	1.94	0.50
1:F:641:LYS:HB2	1:F:644:LYS:NZ	2.27	0.50
1:E:476:TRP:CE2	1:E:602:GLY:HA2	2.46	0.50
1:F:641:LYS:HD2	1:F:644:LYS:HZ3	1.76	0.50
1:A:281:ARG:NH2	1:A:572:TYR:O	2.45	0.49
1:A:476:TRP:CD1	1:A:476:TRP:N	2.80	0.49
1:C:397:LYS:HE3	1:C:433:TRP:CE2	2.48	0.49
1:H:284:ARG:HH21	1:H:450:SER:HB3	1.77	0.49
1:A:718:LEU:HA	1:G:694:GLN:HE22	1.77	0.49
1:D:301:TYR:OH	1:D:593:ASP:OD2	2.22	0.49
1:G:771:ARG:HB2	1:G:774:LEU:HB2	1.94	0.49
1:E:659:ARG:HB3	1:E:670:LYS:HB3	1.94	0.49
1:C:342:ILE:HG23	1:C:470:LYS:HD2	1.95	0.49
1:E:440:ARG:NH2	1:E:488:GLU:OE1	2.46	0.49
1:A:567:LEU:HD22	1:A:571:LYS:HE2	1.93	0.49
1:H:771:ARG:HB2	1:H:774:LEU:HB2	1.95	0.49
1:F:293:TRP:CZ2	1:F:308:GLY:HA3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:322:VAL:HG11	1:F:327:ARG:HD3	1.93	0.48
1:B:489:ALA:HB1	1:B:566:ALA:HA	1.96	0.48
1:D:354:ARG:HD3	1:D:459:ARG:HH21	1.77	0.48
1:A:550:ASN:HA	1:A:553:LEU:HD23	1.95	0.48
1:A:626:GLU:HB3	1:A:679:ALA:HB1	1.94	0.48
1:B:488:GLU:OE2	1:B:565:LEU:HD21	2.14	0.48
1:E:628:GLU:OE2	1:E:656:ARG:NE	2.47	0.48
1:F:273:PRO:HB2	1:F:278:ILE:HD11	1.95	0.48
1:A:455:MET:HB3	1:A:581:VAL:HG22	1.95	0.48
1:F:635:ASP:HA	1:F:639:LEU:HA	1.96	0.48
1:F:381:TRP:CE2	1:F:649:LEU:HB3	2.48	0.48
1:C:349:PRO:HG2	1:C:590:THR:HG21	1.96	0.48
1:H:524:ASN:HD22	1:H:705:TRP:HD1	1.61	0.48
1:E:812:LEU:O	1:E:816:ASN:ND2	2.46	0.48
1:A:569:VAL:O	1:A:573:THR:HB	2.14	0.47
1:H:454:ASN:HB2	1:H:477:TYR:HB2	1.96	0.47
1:C:643:GLU:HB2	1:C:647:ARG:NH1	2.25	0.47
1:D:402:ASN:HA	1:D:403:LYS:C	2.35	0.47
1:D:843:LYS:HD3	1:D:853:ILE:HD12	1.95	0.47
1:F:389:ARG:HH21	1:F:503:ASN:HA	1.79	0.47
1:A:513:LEU:HD23	1:A:516:LEU:HD12	1.97	0.47
1:E:441:GLU:HG3	1:E:445:ARG:NH1	2.30	0.47
1:H:620:GLN:HE21	1:H:669:VAL:HG21	1.79	0.47
1:C:413:ILE:HG22	1:C:580:LYS:HD2	1.96	0.47
1:D:811:MET:HA	1:D:814:VAL:HG12	1.95	0.47
1:F:654:TRP:HE1	1:F:658:LYS:HE3	1.79	0.47
1:H:409:ALA:HB3	1:H:477:TYR:CD2	2.49	0.47
1:E:304:TRP:CE2	1:E:597:ARG:HD2	2.50	0.47
1:F:625:MET:HG3	1:F:648:TRP:CE2	2.49	0.47
1:B:368:GLN:HG2	1:B:637:TRP:CD1	2.49	0.47
1:C:483:ARG:NH2	1:C:605:GLN:HA	2.30	0.47
1:D:718:LEU:HD21	1:D:841:LEU:HD23	1.96	0.47
1:E:516:LEU:HD11	1:E:800:HIS:CD2	2.50	0.47
1:B:523:MET:HE3	1:B:670:LYS:HB2	1.96	0.47
1:D:809:GLU:OE1	1:D:817:ARG:NH2	2.44	0.46
1:E:387:GLY:HA3	1:E:557:GLN:NE2	2.30	0.46
1:A:817:ARG:HA	1:A:821:GLU:HB3	1.97	0.46
1:C:744:PRO:HG2	1:C:748:TRP:CE2	2.49	0.46
1:F:856:ARG:H	1:F:856:ARG:HD2	1.80	0.46
1:G:369:GLU:HG2	1:G:372:ARG:HH22	1.80	0.46
1:F:619:VAL:HG21	1:F:688:LYS:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLN:HE21	1:E:675:ARG:HG2	1.79	0.46
1:B:439:GLU:HB3	1:B:485:LEU:HD11	1.97	0.46
1:B:280:ARG:HG2	1:B:449:HIS:CD2	2.51	0.46
1:A:291:GLU:OE2	1:A:291:GLU:N	2.48	0.46
1:F:389:ARG:NH2	1:F:503:ASN:HA	2.31	0.46
1:G:286:ARG:HG3	1:G:293:TRP:CE2	2.51	0.46
1:D:462:LYS:HD2	1:D:470:LYS:O	2.16	0.46
1:E:287:ASN:HA	1:E:290:ALA:HB2	1.97	0.46
1:G:718:LEU:HD11	1:G:841:LEU:HD23	1.98	0.45
1:A:731:ARG:HD3	1:A:736:LEU:HD21	1.98	0.45
1:B:637:TRP:CZ2	1:F:697:LYS:HG3	2.51	0.45
1:F:462:LYS:HB3	1:F:463:GLN:CB	2.46	0.45
1:C:280:ARG:HD3	1:C:449:HIS:NE2	2.31	0.45
1:G:476:TRP:CD1	1:G:476:TRP:N	2.85	0.45
1:H:354:ARG:NH1	1:H:358:GLU:OE2	2.50	0.45
1:C:318:ALA:N	1:C:319:SER:HA	2.28	0.45
1:G:581:VAL:HG23	1:G:593:ASP:HB2	1.98	0.45
1:H:404:VAL:HA	1:H:405:ARG:HA	1.56	0.45
1:D:442:HIS:CD2	1:D:445:ARG:HH21	2.34	0.45
1:F:739:ARG:HE	1:F:739:ARG:HB2	1.66	0.45
1:B:278:ILE:HA	1:B:281:ARG:NH2	2.32	0.45
1:B:281:ARG:HG2	1:B:452:VAL:HG22	1.98	0.45
1:C:812:LEU:HD23	1:C:835:TRP:CE2	2.51	0.45
1:A:287:ASN:HA	1:A:290:ALA:HB2	1.99	0.45
1:A:462:LYS:NZ	1:A:470:LYS:HB3	2.32	0.45
1:D:555:THR:HB	1:D:563:ARG:HG3	1.99	0.45
1:E:569:VAL:O	1:E:573:THR:HB	2.17	0.45
1:H:478:MET:HB2	1:H:483:ARG:NH1	2.32	0.45
1:C:641:LYS:O	1:C:644:LYS:HG2	2.18	0.44
1:F:314:THR:HB	1:F:590:THR:HG21	1.99	0.44
1:F:724:ARG:HD3	1:F:828:ASP:HB3	1.99	0.44
1:G:654:TRP:HD1	1:G:658:LYS:HE2	1.80	0.44
1:A:364:VAL:HB	1:A:542:ARG:NH1	2.29	0.44
1:D:468:LYS:HA	1:D:468:LYS:HD2	1.75	0.44
1:E:465:GLU:H	1:E:466:PHE:CB	2.29	0.44
1:F:521:GLU:CG	1:F:525:ARG:HH11	2.30	0.44
1:F:771:ARG:HB2	1:F:774:LEU:HB2	2.00	0.44
1:B:462:LYS:HG3	1:B:463:GLN:HG3	1.98	0.44
1:C:648:TRP:CZ2	1:C:656:ARG:HD2	2.52	0.44
1:E:486:GLU:OE2	1:E:606:VAL:N	2.48	0.44
1:G:371:THR:O	1:G:375:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:CYS:HB3	1:B:478:MET:HE1	1.98	0.44
1:B:526:ALA:HB1	1:B:659:ARG:HH11	1.81	0.44
1:C:269:CYS:SG	1:C:270:ALA:N	2.90	0.44
1:E:639:LEU:HD22	1:E:642:PRO:HA	2.00	0.44
1:A:414:PHE:HE2	1:A:450:SER:HA	1.82	0.44
1:C:855:HIS:ND1	1:C:857:PRO:HD2	2.33	0.44
1:F:374:VAL:HG21	1:F:682:PHE:HE2	1.82	0.44
1:G:523:MET:O	1:G:670:LYS:HD2	2.17	0.44
1:H:339:VAL:HG23	1:H:738:GLY:HA2	2.00	0.44
1:F:286:ARG:HD3	1:F:293:TRP:NE1	2.32	0.44
1:F:451:CYS:HB3	1:F:478:MET:HE1	2.00	0.44
1:C:325:VAL:HG12	1:C:753:THR:HG22	2.00	0.44
1:A:271:GLU:HG2	1:A:363:ARG:NH2	2.32	0.43
1:B:465:GLU:HB2	1:B:466:PHE:CD1	2.53	0.43
1:E:573:THR:O	1:E:577:LYS:HG2	2.18	0.43
1:A:463:GLN:HG2	1:A:464:GLY:H	1.84	0.43
1:E:343:ALA:HB2	1:E:742:VAL:HG22	2.01	0.43
1:F:515:ARG:NH1	1:F:818:VAL:O	2.51	0.43
1:B:724:ARG:HD3	1:B:828:ASP:HB3	2.00	0.43
1:A:470:LYS:HE3	1:A:473:ARG:HH21	1.83	0.43
1:A:856:ARG:NH2	1:G:459:ARG:HH22	2.17	0.43
1:D:284:ARG:NH1	1:D:416:GLU:OE2	2.51	0.43
1:E:420:TRP:CD1	1:E:426:ALA:HA	2.53	0.43
1:H:540:ASP:OD2	1:H:603:SER:HB3	2.18	0.43
1:C:286:ARG:HG3	1:C:293:TRP:CE2	2.53	0.43
1:C:643:GLU:CB	1:C:647:ARG:HH11	2.29	0.43
1:C:654:TRP:CD1	1:C:658:LYS:HE3	2.53	0.43
1:E:293:TRP:CZ2	1:E:308:GLY:HA3	2.54	0.43
1:F:640:ARG:HG3	1:F:641:LYS:HG3	2.00	0.43
1:A:586:GLU:O	1:A:589:LYS:HG2	2.19	0.43
1:F:648:TRP:HD1	1:F:649:LEU:HG	1.84	0.43
1:B:573:THR:HG22	1:B:574:TYR:CD1	2.53	0.43
1:F:476:TRP:N	1:F:476:TRP:HD1	2.13	0.43
1:H:468:LYS:HB3	1:H:712:SER:HA	2.00	0.43
1:A:695:GLU:OE2	1:A:696:TRP:NE1	2.52	0.43
1:B:629:GLU:OE1	1:B:675:ARG:NH1	2.49	0.43
1:F:621:LEU:HA	1:F:621:LEU:HD12	1.90	0.43
1:F:524:ASN:HD22	1:F:705:TRP:HD1	1.65	0.43
1:G:393:ARG:NH2	1:G:399:GLU:OE2	2.52	0.43
1:A:476:TRP:CE2	1:A:602:GLY:HA2	2.54	0.43
1:C:718:LEU:HD11	1:C:841:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:ARG:NH2	1:F:572:TYR:O	2.52	0.43
1:B:465:GLU:HB2	1:B:466:PHE:CG	2.54	0.42
1:C:514:GLN:NE2	1:C:514:GLN:H	2.13	0.42
1:E:342:ILE:HD13	1:E:462:LYS:HD3	2.00	0.42
1:F:280:ARG:HG2	1:F:449:HIS:ND1	2.34	0.42
1:F:440:ARG:NH2	1:F:488:GLU:OE1	2.51	0.42
1:F:364:VAL:HG21	1:F:542:ARG:HD3	2.01	0.42
1:H:373:GLN:HB2	1:H:373:GLN:HE21	1.62	0.42
1:B:639:LEU:HD12	1:B:642:PRO:HA	2.01	0.42
1:C:342:ILE:HD12	1:C:738:GLY:HA3	2.00	0.42
1:C:463:GLN:HE22	1:C:469:ALA:HB3	1.84	0.42
1:C:477:TYR:HA	1:C:483:ARG:HH11	1.84	0.42
1:D:519:ILE:HA	1:D:522:GLU:HG2	2.01	0.42
1:E:314:THR:HB	1:E:590:THR:HG21	2.01	0.42
1:E:533:ALA:HB2	1:E:668:VAL:HG22	2.01	0.42
1:C:318:ALA:H	1:C:319:SER:CA	2.31	0.42
1:H:293:TRP:CZ2	1:H:308:GLY:HA3	2.53	0.42
1:G:293:TRP:CZ2	1:G:308:GLY:HA3	2.54	0.42
1:B:287:ASN:HA	1:B:290:ALA:HB2	2.02	0.42
1:B:293:TRP:CZ2	1:B:308:GLY:HA3	2.54	0.42
1:B:573:THR:O	1:B:577:LYS:HG2	2.20	0.42
1:C:835:TRP:CE3	1:C:838:ILE:HD12	2.53	0.42
1:D:354:ARG:CZ	1:F:856:ARG:HG3	2.49	0.42
1:F:853:ILE:H	1:F:853:ILE:HG13	1.45	0.42
1:A:489:ALA:O	1:A:562:HIS:NE2	2.43	0.42
1:C:317:SER:HB2	1:C:318:ALA:HB2	2.01	0.42
1:C:390:LYS:HE2	1:C:390:LYS:HB3	1.81	0.42
1:C:639:LEU:HA	1:C:639:LEU:HD22	1.66	0.42
1:E:421:LYS:HE3	1:E:421:LYS:HB2	1.86	0.42
1:E:597:ARG:NE	1:E:599:ASP:OD1	2.50	0.42
1:F:468:LYS:HB3	1:F:469:ALA:H	1.56	0.42
1:E:284:ARG:O	1:E:288:GLU:HB2	2.19	0.42
1:F:341:GLY:HA2	1:F:344:MET:HG2	2.01	0.42
1:A:276:LYS:HE3	1:A:276:LYS:HB2	1.84	0.42
1:E:372:ARG:HD3	1:E:546:PHE:CE1	2.55	0.42
1:E:625:MET:HG2	1:E:630:VAL:HB	2.02	0.42
1:E:733:GLN:OE1	1:E:773:ASP:HB2	2.20	0.42
1:F:625:MET:HG3	1:F:648:TRP:CD2	2.54	0.42
1:B:721:LYS:HG3	1:H:696:TRP:CZ2	2.55	0.42
1:A:629:GLU:HG3	1:A:675:ARG:NH1	2.35	0.42
1:D:834:LYS:HB2	1:D:837:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:476:TRP:HD1	1:E:476:TRP:N	2.18	0.42
1:D:476:TRP:CD1	1:D:476:TRP:N	2.88	0.42
1:D:478:MET:HB2	1:D:483:ARG:CZ	2.49	0.42
1:H:416:GLU:HG2	1:H:435:LEU:HD21	2.01	0.42
1:B:342:ILE:HD11	1:B:735:GLU:HA	2.01	0.41
1:C:407:ASN:ND2	1:C:408:ALA:H	2.18	0.41
1:C:453:TYR:CD2	1:C:476:TRP:HB3	2.55	0.41
1:C:468:LYS:HB3	1:C:468:LYS:HE2	1.87	0.41
1:E:352:GLN:HB2	1:E:457:GLY:HA3	2.01	0.41
1:F:441:GLU:OE2	1:F:444:LEU:HD12	2.20	0.41
1:F:393:ARG:NH1	1:F:496:ASP:OD1	2.48	0.41
1:H:489:ALA:HB1	1:H:566:ALA:HA	2.02	0.41
1:B:454:ASN:O	1:B:476:TRP:HA	2.20	0.41
1:H:436:VAL:HG11	1:H:484:PHE:CD2	2.55	0.41
1:E:634:GLN:HE22	1:E:640:ARG:HD3	1.85	0.41
1:E:724:ARG:HD2	1:E:826:MET:SD	2.60	0.41
1:E:772:ARG:HD3	1:E:853:ILE:HG13	2.01	0.41
1:F:526:ALA:HB1	1:F:659:ARG:NH1	2.35	0.41
1:D:368:GLN:HE21	1:D:368:GLN:HB3	1.75	0.41
1:D:656:ARG:HA	1:D:656:ARG:HD3	1.91	0.41
1:E:859:THR:O	1:E:863:GLU:HG3	2.20	0.41
1:F:616:ASN:O	1:F:620:GLN:HG2	2.19	0.41
1:A:281:ARG:HH21	1:A:572:TYR:HB3	1.86	0.41
1:A:573:THR:O	1:A:577:LYS:HG2	2.21	0.41
1:B:414:PHE:HE2	1:B:450:SER:HA	1.85	0.41
1:C:815:TRP:CE2	1:C:838:ILE:HD13	2.56	0.41
1:E:681:ARG:HG2	1:E:696:TRP:CZ3	2.56	0.41
1:A:583:ARG:NE	1:A:593:ASP:OD2	2.53	0.41
1:A:617:LEU:O	1:A:621:LEU:HB2	2.21	0.41
1:A:724:ARG:HD2	1:A:826:MET:SD	2.61	0.41
1:B:470:LYS:HE2	1:B:739:ARG:NH2	2.36	0.41
1:F:342:ILE:HD12	1:F:738:GLY:HA3	2.02	0.41
1:F:354:ARG:HG3	1:F:357:LYS:HE3	2.02	0.41
1:F:416:GLU:HB3	1:F:435:LEU:HD21	2.01	0.41
1:F:625:MET:HB3	1:F:631:LEU:HD11	2.02	0.41
1:F:616:ASN:HD21	1:F:667:CYS:HB3	1.85	0.41
1:B:285:ILE:HG12	1:B:414:PHE:CE1	2.56	0.41
1:D:406:SER:OG	1:D:407:ASN:N	2.50	0.41
1:E:371:THR:O	1:E:375:MET:HG3	2.20	0.41
1:E:634:GLN:NE2	1:E:640:ARG:HD3	2.36	0.41
1:C:471:GLY:O	1:C:473:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:737:ILE:HG22	1:F:741:ARG:HD2	2.03	0.41
1:C:636:LEU:HD12	1:C:636:LEU:HA	1.96	0.41
1:F:311:GLU:N	1:F:311:GLU:OE1	2.50	0.41
1:F:733:GLN:OE1	1:F:773:ASP:HB2	2.21	0.41
1:H:463:GLN:HG2	1:H:464:GLY:H	1.86	0.41
1:H:744:PRO:HG2	1:H:748:TRP:CE2	2.56	0.41
1:H:479:TRP:CZ2	1:H:481:GLY:HA3	2.56	0.41
1:A:293:TRP:CZ2	1:A:308:GLY:HA3	2.55	0.41
1:B:465:GLU:N	1:B:466:PHE:HB2	2.33	0.41
1:E:605:GLN:HB2	1:E:608:THR:OG1	2.22	0.41
1:H:413:ILE:HG12	1:H:580:LYS:HZ3	1.86	0.41
1:A:280:ARG:HD2	1:A:280:ARG:HA	1.97	0.40
1:D:268:SER:OG	1:D:269:CYS:N	2.53	0.40
1:D:304:TRP:CE2	1:D:597:ARG:HD2	2.56	0.40
1:D:360:VAL:O	1:D:362:THR:N	2.48	0.40
1:D:469:ALA:HB3	1:D:731:ARG:HH22	1.86	0.40
1:D:630:VAL:HG21	1:D:648:TRP:CD1	2.56	0.40
1:F:647:ARG:HB2	1:F:647:ARG:HE	1.61	0.40
1:C:346:ASP:OD1	1:C:351:GLY:HA3	2.19	0.40
1:F:312:ALA:O	1:F:590:THR:HG23	2.21	0.40
1:F:656:ARG:O	1:F:660:MET:HG3	2.22	0.40
1:B:476:TRP:CE2	1:B:602:GLY:HA2	2.57	0.40
1:B:638:LEU:HD12	1:B:638:LEU:HA	1.90	0.40
1:B:724:ARG:HD2	1:B:826:MET:SD	2.61	0.40
1:C:478:MET:HB2	1:C:483:ARG:HD3	2.03	0.40
1:B:368:GLN:HB3	1:B:636:LEU:O	2.22	0.40
1:B:641:LYS:HE3	1:B:643:GLU:HB3	2.04	0.40
1:E:652:ASN:O	1:E:656:ARG:HG2	2.22	0.40
1:A:454:ASN:O	1:A:476:TRP:HA	2.22	0.40
1:B:370:GLY:O	1:B:374:VAL:HG23	2.21	0.40
1:F:516:LEU:HD11	1:F:800:HIS:CD2	2.57	0.40
1:H:515:ARG:HD3	1:H:515:ARG:HA	1.91	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:C:280:ARG:NH1	1:E:288:GLU:O[2_656]	2.14	0.06

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	622/639 (97%)	595 (96%)	26 (4%)	1 (0%)	47	82
1	B	619/639 (97%)	588 (95%)	28 (4%)	3 (0%)	29	68
1	C	619/639 (97%)	584 (94%)	30 (5%)	5 (1%)	19	57
1	D	621/639 (97%)	575 (93%)	44 (7%)	2 (0%)	41	76
1	E	620/639 (97%)	587 (95%)	29 (5%)	4 (1%)	25	64
1	F	620/639 (97%)	581 (94%)	34 (6%)	5 (1%)	19	57
1	G	622/639 (97%)	587 (94%)	34 (6%)	1 (0%)	47	82
1	H	621/639 (97%)	587 (94%)	32 (5%)	2 (0%)	41	76
All	All	4964/5112 (97%)	4684 (94%)	257 (5%)	23 (0%)	29	68

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	640	ARG
1	F	271	GLU
1	G	633	MET
1	A	508	VAL
1	C	577	LYS
1	F	461	LYS
1	F	560	GLU
1	H	406	SER
1	H	457	GLY
1	B	320	SER
1	B	748	TRP
1	C	270	ALA
1	C	470	LYS
1	E	409	ALA
1	E	633	MET
1	F	632	GLU
1	C	408	ALA

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Mol	Chain	Res	Type
1	F	642	PRO
1	D	725	SER
1	E	320	SER
1	D	412	ALA
1	E	465	GLU
1	C	538	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	539/549 (98%)	525 (97%)	14 (3%)	46	78
1	B	536/549 (98%)	512 (96%)	24 (4%)	27	64
1	C	536/549 (98%)	515 (96%)	21 (4%)	32	69
1	D	537/549 (98%)	519 (97%)	18 (3%)	37	72
1	E	537/549 (98%)	521 (97%)	16 (3%)	41	75
1	F	537/549 (98%)	519 (97%)	18 (3%)	37	72
1	G	537/549 (98%)	522 (97%)	15 (3%)	43	77
1	H	536/549 (98%)	518 (97%)	18 (3%)	37	72
All	All	4295/4392 (98%)	4151 (97%)	144 (3%)	37	72

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	ARG
1	A	391	ARG
1	A	405	ARG
1	A	413	ILE
1	A	456	MET
1	A	460	GLU
1	A	476	TRP
1	A	479	TRP
1	A	586	GLU

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Mol	Chain	Res	Type
1	A	639	LEU
1	A	818	VAL
1	A	852	LEU
1	A	887	SER
1	A	890	VAL
1	B	281	ARG
1	B	284	ARG
1	B	325	VAL
1	B	339	VAL
1	B	459	ARG
1	B	476	TRP
1	B	479	TRP
1	B	514	GLN
1	B	531	MET
1	B	586	GLU
1	B	621	LEU
1	B	624	ASN
1	B	639	LEU
1	B	640	ARG
1	B	647	ARG
1	B	656	ARG
1	B	670	LYS
1	B	673	ASP
1	B	690	ARG
1	B	776	LEU
1	B	799	ILE
1	B	808	THR
1	B	818	VAL
1	B	858	ARG
1	C	269	CYS
1	C	315	GLN
1	C	357	LYS
1	C	473	ARG
1	C	480	LEU
1	C	483	ARG
1	C	514	GLN
1	C	535	ASP
1	C	558	MET
1	C	581	VAL
1	C	601	ARG
1	C	621	LEU
1	C	629	GLU

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Mol	Chain	Res	Type
1	C	639	LEU
1	C	652	ASN
1	C	656	ARG
1	C	775	ARG
1	C	812	LEU
1	C	814	VAL
1	C	858	ARG
1	C	864	ASN
1	D	311	GLU
1	D	315	GLN
1	D	335	VAL
1	D	339	VAL
1	D	357	LYS
1	D	404	VAL
1	D	420	TRP
1	D	456	MET
1	D	480	LEU
1	D	590	THR
1	D	601	ARG
1	D	743	SER
1	D	790	VAL
1	D	794	ARG
1	D	799	ILE
1	D	813	MET
1	D	856	ARG
1	D	883	MET
1	E	314	THR
1	E	344	MET
1	E	363	ARG
1	E	382	LEU
1	E	383	TRP
1	E	421	LYS
1	E	463	GLN
1	E	476	TRP
1	E	479	TRP
1	E	601	ARG
1	E	631	LEU
1	E	637	TRP
1	E	639	LEU
1	E	678	HIS
1	E	790	VAL
1	E	813	MET

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Mol	Chain	Res	Type
1	F	320	SER
1	F	345	THR
1	F	391	ARG
1	F	468	LYS
1	F	476	TRP
1	F	479	TRP
1	F	581	VAL
1	F	590	THR
1	F	621	LEU
1	F	631	LEU
1	F	633	MET
1	F	637	TRP
1	F	644	LYS
1	F	648	TRP
1	F	790	VAL
1	F	814	VAL
1	F	853	ILE
1	F	864	ASN
1	G	321	LEU
1	G	339	VAL
1	G	407	ASN
1	G	413	ILE
1	G	456	MET
1	G	473	ARG
1	G	483	ARG
1	G	531	MET
1	G	581	VAL
1	G	591	VAL
1	G	629	GLU
1	G	643	GLU
1	G	693	THR
1	G	694	GLN
1	G	814	VAL
1	H	325	VAL
1	H	339	VAL
1	H	347	THR
1	H	354	ARG
1	H	373	GLN
1	H	404	VAL
1	H	473	ARG
1	H	621	LEU
1	H	634	GLN

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Mol	Chain	Res	Type
1	H	639	LEU
1	H	656	ARG
1	H	722	ASP
1	H	766	LEU
1	H	807	THR
1	H	852	LEU
1	H	855	HIS
1	H	856	ARG
1	H	871	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	550	ASN
1	B	605	GLN
1	B	762	GLN
1	C	514	GLN
1	C	605	GLN
1	C	864	ASN
1	D	315	GLN
1	D	352	GLN
1	D	368	GLN
1	D	442	HIS
1	D	605	GLN
1	E	557	GLN
1	E	634	GLN
1	F	550	ASN
1	F	765	GLN
1	G	454	ASN
1	G	620	GLN
1	H	373	GLN
1	H	524	ASN
1	H	620	GLN
1	H	694	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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	624/639 (97%)	-0.22	7 (1%) 80 56	29, 59, 86, 109	0
1	B	621/639 (97%)	-0.31	7 (1%) 80 56	22, 45, 69, 110	0
1	C	621/639 (97%)	-0.30	6 (0%) 82 59	26, 46, 85, 107	0
1	D	623/639 (97%)	-0.34	7 (1%) 80 56	26, 39, 68, 103	0
1	E	622/639 (97%)	-0.20	10 (1%) 72 44	28, 59, 90, 130	0
1	F	622/639 (97%)	-0.28	4 (0%) 89 72	27, 53, 80, 113	0
1	G	624/639 (97%)	-0.31	10 (1%) 72 44	31, 44, 80, 99	0
1	H	623/639 (97%)	-0.32	11 (1%) 68 40	24, 37, 70, 94	0
All	All	4980/5112 (97%)	-0.29	62 (1%) 79 54	22, 45, 81, 130	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	416	GLU	4.6
1	G	414	PHE	4.5
1	D	415	GLU	4.4
1	E	464	GLY	4.4
1	E	466	PHE	4.1
1	A	464	GLY	3.9
1	C	414	PHE	3.8
1	D	414	PHE	3.8
1	E	465	GLU	3.7
1	H	412	ALA	3.7
1	E	463	GLN	3.6
1	G	265	ALA	3.5
1	C	407	ASN	3.5
1	E	889	GLN	3.4
1	G	409	ALA	3.4
1	C	413	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	413	ILE	3.3
1	H	413	ILE	3.1
1	E	467	GLY	3.0
1	A	469	ALA	3.0
1	C	415	GLU	3.0
1	H	414	PHE	3.0
1	F	466	PHE	3.0
1	B	465	GLU	3.0
1	H	265	ALA	2.9
1	A	268	SER	2.9
1	H	266	VAL	2.8
1	H	416	GLU	2.7
1	G	416	GLU	2.7
1	G	415	GLU	2.7
1	E	469	ALA	2.7
1	C	412	ALA	2.7
1	A	466	PHE	2.6
1	G	413	ILE	2.6
1	H	407	ASN	2.6
1	G	266	VAL	2.6
1	D	465	GLU	2.6
1	F	467	GLY	2.5
1	A	891	ARG	2.5
1	B	467	GLY	2.4
1	H	415	GLU	2.4
1	A	465	GLU	2.4
1	E	268	SER	2.3
1	G	465	GLU	2.3
1	H	409	ALA	2.3
1	B	461	LYS	2.3
1	G	407	ASN	2.3
1	H	268	SER	2.3
1	B	463	GLN	2.3
1	B	469	ALA	2.2
1	E	468	LYS	2.2
1	D	268	SER	2.2
1	D	419	GLU	2.2
1	F	464	GLY	2.2
1	E	462	LYS	2.2
1	F	465	GLU	2.1
1	B	464	GLY	2.1
1	B	470	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	462	LYS	2.1
1	A	467	GLY	2.1
1	G	888	THR	2.0
1	D	416	GLU	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](#)

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(\AA^2)	Q<0.9
2	ZN	B	1001	1/1	0.99	0.21	54,54,54,54	0
2	ZN	A	1001	1/1	0.99	0.16	58,58,58,58	0
2	ZN	C	1001	1/1	0.99	0.20	69,69,69,69	0
2	ZN	E	1002	1/1	0.99	0.20	52,52,52,52	0
2	ZN	A	1002	1/1	0.99	0.21	42,42,42,42	0
2	ZN	G	1002	1/1	0.99	0.20	44,44,44,44	0
2	ZN	H	1001	1/1	0.99	0.19	49,49,49,49	0
2	ZN	C	1002	1/1	0.99	0.21	42,42,42,42	0
2	ZN	D	1002	1/1	0.99	0.21	44,44,44,44	0
2	ZN	B	1002	1/1	0.99	0.21	47,47,47,47	0
2	ZN	E	1001	1/1	0.99	0.17	65,65,65,65	0
2	ZN	F	1002	1/1	1.00	0.19	46,46,46,46	0
2	ZN	G	1001	1/1	1.00	0.15	54,54,54,54	0
2	ZN	D	1001	1/1	1.00	0.20	48,48,48,48	0
2	ZN	F	1001	1/1	1.00	0.18	46,46,46,46	0
2	ZN	H	1002	1/1	1.00	0.21	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.