



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:07 PM EDT

PDB ID : 6QGM / pdb_00006qgm
Title : VirX1 apo structure
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Deposited on : 2019-01-11
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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Mol	Chain	Length	Quality of chain
1	f	531	% 86% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25688 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 VirX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	524	Total	C	N	O	S	0	0	0
			4273	2724	722	806	21			
1	b	525	Total	C	N	O	S	0	0	0
			4278	2727	723	807	21			
1	c	522	Total	C	N	O	S	0	0	0
			4265	2720	721	803	21			
1	d	526	Total	C	N	O	S	0	0	0
			4285	2731	724	808	22			
1	e	523	Total	C	N	O	S	0	0	0
			4264	2718	721	804	21			
1	f	525	Total	C	N	O	S	0	0	0
			4275	2724	723	807	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	5	VAL	-	insertion	UNP M4SKV1
b	5	VAL	-	insertion	UNP M4SKV1
c	5	VAL	-	insertion	UNP M4SKV1
d	5	VAL	-	insertion	UNP M4SKV1
e	5	VAL	-	insertion	UNP M4SKV1
f	5	VAL	-	insertion	UNP M4SKV1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	a	9	Total	O	0	0
			9	9		
2	b	6	Total	O	0	0
			6	6		
2	c	10	Total	O	0	0
			10	10		

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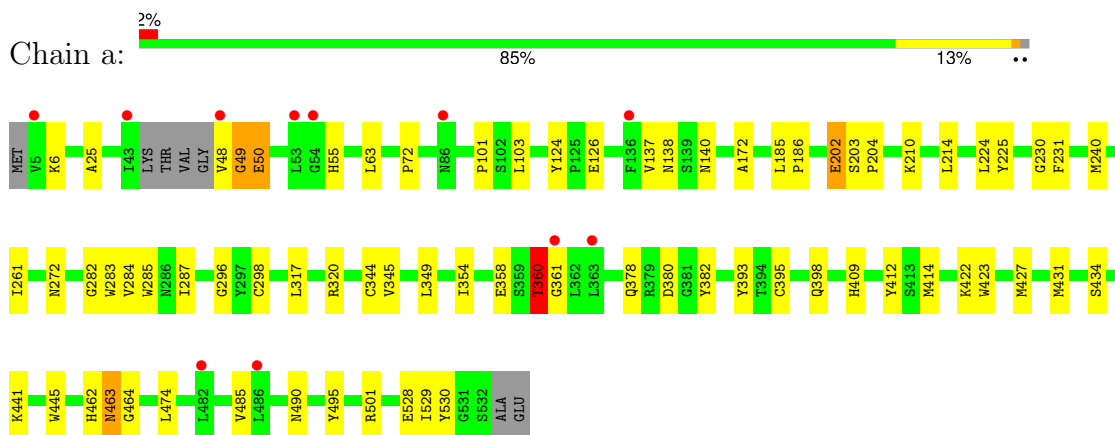
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	d	9	Total	O	0	0
			9	9		
2	e	7	Total	O	0	0
			7	7		
2	f	7	Total	O	0	0
			7	7		

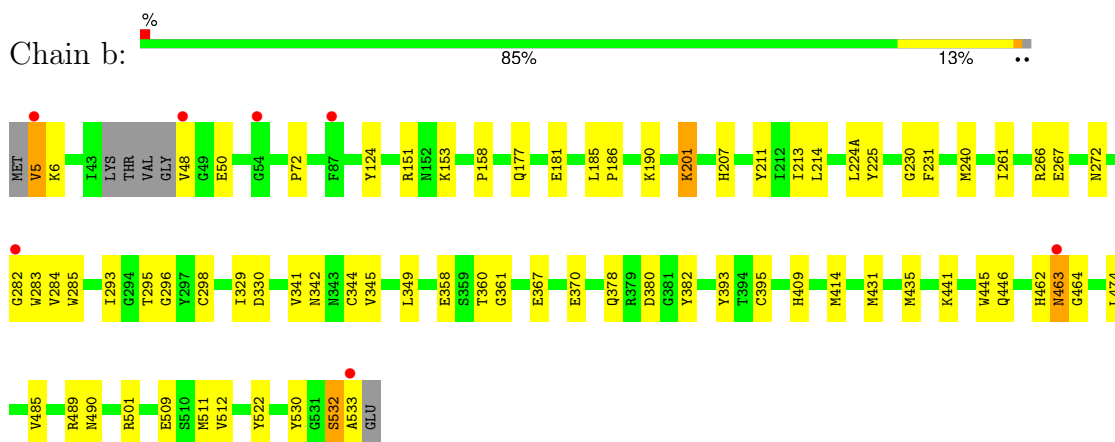
3 Residue-property plots [i](#)

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.

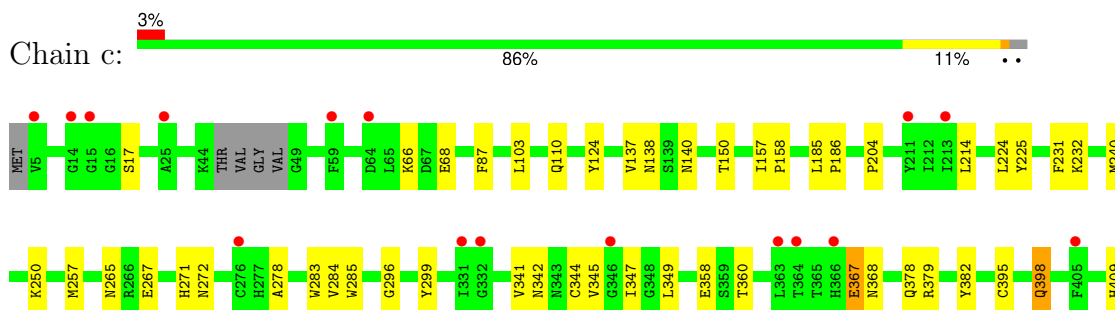
• Molecule 1: VirX1



• Molecule 1: VirX1

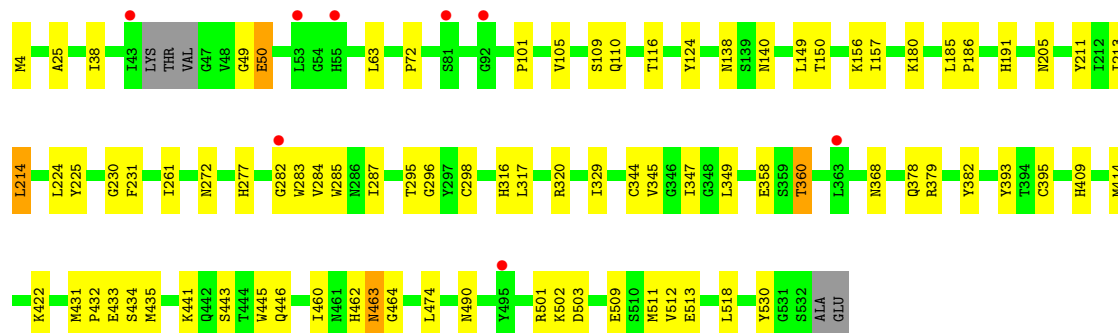
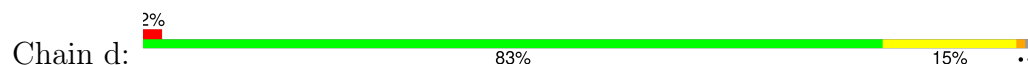


• Molecule 1: VirX1

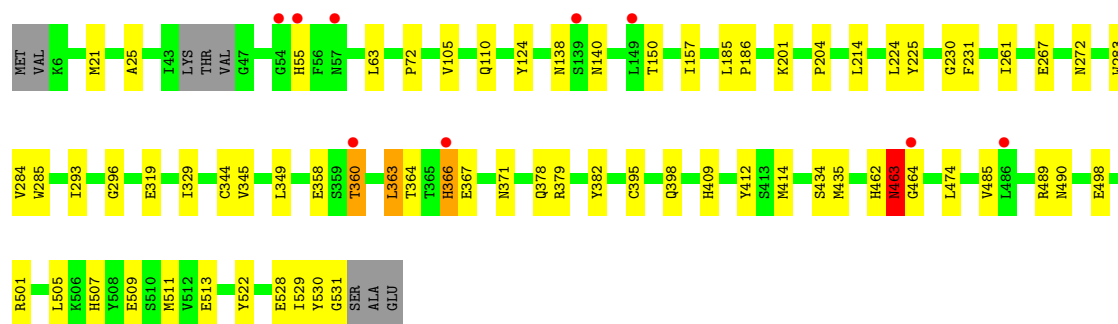
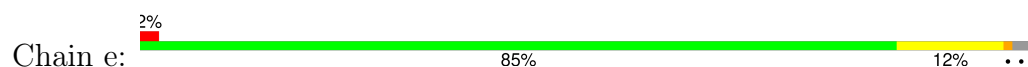




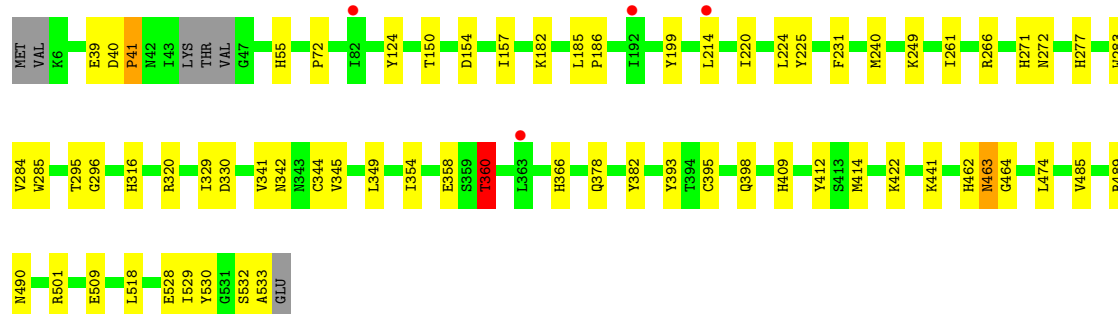
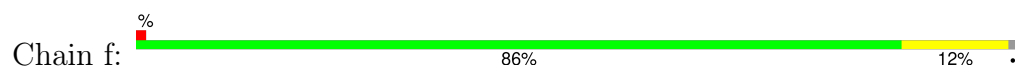
• Molecule 1: VirX1



• Molecule 1: VirX1



• Molecule 1: VirX1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.13Å 172.98Å 110.42Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	87.94 – 2.75 87.94 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (87.94-2.75) 99.0 (87.94-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.216 , 0.259 0.221 , 0.261	Depositor DCC
R_{free} test set	4356 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25688	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.34% 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

5.1 Standard geometry

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	0.98	0/4394	1.40	4/5953 (0.1%)
1	b	0.99	0/4399	1.39	3/5960 (0.1%)
1	c	0.99	0/4386	1.39	3/5941 (0.1%)
1	d	0.99	0/4406	1.38	3/5968 (0.1%)
1	e	0.97	0/4385	1.39	5/5940 (0.1%)
1	f	0.99	0/4396	1.39	6/5955 (0.1%)
All	All	0.98	0/26366	1.39	24/35717 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	366	HIS	CB-CA-C	-7.33	98.62	110.79
1	a	55	HIS	CA-CB-CG	6.82	120.62	113.80
1	e	55	HIS	CA-CB-CG	6.58	120.38	113.80
1	b	360	THR	CB-CA-C	6.46	120.87	110.09
1	c	360	THR	CB-CA-C	6.21	120.46	109.65
1	a	49	GLY	CA-C-O	-6.19	115.94	121.64
1	b	5	VAL	CA-C-N	6.14	129.43	120.71
1	b	5	VAL	C-N-CA	6.14	129.43	120.71
1	d	360	THR	CB-CA-C	5.68	119.58	110.09
1	e	360	THR	CB-CA-C	5.62	119.47	110.09
1	f	55	HIS	CA-CB-CG	-5.47	108.33	113.80
1	f	360	THR	CB-CA-C	5.46	119.20	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	360	THR	CB-CA-C	5.35	119.03	110.09
1	d	49	GLY	CA-C-O	-5.24	116.86	121.58
1	f	366	HIS	CA-CB-CG	5.20	119.00	113.80
1	e	366	HIS	N-CA-CB	5.20	117.76	110.12
1	a	202	GLU	CB-CG-CD	5.14	121.35	112.60
1	d	205	ASN	CA-CB-CG	-5.12	107.48	112.60
1	f	271	HIS	CA-C-N	5.12	131.32	121.54
1	f	271	HIS	C-N-CA	5.12	131.32	121.54
1	f	360	THR	CA-CB-OG1	-5.06	102.00	109.60
1	e	463	ASN	N-CA-CB	5.06	119.04	110.49
1	c	271	HIS	CA-C-N	5.04	131.18	121.54
1	c	271	HIS	C-N-CA	5.04	131.18	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	b	532	SER	Peptide

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	4273	0	4046	54	0
1	b	4278	0	4051	55	0
1	c	4265	0	4042	48	0
1	d	4285	0	4058	65	0
1	e	4264	0	4035	49	0
1	f	4275	0	4045	44	0
2	a	9	0	0	0	0
2	b	6	0	0	0	0
2	c	10	0	0	0	0
2	d	9	0	0	0	0
2	e	7	0	0	0	0
2	f	7	0	0	0	0
All	All	25688	0	24277	266	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 5.

All (266) 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:109:SER:H	1:d:116:THR:HG21	1.43	0.83
1:d:434:SER:O	1:f:441:LYS:HE3	1.83	0.78
1:a:495:TYR:CE2	1:e:498:GLU:HG3	2.20	0.77
1:d:109:SER:N	1:d:116:THR:HG21	2.00	0.77
1:b:240:MET:HE1	1:b:342:ASN:OD1	1.85	0.76
1:c:66:LYS:HG3	1:c:68:GLU:OE1	1.86	0.76
1:d:261:ILE:HD11	1:d:317:LEU:HD13	1.68	0.74
1:a:261:ILE:HD11	1:a:317:LEU:HD13	1.67	0.73
1:d:435:MET:HE1	1:f:393:TYR:HA	1.68	0.73
1:f:240:MET:HE1	1:f:342:ASN:OD1	1.86	0.73
1:c:240:MET:HE1	1:c:342:ASN:OD1	1.89	0.73
1:a:50:GLU:HA	1:a:287:ILE:HD13	1.71	0.71
1:a:434:SER:O	1:c:441:LYS:HE3	1.90	0.71
1:d:379:ARG:NH2	1:e:412:TYR:O	2.24	0.71
1:b:240:MET:HE2	1:b:341:VAL:HG12	1.74	0.70
1:a:378:GLN:HG3	1:b:474:LEU:HD23	1.73	0.69
1:a:412:TYR:O	1:c:379:ARG:NH2	2.26	0.69
1:a:126:GLU:H	1:a:126:GLU:CD	2.01	0.68
1:d:109:SER:HB3	1:d:116:THR:CG2	2.25	0.67
1:d:347:ILE:HD13	1:d:368:ASN:HB3	1.76	0.67
1:a:393:TYR:HA	1:b:435:MET:HE1	1.76	0.67
1:d:211:TYR:CE2	1:d:213:ILE:HD11	2.30	0.67
1:f:240:MET:HE2	1:f:341:VAL:HG12	1.76	0.67
1:c:347:ILE:HD13	1:c:368:ASN:HB3	1.77	0.67
1:a:261:ILE:HG23	1:a:320:ARG:HD2	1.77	0.67
1:d:378:GLN:CG	1:e:474:LEU:HD23	2.25	0.67
1:d:378:GLN:HG3	1:e:474:LEU:HD23	1.77	0.66
1:c:240:MET:HE2	1:c:341:VAL:HG12	1.76	0.66
1:b:177:GLN:O	1:b:181:GLU:HG2	1.96	0.65
1:b:393:TYR:HA	1:c:435:MET:HE1	1.79	0.64
1:d:261:ILE:HG23	1:d:320:ARG:HD2	1.78	0.64
1:a:378:GLN:CG	1:b:474:LEU:HD23	2.27	0.63
1:d:50:GLU:HA	1:d:287:ILE:HD13	1.80	0.63
1:d:441:LYS:HE3	1:e:434:SER:O	1.98	0.63
1:b:261:ILE:HG13	1:b:293:ILE:HB	1.80	0.62
1:f:150:THR:HG21	1:f:157:ILE:CD1	2.29	0.62
1:a:474:LEU:HD23	1:c:378:GLN:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:474:LEU:HD23	1:f:378:GLN:HG3	1.82	0.62
1:d:211:TYR:HE2	1:d:213:ILE:HD11	1.62	0.62
1:a:231:PHE:CZ	1:a:349:LEU:HD13	2.35	0.61
1:d:509:GLU:O	1:d:512:VAL:HG22	1.99	0.61
1:d:231:PHE:CZ	1:d:349:LEU:HD13	2.36	0.61
1:e:378:GLN:HG3	1:f:474:LEU:HD23	1.82	0.61
1:b:509:GLU:O	1:b:512:VAL:HG22	2.01	0.61
1:c:150:THR:HG21	1:c:157:ILE:CD1	2.31	0.61
1:b:211:TYR:CE2	1:b:213:ILE:HD11	2.36	0.60
1:b:532:SER:OG	1:b:533:ALA:N	2.33	0.60
1:f:261:ILE:HG23	1:f:320:ARG:HD2	1.82	0.60
1:a:474:LEU:HD23	1:c:378:GLN:CG	2.31	0.60
1:b:382:TYR:CE2	1:c:414:MET:HA	2.37	0.60
1:e:261:ILE:HG13	1:e:293:ILE:HB	1.81	0.60
1:d:435:MET:HE1	1:f:393:TYR:CA	2.31	0.60
1:a:495:TYR:CZ	1:e:498:GLU:HG3	2.36	0.60
1:b:151:ARG:HB2	1:b:153:LYS:HE3	1.83	0.59
1:d:211:TYR:CE2	1:d:213:ILE:CD1	2.86	0.59
1:e:231:PHE:CZ	1:e:349:LEU:HD13	2.38	0.59
1:e:150:THR:HG21	1:e:157:ILE:CD1	2.31	0.59
1:d:150:THR:HG21	1:d:157:ILE:CD1	2.32	0.58
1:b:211:TYR:CE2	1:b:213:ILE:CD1	2.86	0.58
1:b:378:GLN:HG3	1:c:474:LEU:HD23	1.85	0.58
1:a:414:MET:HA	1:c:382:TYR:CE2	2.39	0.58
1:c:231:PHE:CZ	1:c:349:LEU:HD13	2.39	0.58
1:d:211:TYR:HE2	1:d:213:ILE:CD1	2.16	0.58
1:e:505:LEU:O	1:e:509:GLU:HG2	2.05	0.57
1:b:231:PHE:CZ	1:b:349:LEU:HD13	2.39	0.57
1:f:231:PHE:CZ	1:f:349:LEU:HD13	2.39	0.57
1:e:379:ARG:NH2	1:f:412:TYR:O	2.38	0.56
1:b:211:TYR:HE2	1:b:213:ILE:CD1	2.19	0.56
1:d:109:SER:HB3	1:d:116:THR:HG22	1.87	0.55
1:e:507:HIS:NE2	1:e:511:MET:HE3	2.21	0.55
1:c:158:PRO:HD2	1:c:511:MET:HE1	1.89	0.55
1:f:285:TRP:O	1:f:295:THR:HG23	2.06	0.54
1:b:285:TRP:O	1:b:295:THR:HG23	2.07	0.54
1:f:354:ILE:HD12	1:f:360:THR:HG21	1.90	0.54
1:b:185:LEU:HB2	1:b:186:PRO:HD3	1.90	0.54
1:e:382:TYR:CE2	1:f:414:MET:HA	2.43	0.54
1:b:6:LYS:HE2	1:b:380:ASP:O	2.07	0.54
1:d:185:LEU:HB2	1:d:186:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:285:TRP:O	1:d:295:THR:HG23	2.06	0.54
1:f:40:ASP:C	1:f:41:PRO:O	2.51	0.54
1:e:378:GLN:CG	1:f:474:LEU:HD23	2.38	0.53
1:c:110:GLN:OE1	1:c:110:GLN:HA	2.08	0.53
1:b:393:TYR:CA	1:c:435:MET:HE1	2.39	0.53
1:c:124:TYR:CG	1:c:501:ARG:HD2	2.44	0.53
1:b:158:PRO:HD3	1:b:511:MET:HE1	1.90	0.53
1:d:414:MET:HA	1:f:382:TYR:CE2	2.44	0.53
1:f:124:TYR:CG	1:f:501:ARG:HD2	2.44	0.53
1:f:185:LEU:HB2	1:f:186:PRO:HD3	1.91	0.52
1:a:185:LEU:HB2	1:a:186:PRO:HD3	1.91	0.52
1:a:124:TYR:CG	1:a:501:ARG:HD2	2.44	0.52
1:d:124:TYR:CG	1:d:501:ARG:HD2	2.44	0.52
1:d:474:LEU:HD23	1:f:378:GLN:CG	2.39	0.52
1:d:382:TYR:CE2	1:e:414:MET:HA	2.44	0.52
1:b:151:ARG:HB2	1:b:153:LYS:CE	2.40	0.52
1:c:240:MET:CE	1:c:342:ASN:OD1	2.57	0.52
1:d:277:HIS:HB3	1:d:284:VAL:HG23	1.92	0.52
1:f:358:GLU:OE2	1:f:409:HIS:NE2	2.38	0.51
1:e:185:LEU:HB2	1:e:186:PRO:HD3	1.92	0.51
1:a:495:TYR:CD2	1:e:498:GLU:HG3	2.45	0.51
1:b:124:TYR:CG	1:b:501:ARG:HD2	2.45	0.51
1:c:185:LEU:HB2	1:c:186:PRO:HD3	1.92	0.51
1:e:110:GLN:OE1	1:e:110:GLN:HA	2.11	0.51
1:f:240:MET:CE	1:f:342:ASN:OD1	2.56	0.51
1:a:382:TYR:CE2	1:b:414:MET:HA	2.46	0.51
1:a:528:GLU:C	1:a:529:ILE:HD12	2.36	0.51
1:e:528:GLU:C	1:e:529:ILE:HD12	2.35	0.51
1:c:158:PRO:HD2	1:c:511:MET:CE	2.40	0.50
1:e:124:TYR:CG	1:e:501:ARG:HD2	2.46	0.50
1:f:528:GLU:C	1:f:529:ILE:HD12	2.36	0.50
1:f:40:ASP:OD1	1:f:41:PRO:O	2.30	0.50
1:a:393:TYR:CA	1:b:435:MET:HE1	2.41	0.50
1:f:277:HIS:HB3	1:f:284:VAL:HG23	1.94	0.50
1:c:257:MET:HE3	1:c:299:TYR:CE2	2.47	0.49
1:d:393:TYR:HA	1:e:435:MET:HE1	1.93	0.49
1:c:358:GLU:OE2	1:c:409:HIS:NE2	2.38	0.49
1:b:240:MET:CE	1:b:342:ASN:OD1	2.57	0.48
1:a:124:TYR:CD2	1:a:501:ARG:HD2	2.48	0.48
1:b:211:TYR:HE2	1:b:213:ILE:HD11	1.77	0.48
1:f:266:ARG:HH12	1:f:533:ALA:HB1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:199:TYR:CD1	1:f:199:TYR:C	2.91	0.48
1:a:103:LEU:CG	1:a:137:VAL:HG11	2.44	0.48
1:d:225:TYR:O	1:d:344:CYS:HA	2.13	0.48
1:d:261:ILE:CD1	1:d:317:LEU:HD22	2.43	0.48
1:f:124:TYR:CD2	1:f:501:ARG:HD2	2.49	0.48
1:b:124:TYR:CD2	1:b:501:ARG:HD2	2.48	0.47
1:e:124:TYR:CD2	1:e:501:ARG:HD2	2.48	0.47
1:f:225:TYR:O	1:f:344:CYS:HA	2.14	0.47
1:b:72:PRO:HA	1:b:530:TYR:CE1	2.48	0.47
1:e:284:VAL:HA	1:e:296:GLY:O	2.15	0.47
1:c:103:LEU:HB3	1:c:137:VAL:CG1	2.43	0.47
1:d:124:TYR:CD2	1:d:501:ARG:HD2	2.49	0.47
1:a:103:LEU:HG	1:a:137:VAL:HG11	1.95	0.47
1:a:225:TYR:O	1:a:344:CYS:HA	2.15	0.47
1:c:124:TYR:CD2	1:c:501:ARG:HD2	2.49	0.47
1:b:266:ARG:HH12	1:b:533:ALA:HB1	1.80	0.47
1:b:284:VAL:HA	1:b:296:GLY:O	2.14	0.47
1:c:367:GLU:HG2	1:c:398:GLN:OE1	2.15	0.47
1:e:382:TYR:CZ	1:f:414:MET:HA	2.49	0.47
1:f:284:VAL:HG21	1:f:316:HIS:CD2	2.50	0.47
1:c:284:VAL:HA	1:c:296:GLY:O	2.15	0.47
1:b:225:TYR:O	1:b:344:CYS:HA	2.15	0.47
1:c:225:TYR:O	1:c:344:CYS:HA	2.14	0.47
1:d:277:HIS:HB3	1:d:284:VAL:CG2	2.45	0.46
1:a:284:VAL:HA	1:a:296:GLY:O	2.14	0.46
1:e:225:TYR:O	1:e:344:CYS:HA	2.15	0.46
1:c:283:TRP:CZ3	1:c:285:TRP:HB3	2.50	0.46
1:c:231:PHE:CE1	1:c:349:LEU:HD13	2.50	0.46
1:a:358:GLU:OE2	1:a:409:HIS:NE2	2.38	0.46
1:d:284:VAL:HA	1:d:296:GLY:O	2.16	0.46
1:e:105:VAL:HG12	1:e:105:VAL:O	2.15	0.46
1:f:284:VAL:HA	1:f:296:GLY:O	2.16	0.46
1:c:158:PRO:CD	1:c:511:MET:HE1	2.46	0.46
1:f:231:PHE:CE1	1:f:349:LEU:HD13	2.51	0.46
1:f:277:HIS:HB3	1:f:284:VAL:CG2	2.45	0.46
1:b:378:GLN:CG	1:c:474:LEU:HD23	2.45	0.45
1:c:462:HIS:O	1:c:464:GLY:N	2.49	0.45
1:d:231:PHE:CE1	1:d:349:LEU:HD13	2.51	0.45
1:d:284:VAL:HG21	1:d:316:HIS:CD2	2.50	0.45
1:f:72:PRO:HA	1:f:530:TYR:CE1	2.51	0.45
1:d:156:LYS:O	1:d:511:MET:HE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:462:HIS:O	1:f:464:GLY:N	2.50	0.45
1:a:72:PRO:HA	1:a:530:TYR:CE1	2.52	0.45
1:a:283:TRP:CZ3	1:a:285:TRP:HB3	2.52	0.45
1:a:50:GLU:OE1	1:a:172:ALA:HB2	2.17	0.45
1:a:231:PHE:CE1	1:a:349:LEU:HD13	2.52	0.45
1:a:462:HIS:O	1:a:464:GLY:N	2.50	0.45
1:a:202:GLU:OE1	1:a:210:LYS:HD2	2.17	0.45
1:d:462:HIS:O	1:d:464:GLY:N	2.50	0.45
1:b:441:LYS:CE	1:c:436:GLY:O	2.65	0.45
1:a:6:LYS:HD3	1:a:380:ASP:O	2.17	0.45
1:d:431:MET:HG2	1:d:445:TRP:HB3	1.99	0.45
1:e:231:PHE:CE1	1:e:349:LEU:HD13	2.52	0.45
1:d:72:PRO:HA	1:d:530:TYR:CE1	2.52	0.44
1:e:72:PRO:HA	1:e:530:TYR:CE1	2.51	0.44
1:e:283:TRP:CZ3	1:e:285:TRP:HB3	2.52	0.44
1:a:126:GLU:CD	1:a:126:GLU:N	2.71	0.44
1:d:393:TYR:CA	1:e:435:MET:HE1	2.47	0.44
1:d:502:LYS:HG3	1:d:503:ASP:N	2.32	0.44
1:b:462:HIS:O	1:b:464:GLY:N	2.50	0.44
1:b:224(A):LEU:HD11	1:b:345:VAL:HG23	2.00	0.44
1:c:265:ASN:OD1	1:c:267:GLU:HG2	2.18	0.44
1:e:105:VAL:O	1:e:105:VAL:CG1	2.64	0.44
1:b:431:MET:HG2	1:b:445:TRP:HB3	2.00	0.44
1:a:354:ILE:HD12	1:a:360:THR:HG21	2.00	0.44
1:c:103:LEU:HD23	1:c:137:VAL:HG11	1.99	0.44
1:b:266:ARG:HH12	1:b:533:ALA:CB	2.30	0.43
1:b:358:GLU:OE2	1:b:409:HIS:NE2	2.39	0.43
1:c:462:HIS:O	1:c:463:ASN:C	2.61	0.43
1:d:283:TRP:CZ3	1:d:285:TRP:HB3	2.52	0.43
1:a:240:MET:HE3	1:a:240:MET:HA	2.00	0.43
1:d:105:VAL:HG12	1:d:105:VAL:O	2.18	0.43
1:d:378:GLN:HG2	1:e:474:LEU:CD2	2.48	0.43
1:f:462:HIS:O	1:f:463:ASN:C	2.61	0.43
1:b:267:GLU:HG2	1:b:522:TYR:CD2	2.53	0.43
1:d:105:VAL:O	1:d:105:VAL:CG1	2.66	0.43
1:e:267:GLU:HG3	1:e:522:TYR:CD2	2.53	0.43
1:a:101:PRO:HG3	1:b:489:ARG:NH2	2.33	0.43
1:e:358:GLU:OE2	1:e:409:HIS:NE2	2.38	0.43
1:f:154:ASP:C	1:f:154:ASP:OD1	2.61	0.43
1:a:230:GLY:HA2	1:a:349:LEU:HB2	2.00	0.43
1:b:283:TRP:CZ3	1:b:285:TRP:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:101:PRO:HB3	1:e:489:ARG:NH2	2.34	0.43
1:e:462:HIS:O	1:e:464:GLY:N	2.51	0.43
1:e:530:TYR:O	1:e:531:GLY:O	2.37	0.43
1:d:230:GLY:HA2	1:d:349:LEU:HB2	2.00	0.43
1:d:358:GLU:OE2	1:d:409:HIS:NE2	2.37	0.43
1:d:432:PRO:HG2	1:d:433:GLU:OE1	2.19	0.43
1:b:441:LYS:HE3	1:c:434:SER:O	2.19	0.43
1:e:367:GLU:OE1	1:e:371:ASN:ND2	2.52	0.43
1:d:224:LEU:HD11	1:d:345:VAL:HG23	2.00	0.43
1:e:462:HIS:O	1:e:463:ASN:C	2.62	0.43
1:b:462:HIS:O	1:b:463:ASN:C	2.62	0.42
1:a:224:LEU:HD11	1:a:345:VAL:HG23	2.01	0.42
1:b:5:VAL:HG21	1:c:416:THR:HG21	2.00	0.42
1:d:378:GLN:HG2	1:e:474:LEU:HD23	1.98	0.42
1:a:48:VAL:HG12	1:a:49:GLY:N	2.35	0.42
1:b:201:LYS:HD3	1:b:207:HIS:HA	2.01	0.42
1:f:283:TRP:CZ3	1:f:285:TRP:HB3	2.54	0.42
1:a:414:MET:HA	1:c:382:TYR:CZ	2.54	0.42
1:c:224:LEU:HD11	1:c:345:VAL:HG23	2.01	0.42
1:d:414:MET:HA	1:f:382:TYR:CZ	2.54	0.42
1:e:230:GLY:HA2	1:e:349:LEU:HB2	2.01	0.42
1:a:431:MET:HG2	1:a:445:TRP:HB3	2.02	0.42
1:b:50:GLU:OE2	1:b:361:GLY:HA3	2.20	0.42
1:d:462:HIS:O	1:d:463:ASN:C	2.63	0.42
1:e:360:THR:O	1:e:363:LEU:HB3	2.20	0.42
1:a:529:ILE:HD12	1:a:529:ILE:N	2.35	0.42
1:b:231:PHE:CE1	1:b:349:LEU:HD13	2.55	0.42
1:b:382:TYR:CZ	1:c:414:MET:HA	2.55	0.42
1:c:158:PRO:CD	1:c:511:MET:CE	2.97	0.42
1:d:38:ILE:HG21	1:d:214:LEU:HD11	2.02	0.42
1:a:103:LEU:HB3	1:a:137:VAL:CG1	2.50	0.41
1:d:25:ALA:HA	1:d:63:LEU:HD21	2.01	0.41
1:a:423:TRP:HA	1:a:427:MET:CE	2.49	0.41
1:d:149:LEU:HD12	1:d:149:LEU:HA	1.92	0.41
1:e:21:MET:HE1	1:e:366:HIS:CD2	2.55	0.41
1:f:528:GLU:HB2	1:f:529:ILE:HD12	2.03	0.41
1:a:528:GLU:HB2	1:a:529:ILE:HD12	2.02	0.41
1:b:367:GLU:O	1:b:370:GLU:HG2	2.21	0.41
1:a:462:HIS:O	1:a:463:ASN:C	2.63	0.41
1:d:180:LYS:NZ	1:d:191:HIS:CE1	2.88	0.41
1:e:224:LEU:HD11	1:e:345:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:87:PHE:CD1	1:c:278:ALA:HB2	2.56	0.41
1:c:103:LEU:CG	1:c:137:VAL:HG11	2.51	0.41
1:c:138:ASN:OD1	1:c:140:ASN:N	2.54	0.41
1:c:491:ASN:OD1	1:c:491:ASN:N	2.54	0.41
1:d:138:ASN:OD1	1:d:140:ASN:N	2.54	0.41
1:e:529:ILE:HD12	1:e:529:ILE:N	2.35	0.41
1:f:224:LEU:HD11	1:f:345:VAL:HG23	2.03	0.41
1:a:25:ALA:HA	1:a:63:LEU:HD21	2.03	0.41
1:a:441:LYS:HE2	1:b:446:GLN:OE1	2.21	0.41
1:d:150:THR:HB	1:d:518:LEU:HD22	2.02	0.41
1:a:203:SER:HB2	1:a:204:PRO:HD2	2.02	0.40
1:d:282:GLY:HA3	1:d:298:CYS:O	2.21	0.40
1:d:434:SER:O	1:f:441:LYS:CE	2.61	0.40
1:e:25:ALA:HA	1:e:63:LEU:HD21	2.03	0.40
1:a:138:ASN:OD1	1:a:140:ASN:N	2.54	0.40
1:b:441:LYS:HE3	1:c:436:GLY:O	2.22	0.40
1:d:443:SER:HA	1:d:446:GLN:NE2	2.36	0.40
1:e:138:ASN:OD1	1:e:140:ASN:N	2.54	0.40
1:f:150:THR:HB	1:f:518:LEU:HD22	2.03	0.40
1:b:282:GLY:HA3	1:b:298:CYS:O	2.21	0.40
1:b:230:GLY:HA2	1:b:349:LEU:HB2	2.02	0.40
1:e:528:GLU:HB2	1:e:529:ILE:HD12	2.03	0.40
1:a:261:ILE:HD12	1:a:317:LEU:HD22	2.04	0.40
1:a:282:GLY:HA3	1:a:298:CYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	a	520/531 (98%)	488 (94%)	29 (6%)	3 (1%)	21 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	521/531 (98%)	490 (94%)	29 (6%)	2 (0%)	30	50
1	c	518/531 (98%)	488 (94%)	28 (5%)	2 (0%)	30	50
1	d	522/531 (98%)	492 (94%)	28 (5%)	2 (0%)	30	50
1	e	519/531 (98%)	489 (94%)	27 (5%)	3 (1%)	21	38
1	f	521/531 (98%)	492 (94%)	25 (5%)	4 (1%)	16	30
All	All	3121/3186 (98%)	2939 (94%)	166 (5%)	16 (0%)	24	43

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	272	ASN
1	a	463	ASN
1	b	272	ASN
1	b	463	ASN
1	c	272	ASN
1	c	463	ASN
1	d	272	ASN
1	d	463	ASN
1	e	272	ASN
1	f	41	PRO
1	f	272	ASN
1	f	463	ASN
1	e	463	ASN
1	e	364	THR
1	f	532	SER
1	a	361	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	459/464 (99%)	451 (98%)	8 (2%)	53	71
1	b	459/464 (99%)	450 (98%)	9 (2%)	48	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	458/464 (99%)	447 (98%)	11 (2%)	43	65
1	d	460/464 (99%)	449 (98%)	11 (2%)	43	65
1	e	457/464 (98%)	446 (98%)	11 (2%)	43	65
1	f	458/464 (99%)	443 (97%)	15 (3%)	33	57
All	All	2751/2784 (99%)	2686 (98%)	65 (2%)	43	65

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	50	GLU
1	a	214	LEU
1	a	360	THR
1	a	395	CYS
1	a	398	GLN
1	a	422	LYS
1	a	485	VAL
1	a	490	ASN
1	b	48	VAL
1	b	190	LYS
1	b	201	LYS
1	b	214	LEU
1	b	329	ILE
1	b	330	ASP
1	b	395	CYS
1	b	485	VAL
1	b	490	ASN
1	c	17	SER
1	c	204	PRO
1	c	214	LEU
1	c	232	LYS
1	c	250	LYS
1	c	367	GLU
1	c	395	CYS
1	c	398	GLN
1	c	490	ASN
1	c	491	ASN
1	c	511	MET
1	d	4	MET
1	d	50	GLU
1	d	110	GLN
1	d	214	LEU

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Mol	Chain	Res	Type
1	d	329	ILE
1	d	360	THR
1	d	395	CYS
1	d	422	LYS
1	d	460	ILE
1	d	490	ASN
1	d	513	GLU
1	e	201	LYS
1	e	204	PRO
1	e	214	LEU
1	e	319	GLU
1	e	329	ILE
1	e	363	LEU
1	e	395	CYS
1	e	398	GLN
1	e	485	VAL
1	e	490	ASN
1	e	513	GLU
1	f	39	GLU
1	f	182	LYS
1	f	214	LEU
1	f	220	ILE
1	f	249	LYS
1	f	329	ILE
1	f	330	ASP
1	f	360	THR
1	f	395	CYS
1	f	398	GLN
1	f	422	LYS
1	f	485	VAL
1	f	489	ARG
1	f	490	ASN
1	f	509	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	161	ASN
1	a	507	HIS
1	b	193	GLN
1	b	207	HIS
1	b	253	ASN

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Mol	Chain	Res	Type
1	b	281	ASN
1	b	398	GLN
1	c	61	HIS
1	c	207	HIS
1	c	253	ASN
1	c	429	ASN
1	d	191	HIS
1	d	207	HIS
1	d	253	ASN
1	d	342	ASN
1	d	507	HIS
1	e	207	HIS
1	e	208	ASN
1	e	253	ASN
1	e	366	HIS
1	e	371	ASN
1	f	110	GLN
1	f	191	HIS
1	f	207	HIS
1	f	253	ASN
1	f	281	ASN
1	f	366	HIS
1	f	398	GLN
1	f	446	GLN
1	f	507	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	524/531 (98%)	0.22	11 (2%) 63 61	46, 61, 80, 100	0
1	b	525/531 (98%)	0.14	7 (1%) 75 75	43, 61, 79, 96	0
1	c	522/531 (98%)	0.36	18 (3%) 48 46	47, 66, 89, 110	0
1	d	526/531 (99%)	0.31	8 (1%) 72 71	51, 68, 90, 108	0
1	e	523/531 (98%)	0.25	9 (1%) 69 67	49, 66, 87, 103	0
1	f	525/531 (98%)	0.19	4 (0%) 82 82	45, 65, 84, 108	0
All	All	3145/3186 (98%)	0.24	57 (1%) 67 65	43, 65, 86, 110	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	59	PHE	4.9
1	e	54	GLY	4.5
1	c	363	LEU	3.4
1	e	366	HIS	3.1
1	a	5	VAL	3.1
1	c	495	TYR	3.0
1	a	136	PHE	3.0
1	d	81	SER	2.9
1	b	463	ASN	2.8
1	a	363	LEU	2.7
1	c	366	HIS	2.7
1	e	360	THR	2.7
1	d	43	ILE	2.7
1	d	53	LEU	2.7
1	e	57	ASN	2.7
1	a	486	LEU	2.6
1	a	43	ILE	2.6
1	c	213	ILE	2.6
1	a	54	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	a	48	VAL	2.6
1	e	55	HIS	2.5
1	c	64	ASP	2.5
1	c	5	VAL	2.5
1	e	139	SER	2.5
1	a	53	LEU	2.5
1	a	361	GLY	2.5
1	c	331	ILE	2.4
1	c	25	ALA	2.4
1	a	86	ASN	2.4
1	c	405	PHE	2.3
1	b	282	GLY	2.3
1	c	15	GLY	2.3
1	e	486	LEU	2.3
1	f	214	LEU	2.3
1	c	364	THR	2.2
1	b	5	VAL	2.2
1	b	48	VAL	2.2
1	b	533	ALA	2.2
1	c	276	CYS	2.2
1	d	495	TYR	2.2
1	b	54	GLY	2.2
1	c	346	GLY	2.2
1	e	149	LEU	2.2
1	f	363	LEU	2.2
1	d	282	GLY	2.2
1	d	363	LEU	2.2
1	c	486	LEU	2.2
1	e	464	GLY	2.1
1	f	82	ILE	2.1
1	a	482	LEU	2.1
1	c	332	GLY	2.1
1	d	55	HIS	2.1
1	d	92	GLY	2.1
1	b	87	PHE	2.1
1	c	14	GLY	2.0
1	f	192	ILE	2.0
1	c	211	TYR	2.0

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.