



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:04 PM UTC

PDB ID : 4OHS / pdb_00004ohs
Title : The structure of a far-red fluorescent protein, AQ143
Authors : Wannier, T.M.; Mayo, S.L.
Deposited on : 2014-01-17
Resolution : 2.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

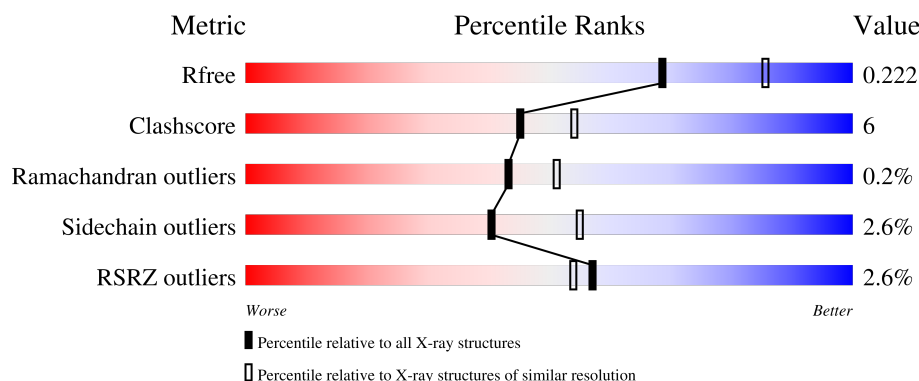
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	238	 2% 85% 6% • 7%
1	B	238	 2% 85% 7% • 5%
1	C	238	 3% 77% 13% • 6%
1	D	238	 % 84% 8% 8%
1	E	238	 % 79% 13% • 8%

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Mol	Chain	Length	Quality of chain
1	F	238	4% 84% 9% • 5%
1	G	238	3% 79% 11% • 9%
1	H	238	4% 72% 17% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14612 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 FAR-RED FLUORESCENT PROTEIN AQ143.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	5	0
			1789	1140	304	330	15			
1	B	226	Total	C	N	O	S	0	4	0
			1826	1164	310	337	15			
1	C	222	Total	C	N	O	S	1	4	0
			1789	1140	301	333	15			
1	D	218	Total	C	N	O	S	0	5	0
			1780	1135	302	328	15			
1	E	218	Total	C	N	O	S	0	3	0
			1765	1125	297	328	15			
1	F	226	Total	C	N	O	S	0	3	0
			1811	1154	307	335	15			
1	G	215	Total	C	N	O	S	0	3	0
			1734	1107	292	320	15			
1	H	217	Total	C	N	O	S	0	4	0
			1759	1122	297	325	15			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

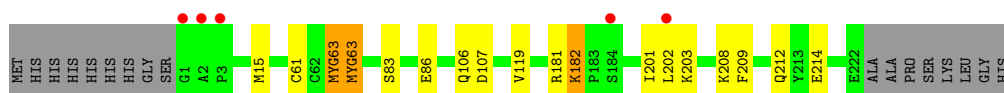
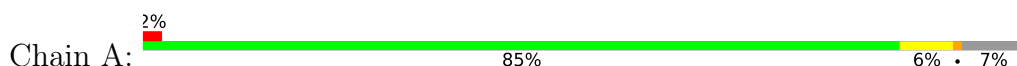
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total 63	O 63	0	0
3	B	59	Total 59	O 59	0	0
3	C	44	Total 44	O 44	0	0
3	D	39	Total 39	O 39	0	0
3	E	46	Total 46	O 46	0	0
3	F	49	Total 49	O 49	0	0
3	G	26	Total 26	O 26	0	0
3	H	29	Total 29	O 29	0	0

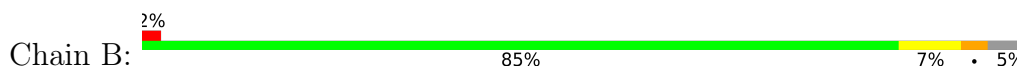
3 Residue-property plots [i](#)

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.

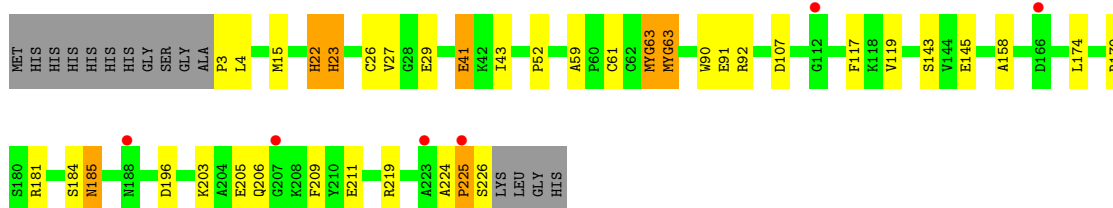
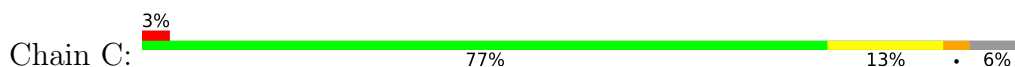
• Molecule 1: FAR-RED FLUORESCENT PROTEIN AQ143



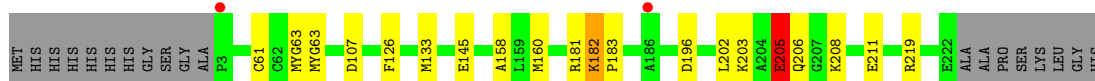
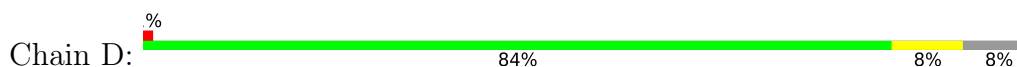
• Molecule 1: FAR-RED FLUORESCENT PROTEIN AQ143



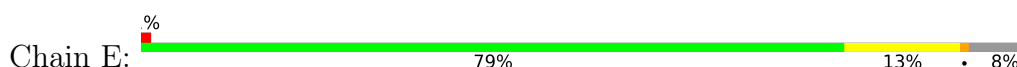
• Molecule 1: FAR-RED FLUORESCENT PROTEIN AQ143

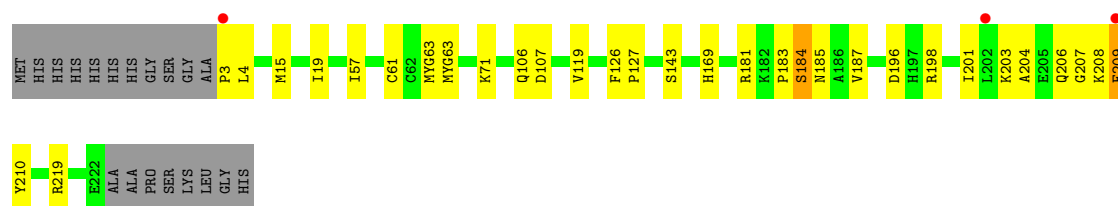


• Molecule 1: FAR-RED FLUORESCENT PROTEIN AQ143

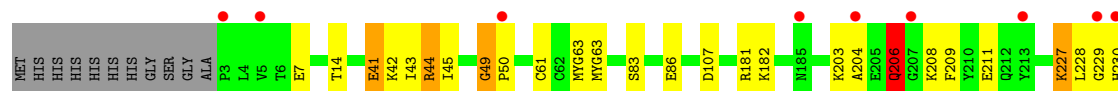
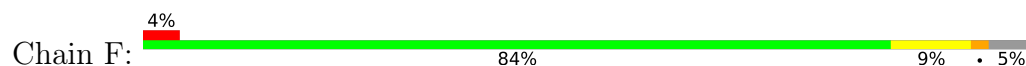


• Molecule 1: FAR-RED FLUORESCENT PROTEIN AQ143

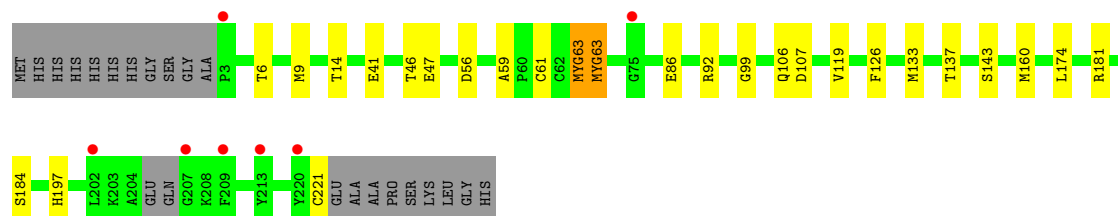
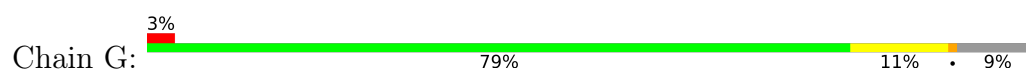




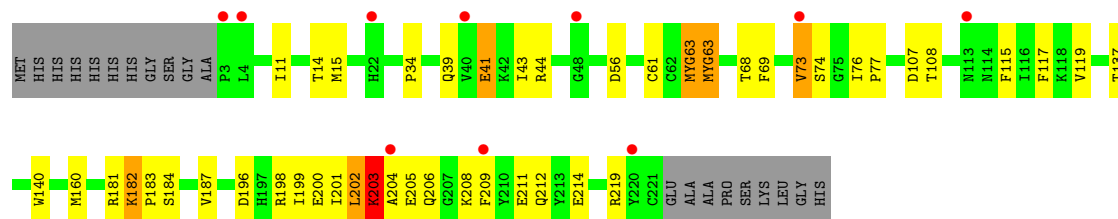
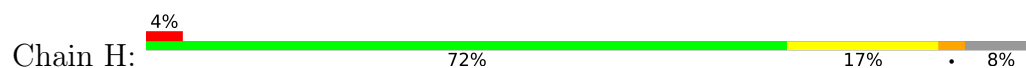
• Molecule 1: FAR-RED FLUORESCENT PROTEIN AQ143



• Molecule 1: FAR-RED FLUORESCENT PROTEIN AQ143



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.97Å 68.11Å 132.79Å 98.38° 90.74° 110.47°	Depositor
Resolution (Å)	37.33 – 2.19 37.33 – 2.19	Depositor EDS
% Data completeness (in resolution range)	86.1 (37.33-2.19) 86.1 (37.33-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.190 , 0.221 0.193 , 0.222	Depositor DCC
R_{free} test set	3651 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.780	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14612	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NRQ, CH6, CL

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	0.41	0/1800	0.77	2/2428 (0.1%)
1	B	0.44	0/1836	0.80	4/2477 (0.2%)
1	C	0.56	3/1801 (0.2%)	0.94	14/2431 (0.6%)
1	D	0.40	0/1791	0.76	3/2415 (0.1%)
1	E	0.46	0/1769	0.78	2/2386 (0.1%)
1	F	0.49	0/1817	0.86	4/2453 (0.2%)
1	G	0.36	0/1737	0.81	4/2343 (0.2%)
1	H	0.50	2/1767 (0.1%)	0.82	6/2385 (0.3%)
All	All	0.46	5/14318 (0.0%)	0.82	39/19318 (0.2%)

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	C	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	23[A]	HIS	CA-C	6.42	1.61	1.52
1	C	23[B]	HIS	CA-C	6.42	1.61	1.52
1	H	77	PRO	N-CD	5.35	1.55	1.47
1	C	225	PRO	N-CD	5.32	1.55	1.47
1	H	76	ILE	C-N	5.30	1.40	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	61	CYS	CA-C-N	11.30	142.04	121.70
1	G	61	CYS	C-N-CA	11.30	142.04	121.70
1	B	61	CYS	CA-C-N	10.38	140.38	121.70
1	B	61	CYS	C-N-CA	10.38	140.38	121.70
1	C	22	HIS	CA-C-N	-8.91	106.59	121.39
1	C	22	HIS	C-N-CA	-8.91	106.59	121.39
1	F	49	GLY	C-N-CD	8.57	139.45	120.60
1	E	61	CYS	CA-C-N	8.40	136.81	121.70
1	E	61	CYS	C-N-CA	8.40	136.81	121.70
1	F	61	CYS	CA-C-N	7.74	135.63	121.70
1	F	61	CYS	C-N-CA	7.74	135.63	121.70
1	C	23[A]	HIS	N-CA-C	7.25	121.21	110.48
1	C	23[B]	HIS	N-CA-C	7.25	121.21	110.48
1	H	61	CYS	CA-C-N	7.17	134.60	121.70
1	H	61	CYS	C-N-CA	7.17	134.60	121.70
1	G	59	ALA	CA-C-N	-6.47	113.26	120.45
1	G	59	ALA	C-N-CA	-6.47	113.26	120.45
1	B	59	ALA	CA-C-N	-6.12	114.59	120.83
1	B	59	ALA	C-N-CA	-6.12	114.59	120.83
1	C	59	ALA	CA-C-N	-6.07	113.72	120.45
1	C	59	ALA	C-N-CA	-6.07	113.72	120.45
1	C	23[A]	HIS	N-CA-CB	-6.01	101.16	110.29
1	C	23[B]	HIS	N-CA-CB	-6.01	101.16	110.29
1	D	61	CYS	CA-C-N	5.92	132.35	121.70
1	D	61	CYS	C-N-CA	5.92	132.35	121.70
1	C	61	CYS	CA-C-N	5.91	132.33	121.70
1	C	61	CYS	C-N-CA	5.91	132.33	121.70
1	H	76	ILE	CA-C-N	-5.83	113.76	119.76
1	H	76	ILE	C-N-CA	-5.83	113.76	119.76
1	C	23[A]	HIS	O-C-N	-5.73	116.49	122.96
1	C	23[B]	HIS	O-C-N	-5.73	116.49	122.96
1	A	61	CYS	CA-C-N	5.67	131.90	121.70
1	A	61	CYS	C-N-CA	5.67	131.90	121.70
1	C	224	ALA	CA-C-N	-5.56	112.89	119.84
1	C	224	ALA	C-N-CA	-5.56	112.89	119.84
1	H	182	LYS	CA-C-N	5.51	125.52	119.90
1	H	182	LYS	C-N-CA	5.51	125.52	119.90
1	D	205	GLU	N-CA-C	5.04	117.45	109.24
1	F	45	ILE	CB-CA-C	-5.01	106.96	112.68

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	23[A]	HIS	Mainchain
1	C	23[B]	HIS	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1789	0	1723	9	0
1	B	1826	0	1756	18	0
1	C	1789	0	1717	21	0
1	D	1780	0	1713	10	0
1	E	1765	0	1693	17	0
1	F	1811	0	1734	29	0
1	G	1734	0	1661	13	0
1	H	1759	0	1683	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	63	0	0	0	0
3	B	59	0	0	0	0
3	C	44	0	0	2	0
3	D	39	0	0	2	0
3	E	46	0	0	0	0
3	F	49	0	0	1	0
3	G	26	0	0	1	0
3	H	29	0	0	1	0
All	All	14612	0	13680	156	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 6.

All (156) 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:B:203:LYS:HE3	1:B:211:GLU:OE1	1.40	1.19
1:H:11:ILE:HD11	1:H:41:GLU:HG3	1.21	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:LYS:HE2	1:H:205:GLU:HB2	1.33	1.10
1:F:203:LYS:HA	1:F:204:ALA:HB3	1.06	1.05
1:C:203:LYS:HD2	1:C:211:GLU:OE1	1.61	0.99
1:F:203:LYS:HA	1:F:204:ALA:CB	1.89	0.99
1:F:44:ARG:HH12	1:F:209:PHE:HB2	1.26	0.97
1:H:203:LYS:CE	1:H:205:GLU:HB2	1.95	0.97
1:F:229:GLY:HA2	1:F:230:HIS:HB2	1.44	0.96
1:F:203:LYS:CA	1:F:204:ALA:HB3	1.98	0.94
1:H:73:VAL:HG12	1:H:74:SER:HA	1.50	0.93
1:H:11:ILE:CD1	1:H:41:GLU:HG3	2.00	0.91
1:F:44:ARG:NH1	1:F:209:PHE:HB2	1.87	0.88
1:F:229:GLY:CA	1:F:230:HIS:HB2	2.05	0.86
1:F:44:ARG:HG2	1:F:44:ARG:HH11	1.41	0.82
1:C:203:LYS:CD	1:C:211:GLU:OE1	2.29	0.81
1:F:206:GLN:HB3	1:F:208:LYS:H	1.46	0.81
1:H:203:LYS:HE2	1:H:205:GLU:CB	2.13	0.77
1:C:41:GLU:HG2	1:C:43:ILE:HD11	1.68	0.76
1:H:107:ASP:OD2	1:H:181:ARG:NH2	2.19	0.75
1:F:107:ASP:OD2	1:F:181:ARG:NH2	2.20	0.75
1:G:107:ASP:OD1	1:G:181:ARG:NH2	2.19	0.75
1:C:107:ASP:OD2	1:C:181:ARG:NH2	2.19	0.74
1:G:99:GLY:O	3:G:325:HOH:O	2.06	0.74
1:F:42:LYS:HD3	1:F:209:PHE:HZ	1.51	0.73
1:B:228:LEU:H	1:B:228:LEU:HD23	1.53	0.73
1:H:205:GLU:O	1:H:209:PHE:HB3	1.89	0.73
1:B:107:ASP:OD2	1:B:181:ARG:NH2	2.21	0.73
1:H:203:LYS:HE3	1:H:204:ALA:H	1.51	0.73
1:E:107:ASP:OD2	1:E:181:ARG:NH2	2.23	0.72
1:A:107:ASP:OD2	1:A:181:ARG:NH2	2.21	0.72
1:C:184:SER:OG	1:C:185:ASN:OD1	2.08	0.72
1:D:107:ASP:OD2	1:D:181:ARG:NH2	2.21	0.71
1:H:11:ILE:HD12	1:H:41:GLU:OE1	1.92	0.69
1:H:203:LYS:CD	1:H:205:GLU:HB2	2.23	0.68
1:H:203:LYS:HD3	1:H:205:GLU:CB	2.24	0.68
1:H:56:ASP:OD2	1:H:137:THR:OG1	2.09	0.68
1:C:117:PHE:HD2	3:C:444:HOH:O	1.77	0.67
1:H:108:THR:HG23	1:H:117:PHE:HE1	1.60	0.66
1:H:203:LYS:HD3	1:H:205:GLU:HB2	1.78	0.66
1:H:73:VAL:CG1	1:H:74:SER:HA	2.24	0.66
1:B:228:LEU:H	1:B:228:LEU:CD2	2.09	0.65
1:H:41:GLU:OE2	1:H:43:ILE:HD11	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:HIS:ND1	1:C:52:PRO:HG3	2.15	0.61
1:H:202:LEU:O	1:H:203:LYS:HB3	2.00	0.61
1:C:205:GLU:O	1:C:206:GLN:HB2	2.00	0.60
1:H:203:LYS:HE3	1:H:204:ALA:N	2.16	0.59
1:B:49:GLY:HA3	1:B:208:LYS:HE2	1.85	0.59
1:H:199:ILE:HD11	1:H:214:GLU:OE1	2.03	0.58
1:F:44:ARG:HG3	1:F:209:PHE:CD1	2.39	0.58
1:B:205:GLU:O	1:B:206:GLN:HB2	2.03	0.58
1:D:205:GLU:HG2	3:D:420:HOH:O	2.03	0.58
1:B:226:SER:HB2	1:E:198:ARG:HD3	1.87	0.57
1:G:56:ASP:OD2	1:G:137:THR:OG1	2.15	0.56
1:H:117:PHE:HD2	3:H:329:HOH:O	1.88	0.56
1:H:203:LYS:HE2	1:H:205:GLU:N	2.19	0.56
1:C:41:GLU:HG2	1:C:43:ILE:CD1	2.36	0.56
1:G:63[A]:CH6:HE1	1:G:160:MET:SD	2.46	0.56
1:B:203:LYS:CE	1:B:211:GLU:OE1	2.33	0.55
1:C:15:MET:HE2	1:C:119:VAL:HG11	1.89	0.55
1:G:221:CYS:SG	1:H:198:ARG:NH2	2.79	0.55
1:G:63[A]:CH6:HB2	1:G:197:HIS:CD2	2.42	0.55
1:C:185:ASN:OD1	1:C:185:ASN:N	2.36	0.55
1:C:225:PRO:O	1:C:226:SER:HB3	2.05	0.54
1:A:201:ILE:HD13	1:A:212:GLN:HG3	1.89	0.54
1:E:209:PHE:C	1:E:209:PHE:CD1	2.85	0.54
1:G:6:THR:H	1:G:9:MET:HE3	1.73	0.54
1:H:15:MET:HE2	1:H:119:VAL:HG11	1.89	0.53
1:E:183:PRO:O	1:E:185:ASN:N	2.41	0.53
1:B:206:GLN:C	1:B:208:LYS:N	2.66	0.53
1:H:203:LYS:HD3	1:H:205:GLU:HB3	1.90	0.53
1:A:83:SER:HA	1:A:182:LYS:HG3	1.91	0.52
1:F:44:ARG:HG3	1:F:209:PHE:HD1	1.73	0.52
1:B:228:LEU:CD2	1:B:228:LEU:N	2.73	0.52
1:F:44:ARG:HH11	1:F:44:ARG:CG	2.14	0.52
1:B:206:GLN:C	1:B:208:LYS:H	2.17	0.51
1:D:182:LYS:HG3	1:D:183:PRO:HD2	1.92	0.51
1:F:44:ARG:NH1	1:F:44:ARG:HG2	2.16	0.51
1:H:203:LYS:HG3	1:H:204:ALA:N	2.25	0.51
1:B:15:MET:HE2	1:B:119:VAL:HG11	1.93	0.51
1:B:206:GLN:O	1:B:208:LYS:N	2.44	0.50
1:D:160:MET:HA	3:D:439:HOH:O	2.11	0.50
1:C:196:ASP:OD2	1:C:219:ARG:NE	2.42	0.50
1:F:206:GLN:NE2	1:F:208:LYS:NZ	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:ARG:HD3	1:G:174:LEU:HD23	1.94	0.49
1:F:44:ARG:NH1	1:F:44:ARG:CG	2.73	0.49
1:D:203:LYS:HD2	1:D:211:GLU:OE1	2.12	0.48
1:C:91:GLU:OE2	1:C:179:ARG:NE	2.32	0.48
1:H:11:ILE:CD1	1:H:41:GLU:CG	2.84	0.48
1:H:11:ILE:HG22	1:H:115:PHE:HB2	1.95	0.48
1:A:202:LEU:C	1:A:203:LYS:HG2	2.37	0.48
1:F:206:GLN:NE2	1:F:208:LYS:HZ3	2.11	0.48
1:A:15:MET:HE2	1:A:119:VAL:HG11	1.96	0.47
1:E:196:ASP:OD2	1:E:219:ARG:NE	2.35	0.47
1:G:63[A]:CH6:OH	1:G:174:LEU:HD22	2.14	0.47
1:C:63[A]:CH6:HA32	1:C:90:TRP:CZ2	2.50	0.47
1:E:15:MET:HE2	1:E:119:VAL:HG11	1.97	0.46
1:H:201:ILE:HG12	1:H:212:GLN:HG3	1.96	0.46
1:H:108:THR:HG23	1:H:117:PHE:CE1	2.46	0.46
1:F:227:LYS:HA	1:F:227:LYS:HD2	1.59	0.46
1:H:183:PRO:O	1:H:187:VAL:HG23	2.16	0.46
1:C:145:GLU:HA	1:C:158:ALA:HB2	1.98	0.46
1:H:34:PRO:HA	1:H:69:PHE:HA	1.97	0.45
1:E:19:ILE:HD13	1:E:57:ILE:HD11	1.99	0.45
1:E:206:GLN:O	1:E:208:LYS:HG3	2.15	0.45
1:H:202:LEU:HD12	1:H:211:GLU:HB3	1.98	0.45
1:D:206:GLN:O	1:D:208:LYS:HG3	2.17	0.45
1:F:41:GLU:CG	1:F:43:ILE:HD11	2.47	0.45
1:C:22:HIS:HB3	3:C:429:HOH:O	2.17	0.45
1:F:7:GLU:OE1	3:F:343:HOH:O	2.20	0.45
1:C:92:ARG:HD3	1:C:174:LEU:HD23	1.98	0.44
1:H:196:ASP:OD2	1:H:219:ARG:NE	2.40	0.44
1:H:203:LYS:HE2	1:H:205:GLU:CA	2.47	0.44
1:C:3:PRO:N	1:C:4:LEU:HA	2.33	0.44
1:G:86:GLU:HB3	1:G:181:ARG:HB2	1.99	0.44
1:B:229:GLY:HA2	1:B:230:HIS:HA	1.68	0.44
1:H:182:LYS:HG3	1:H:183:PRO:HD2	1.98	0.44
1:B:63[A]:CH6:HB12	1:B:214:GLU:OE1	2.18	0.44
1:B:227:LYS:HG2	1:B:228:LEU:HD22	1.99	0.44
1:F:44:ARG:NH1	1:F:209:PHE:CB	2.70	0.44
1:E:3:PRO:N	1:E:4:LEU:HA	2.32	0.44
1:A:63[A]:CH6:HB12	1:A:214:GLU:OE1	2.19	0.43
1:C:203:LYS:HD3	1:C:211:GLU:OE1	2.17	0.43
1:H:205:GLU:HA	1:H:206:GLN:HA	1.63	0.43
1:D:126:PHE:HB2	1:D:133:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ASP:OD2	1:D:219:ARG:NE	2.40	0.43
1:F:42:LYS:HG2	1:F:211:GLU:HG3	2.01	0.43
1:E:183:PRO:C	1:E:185:ASN:H	2.27	0.42
1:H:44:ARG:HA	1:H:208:LYS:O	2.19	0.42
1:H:140:TRP:CE3	1:H:160:MET:HE2	2.54	0.42
1:F:41:GLU:OE2	1:F:43:ILE:HD11	2.20	0.42
1:E:209:PHE:C	1:E:209:PHE:HD1	2.27	0.42
1:B:150:ARG:NH2	1:E:169:HIS:O	2.53	0.42
1:D:202:LEU:HB2	1:D:211:GLU:HB3	2.01	0.42
1:F:83:SER:HA	1:F:182:LYS:HG3	2.01	0.42
1:A:106:GLN:HG2	1:A:119:VAL:HG22	2.02	0.42
1:A:208:LYS:HD3	1:A:209:PHE:CZ	2.54	0.42
1:E:203:LYS:HG3	1:E:204:ALA:N	2.35	0.42
1:A:86:GLU:HB3	1:A:181:ARG:HB2	2.01	0.41
1:H:200:GLU:OE1	1:H:200:GLU:HA	2.19	0.41
1:G:106:GLN:HG2	1:G:119:VAL:HG22	2.02	0.41
1:G:126:PHE:HB2	1:G:133:MET:HE3	2.03	0.41
1:D:145:GLU:HA	1:D:158:ALA:HB2	2.03	0.41
1:E:126:PHE:HA	1:E:127:PRO:HD3	1.96	0.41
1:E:183:PRO:C	1:E:185:ASN:N	2.77	0.41
1:E:207:GLY:HA2	1:E:210:TYR:OH	2.20	0.41
1:F:49:GLY:HA2	1:F:50:PRO:HA	1.71	0.41
1:F:41:GLU:CD	1:F:43:ILE:HD11	2.45	0.41
1:F:41:GLU:OE2	1:F:43:ILE:CD1	2.69	0.41
1:H:39:GLN:NE2	1:H:63[A]:CH6:HE3	2.35	0.41
1:H:202:LEU:HB2	1:H:211:GLU:HB3	2.03	0.41
1:E:106:GLN:HG2	1:E:119:VAL:HG22	2.03	0.41
1:B:106:GLN:HG2	1:B:119:VAL:HG22	2.03	0.40
1:F:86:GLU:HB3	1:F:181:ARG:HB2	2.02	0.40
1:G:46:THR:OG1	1:G:47:GLU:N	2.53	0.40
1:C:15:MET:HB3	1:C:26:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/238 (92%)	215 (99%)	3 (1%)	0	100	100
1	B	223/238 (94%)	217 (97%)	6 (3%)	0	100	100
1	C	219/238 (92%)	212 (97%)	7 (3%)	0	100	100
1	D	216/238 (91%)	209 (97%)	7 (3%)	0	100	100
1	E	214/238 (90%)	209 (98%)	4 (2%)	1 (0%)	24	27
1	F	222/238 (93%)	216 (97%)	5 (2%)	1 (0%)	24	27
1	G	209/238 (88%)	208 (100%)	1 (0%)	0	100	100
1	H	214/238 (90%)	207 (97%)	6 (3%)	1 (0%)	24	27
All	All	1735/1904 (91%)	1693 (98%)	39 (2%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	184	SER
1	F	206	GLN
1	H	203	LYS

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	189/198 (96%)	188 (100%)	1 (0%)	81	90
1	B	193/198 (98%)	186 (96%)	7 (4%)	31	42
1	C	190/198 (96%)	184 (97%)	6 (3%)	34	47
1	D	189/198 (96%)	187 (99%)	2 (1%)	65	79
1	E	187/198 (94%)	181 (97%)	6 (3%)	34	47
1	F	190/198 (96%)	184 (97%)	6 (3%)	34	47
1	G	183/198 (92%)	179 (98%)	4 (2%)	45	61
1	H	186/198 (94%)	179 (96%)	7 (4%)	29	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1507/1584 (95%)	1468 (97%)	39 (3%)	40 55

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	LYS
1	B	67	LYS
1	B	143	SER
1	B	206	GLN
1	B	208	LYS
1	B	227	LYS
1	B	228	LEU
1	B	230	HIS
1	C	27	VAL
1	C	29	GLU
1	C	41	GLU
1	C	143	SER
1	C	185	ASN
1	C	209	PHE
1	D	182	LYS
1	D	205	GLU
1	E	71	LYS
1	E	143	SER
1	E	184	SER
1	E	187	VAL
1	E	201	ILE
1	E	209	PHE
1	F	14	THR
1	F	41	GLU
1	F	44	ARG
1	F	206	GLN
1	F	227	LYS
1	F	228	LEU
1	G	14	THR
1	G	41	GLU
1	G	143	SER
1	G	184	SER
1	H	14	THR
1	H	41	GLU
1	H	68	THR
1	H	73	VAL
1	H	184	SER

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Mol	Chain	Res	Type
1	H	202	LEU
1	H	203	LYS

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

Mol	Chain	Res	Type
1	A	105	HIS
1	A	125	ASN
1	A	157	GLN
1	B	105	HIS
1	B	129	ASN
1	B	134	GLN
1	B	157	GLN
1	C	39	GLN
1	C	157	GLN
1	D	39	GLN
1	E	125	ASN
1	E	157	GLN
1	F	113	ASN
1	F	120	ASN
1	F	157	GLN
1	F	206	GLN
1	G	105	HIS
1	G	125	ASN
1	G	157	GLN
1	G	197	HIS
1	H	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CH6	C	63[A]	1	23,24,25	2.95	4 (17%)	28,32,34	2.54	13 (46%)
1	CH6	D	63[A]	1	23,24,25	3.10	5 (21%)	28,32,34	2.79	9 (32%)
1	CH6	F	63[A]	1	23,24,25	3.10	4 (17%)	28,32,34	2.56	11 (39%)
1	NRQ	H	63[B]	-	24,24,25	3.16	3 (12%)	24,32,34	2.67	9 (37%)
1	NRQ	G	63[B]	-	24,24,25	3.14	3 (12%)	24,32,34	2.90	8 (33%)
1	CH6	E	63[A]	1	23,24,25	3.06	5 (21%)	28,32,34	2.96	10 (35%)
1	CH6	G	63[A]	1	23,24,25	2.90	5 (21%)	28,32,34	2.79	10 (35%)
1	NRQ	E	63[B]	-	24,24,25	3.30	3 (12%)	24,32,34	2.78	9 (37%)
1	NRQ	D	63[B]	-	24,24,25	3.24	3 (12%)	24,32,34	2.55	8 (33%)
1	CH6	H	63[A]	1	23,24,25	3.11	4 (17%)	28,32,34	2.71	11 (39%)
1	NRQ	C	63[B]	-	24,24,25	3.26	4 (16%)	24,32,34	2.57	8 (33%)
1	NRQ	F	63[B]	-	24,24,25	3.19	3 (12%)	24,32,34	2.54	7 (29%)
1	NRQ	B	63[B]	-	24,24,25	3.30	4 (16%)	24,32,34	2.81	9 (37%)
1	NRQ	A	63[B]	-	24,24,25	3.19	3 (12%)	24,32,34	2.85	9 (37%)
1	CH6	B	63[A]	1	23,24,25	2.94	4 (17%)	28,32,34	2.74	9 (32%)
1	CH6	A	63[A]	1	23,24,25	2.95	4 (17%)	28,32,34	3.11	11 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CH6	C	63[A]	1	-	5/12/31/32	0/2/2/2
1	CH6	D	63[A]	1	-	5/12/31/32	0/2/2/2
1	CH6	F	63[A]	1	-	5/12/31/32	0/2/2/2
1	NRQ	H	63[B]	-	-	5/9/31/32	0/2/2/2
1	NRQ	G	63[B]	-	-	5/9/31/32	0/2/2/2
1	CH6	E	63[A]	1	-	5/12/31/32	0/2/2/2
1	CH6	G	63[A]	1	-	6/12/31/32	0/2/2/2
1	NRQ	E	63[B]	-	-	5/9/31/32	0/2/2/2
1	NRQ	D	63[B]	-	-	6/9/31/32	0/2/2/2
1	CH6	H	63[A]	1	-	5/12/31/32	0/2/2/2
1	NRQ	C	63[B]	-	-	5/9/31/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NRQ	F	63[B]	-	-	5/9/31/32	0/2/2/2
1	NRQ	B	63[B]	-	-	6/9/31/32	0/2/2/2
1	NRQ	A	63[B]	-	-	5/9/31/32	0/2/2/2
1	CH6	B	63[A]	1	-	4/12/31/32	0/2/2/2
1	CH6	A	63[A]	1	-	7/12/31/32	0/2/2/2

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63[B]	NRQ	CB2-CA2	15.12	1.49	1.35
1	B	63[B]	NRQ	CB2-CA2	15.03	1.49	1.35
1	D	63[B]	NRQ	CB2-CA2	14.85	1.49	1.35
1	C	63[B]	NRQ	CB2-CA2	14.79	1.49	1.35
1	F	63[B]	NRQ	CB2-CA2	14.54	1.49	1.35
1	A	63[B]	NRQ	CB2-CA2	14.51	1.49	1.35
1	H	63[B]	NRQ	CB2-CA2	14.51	1.49	1.35
1	G	63[B]	NRQ	CB2-CA2	14.28	1.48	1.35
1	H	63[A]	CH6	CB2-CA2	13.88	1.48	1.35
1	D	63[A]	CH6	CB2-CA2	13.80	1.48	1.35
1	F	63[A]	CH6	CB2-CA2	13.77	1.48	1.35
1	E	63[A]	CH6	CB2-CA2	13.61	1.48	1.35
1	A	63[A]	CH6	CB2-CA2	13.00	1.47	1.35
1	C	63[A]	CH6	CB2-CA2	12.92	1.47	1.35
1	B	63[A]	CH6	CB2-CA2	12.92	1.47	1.35
1	G	63[A]	CH6	CB2-CA2	12.72	1.47	1.35
1	B	63[A]	CH6	O2-C2	2.96	1.29	1.23
1	G	63[A]	CH6	O2-C2	2.91	1.29	1.23
1	F	63[B]	NRQ	O2-C2	2.91	1.29	1.23
1	C	63[B]	NRQ	C2-N3	-2.90	1.33	1.40
1	C	63[A]	CH6	O2-C2	2.90	1.29	1.23
1	B	63[B]	NRQ	O2-C2	2.89	1.29	1.23
1	C	63[B]	NRQ	O2-C2	2.89	1.29	1.23
1	E	63[B]	NRQ	O2-C2	2.87	1.28	1.23
1	F	63[A]	CH6	O2-C2	2.84	1.28	1.23
1	A	63[B]	NRQ	C2-N3	-2.84	1.33	1.40
1	E	63[A]	CH6	O2-C2	2.83	1.28	1.23
1	B	63[B]	NRQ	C2-N3	-2.83	1.33	1.40
1	H	63[A]	CH6	O2-C2	2.83	1.28	1.23
1	G	63[B]	NRQ	C2-N3	-2.83	1.33	1.40
1	G	63[B]	NRQ	O2-C2	2.82	1.28	1.23
1	A	63[A]	CH6	O2-C2	2.82	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63[B]	NRQ	O2-C2	2.82	1.28	1.23
1	H	63[B]	NRQ	O2-C2	2.82	1.28	1.23
1	D	63[B]	NRQ	O2-C2	2.82	1.28	1.23
1	D	63[B]	NRQ	C2-N3	-2.79	1.33	1.40
1	D	63[A]	CH6	O2-C2	2.79	1.28	1.23
1	H	63[B]	NRQ	C2-N3	-2.79	1.33	1.40
1	E	63[B]	NRQ	C2-N3	-2.77	1.33	1.40
1	F	63[B]	NRQ	C2-N3	-2.71	1.33	1.40
1	G	63[A]	CH6	C2-N3	-2.68	1.33	1.40
1	H	63[A]	CH6	C2-N3	-2.67	1.33	1.40
1	B	63[A]	CH6	C2-N3	-2.65	1.33	1.40
1	A	63[A]	CH6	C2-N3	-2.60	1.34	1.40
1	C	63[A]	CH6	C2-N3	-2.58	1.34	1.40
1	F	63[A]	CH6	C2-N3	-2.55	1.34	1.40
1	D	63[A]	CH6	C2-N3	-2.55	1.34	1.40
1	C	63[A]	CH6	C1-N2	2.54	1.35	1.32
1	A	63[A]	CH6	CA2-N2	-2.48	1.33	1.38
1	E	63[A]	CH6	C2-N3	-2.46	1.34	1.40
1	F	63[A]	CH6	C1-N2	2.40	1.35	1.32
1	G	63[A]	CH6	C1-N2	2.39	1.35	1.32
1	D	63[A]	CH6	C1-N2	2.27	1.35	1.32
1	H	63[A]	CH6	C1-N2	2.26	1.35	1.32
1	B	63[B]	NRQ	C1-CA1	2.24	1.51	1.48
1	E	63[A]	CH6	CA2-N2	-2.22	1.33	1.38
1	B	63[A]	CH6	CA2-N2	-2.20	1.33	1.38
1	C	63[B]	NRQ	C1-CA1	2.16	1.51	1.48
1	G	63[A]	CH6	CA2-N2	-2.15	1.34	1.38
1	E	63[A]	CH6	C1-N2	2.15	1.35	1.32
1	D	63[A]	CH6	CA2-N2	-2.12	1.34	1.38

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63[A]	CH6	CG2-CB2-CA2	-8.80	119.40	129.87
1	E	63[A]	CH6	CG2-CB2-CA2	-8.65	119.58	129.87
1	B	63[A]	CH6	CG2-CB2-CA2	-8.57	119.68	129.87
1	A	63[B]	NRQ	CG2-CB2-CA2	-8.23	120.08	129.87
1	G	63[B]	NRQ	CG2-CB2-CA2	-8.13	120.20	129.87
1	G	63[A]	CH6	CG2-CB2-CA2	-7.74	120.66	129.87
1	E	63[B]	NRQ	CG2-CB2-CA2	-7.62	120.81	129.87
1	G	63[B]	NRQ	O2-C2-CA2	-7.50	126.23	131.02
1	B	63[B]	NRQ	CG2-CB2-CA2	-7.40	121.06	129.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63[A]	CH6	O2-C2-CA2	-7.37	126.31	131.02
1	D	63[A]	CH6	CG2-CB2-CA2	-7.32	121.17	129.87
1	C	63[B]	NRQ	O2-C2-CA2	-6.98	126.57	131.02
1	C	63[A]	CH6	O2-C2-CA2	-6.75	126.71	131.02
1	D	63[A]	CH6	CB2-CA2-C2	6.59	130.34	122.36
1	E	63[A]	CH6	CB2-CA2-C2	6.56	130.31	122.36
1	H	63[A]	CH6	CB2-CA2-C2	6.47	130.19	122.36
1	B	63[B]	NRQ	O2-C2-CA2	-6.34	126.98	131.02
1	A	63[A]	CH6	O2-C2-CA2	-6.17	127.08	131.02
1	F	63[A]	CH6	CB2-CA2-C2	6.06	129.70	122.36
1	H	63[B]	NRQ	CG2-CB2-CA2	-6.05	122.68	129.87
1	H	63[A]	CH6	CG2-CB2-CA2	-6.00	122.74	129.87
1	A	63[B]	NRQ	O2-C2-CA2	-5.99	127.20	131.02
1	D	63[B]	NRQ	CG2-CB2-CA2	-5.84	122.92	129.87
1	F	63[B]	NRQ	O2-C2-CA2	-5.84	127.30	131.02
1	E	63[B]	NRQ	C2-CA2-N2	-5.79	104.81	108.95
1	B	63[B]	NRQ	C2-CA2-N2	-5.73	104.85	108.95
1	D	63[B]	NRQ	C2-CA2-N2	-5.71	104.86	108.95
1	B	63[A]	CH6	CB2-CA2-C2	5.65	129.20	122.36
1	F	63[B]	NRQ	C2-CA2-N2	-5.64	104.91	108.95
1	A	63[A]	CH6	CB2-CA2-C2	5.60	129.15	122.36
1	F	63[B]	NRQ	CG2-CB2-CA2	-5.55	123.27	129.87
1	C	63[B]	NRQ	C2-CA2-N2	-5.51	105.00	108.95
1	E	63[B]	NRQ	O2-C2-CA2	-5.49	127.52	131.02
1	A	63[B]	NRQ	C2-CA2-N2	-5.46	105.04	108.95
1	H	63[B]	NRQ	C2-CA2-N2	-5.42	105.07	108.95
1	F	63[A]	CH6	CG2-CB2-CA2	-5.20	123.68	129.87
1	D	63[A]	CH6	C2-CA2-N2	-5.12	105.28	108.95
1	A	63[A]	CH6	CA1-C1-N3	5.11	131.50	124.84
1	H	63[A]	CH6	C2-CA2-N2	-5.02	105.36	108.95
1	B	63[A]	CH6	O2-C2-CA2	-4.98	127.84	131.02
1	E	63[A]	CH6	O2-C2-CA2	-4.92	127.88	131.02
1	F	63[A]	CH6	C2-CA2-N2	-4.90	105.44	108.95
1	G	63[B]	NRQ	C2-CA2-N2	-4.90	105.44	108.95
1	E	63[A]	CH6	C2-CA2-N2	-4.84	105.48	108.95
1	H	63[B]	NRQ	O2-C2-CA2	-4.83	127.94	131.02
1	F	63[A]	CH6	CA2-N2-C1	4.79	109.55	105.80
1	A	63[A]	CH6	CA2-N2-C1	4.73	109.50	105.80
1	D	63[A]	CH6	CA2-N2-C1	4.66	109.44	105.80
1	A	63[A]	CH6	C2-CA2-N2	-4.59	105.66	108.95
1	E	63[A]	CH6	CA2-N2-C1	4.54	109.35	105.80
1	D	63[B]	NRQ	O2-C2-CA2	-4.53	128.13	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	63[A]	CH6	CA2-N2-C1	4.52	109.33	105.80
1	C	63[A]	CH6	CA2-N2-C1	4.47	109.30	105.80
1	F	63[A]	CH6	O2-C2-CA2	-4.46	128.18	131.02
1	D	63[A]	CH6	O2-C2-CA2	-4.44	128.19	131.02
1	C	63[B]	NRQ	CG2-CB2-CA2	-4.38	124.66	129.87
1	D	63[B]	NRQ	CB2-CA2-C2	4.36	127.65	122.36
1	C	63[A]	CH6	C2-CA2-N2	-4.36	105.83	108.95
1	H	63[A]	CH6	CE-SD-CG1	-4.30	78.04	100.32
1	H	63[B]	NRQ	CE-SD-CG1	-4.30	78.04	100.32
1	B	63[A]	CH6	C2-CA2-N2	-4.13	106.00	108.95
1	C	63[A]	CH6	CA1-C1-N3	4.03	130.09	124.84
1	G	63[A]	CH6	CA1-C1-N3	4.01	130.06	124.84
1	H	63[B]	NRQ	CB2-CA2-C2	3.88	127.06	122.36
1	G	63[A]	CH6	C2-CA2-N2	-3.83	106.21	108.95
1	B	63[A]	CH6	CA2-N2-C1	3.82	108.79	105.80
1	B	63[B]	NRQ	N3-C1-N2	-3.77	108.14	112.62
1	E	63[B]	NRQ	CA2-C2-N3	3.76	106.66	103.50
1	G	63[A]	CH6	CA2-N2-C1	3.74	108.73	105.80
1	D	63[B]	NRQ	CA2-C2-N3	3.70	106.61	103.50
1	C	63[B]	NRQ	CA2-C2-N3	3.70	106.61	103.50
1	E	63[A]	CH6	CA1-C1-N3	3.66	129.61	124.84
1	H	63[B]	NRQ	CA2-C2-N3	3.63	106.55	103.50
1	F	63[B]	NRQ	CA2-C2-N3	3.63	106.55	103.50
1	G	63[B]	NRQ	CA2-C2-N3	3.60	106.52	103.50
1	D	63[A]	CH6	CA2-C2-N3	3.53	106.46	103.50
1	C	63[B]	NRQ	N3-C1-N2	-3.51	108.45	112.62
1	E	63[B]	NRQ	CB2-CA2-C2	3.50	126.60	122.36
1	B	63[B]	NRQ	CA2-C2-N3	3.48	106.43	103.50
1	A	63[B]	NRQ	CA2-C2-N3	3.47	106.42	103.50
1	F	63[B]	NRQ	CB2-CA2-C2	3.46	126.56	122.36
1	E	63[A]	CH6	CB2-CA2-N2	-3.44	124.10	128.76
1	H	63[A]	CH6	CB2-CA2-N2	-3.40	124.14	128.76
1	C	63[A]	CH6	CG2-CB2-CA2	-3.39	125.83	129.87
1	A	63[A]	CH6	CA2-C2-N3	3.36	106.32	103.50
1	G	63[A]	CH6	CA2-C2-N3	3.35	106.31	103.50
1	H	63[A]	CH6	O2-C2-CA2	-3.34	128.89	131.02
1	E	63[A]	CH6	CA2-C2-N3	3.31	106.28	103.50
1	E	63[B]	NRQ	N3-C1-N2	-3.29	108.72	112.62
1	D	63[A]	CH6	CB2-CA2-N2	-3.25	124.35	128.76
1	F	63[B]	NRQ	N3-C1-N2	-3.24	108.77	112.62
1	A	63[B]	NRQ	N3-C1-N2	-3.20	108.82	112.62
1	D	63[B]	NRQ	N3-C1-N2	-3.20	108.83	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63[B]	NRQ	CA2-N2-C1	3.15	109.89	104.09
1	G	63[B]	NRQ	N3-C1-N2	-3.14	108.89	112.62
1	C	63[A]	CH6	CB2-CA2-C2	3.13	126.15	122.36
1	C	63[A]	CH6	CA2-C2-N3	3.11	106.11	103.50
1	D	63[A]	CH6	CA1-C1-N3	3.11	128.89	124.84
1	F	63[B]	NRQ	CA2-N2-C1	3.08	109.77	104.09
1	D	63[B]	NRQ	CA2-N2-C1	3.07	109.75	104.09
1	E	63[B]	NRQ	CA2-N2-C1	3.06	109.73	104.09
1	H	63[A]	CH6	CA2-C2-N3	3.05	106.06	103.50
1	B	63[A]	CH6	CB2-CA2-N2	-3.01	124.67	128.76
1	F	63[A]	CH6	CB2-CA2-N2	-3.01	124.67	128.76
1	F	63[A]	CH6	CA2-C2-N3	2.99	106.01	103.50
1	A	63[B]	NRQ	CA2-N2-C1	2.98	109.58	104.09
1	G	63[A]	CH6	CB2-CA2-C2	2.91	125.89	122.36
1	H	63[B]	NRQ	CA2-N2-C1	2.91	109.45	104.09
1	B	63[A]	CH6	CA1-C1-N3	2.90	128.62	124.84
1	C	63[B]	NRQ	CA2-N2-C1	2.84	109.33	104.09
1	A	63[B]	NRQ	CB2-CA2-C2	2.83	125.78	122.36
1	H	63[B]	NRQ	N3-C1-N2	-2.79	109.31	112.62
1	B	63[A]	CH6	CA2-C2-N3	2.79	105.84	103.50
1	C	63[A]	CH6	N3-C1-N2	-2.74	109.32	111.48
1	F	63[A]	CH6	C2-N3-C1	2.71	109.32	108.07
1	G	63[B]	NRQ	CA2-N2-C1	2.70	109.06	104.09
1	A	63[A]	CH6	CB2-CA2-N2	-2.68	125.13	128.76
1	G	63[A]	CH6	CE1-CD1-CG2	-2.67	117.77	121.22
1	G	63[B]	NRQ	CE1-CD1-CG2	-2.67	117.77	121.22
1	A	63[A]	CH6	CA1-C1-N2	-2.65	118.40	123.57
1	C	63[A]	CH6	C2-N3-C1	2.62	109.28	108.07
1	A	63[A]	CH6	CE1-CD1-CG2	-2.46	118.05	121.22
1	A	63[B]	NRQ	CE1-CD1-CG2	-2.46	118.05	121.22
1	C	63[A]	CH6	CE1-CD1-CG2	-2.45	118.06	121.22
1	C	63[B]	NRQ	CE1-CD1-CG2	-2.45	118.06	121.22
1	C	63[A]	CH6	CD1-CG2-CD2	2.41	121.22	117.65
1	C	63[B]	NRQ	CD1-CG2-CD2	2.41	121.22	117.65
1	G	63[A]	CH6	CD1-CG2-CD2	2.38	121.19	117.65
1	G	63[B]	NRQ	CD1-CG2-CD2	2.38	121.19	117.65
1	A	63[A]	CH6	CD1-CG2-CD2	2.37	121.17	117.65
1	A	63[B]	NRQ	CD1-CG2-CD2	2.37	121.17	117.65
1	F	63[A]	CH6	N3-C1-N2	-2.37	109.62	111.48
1	F	63[A]	CH6	CA1-C1-N3	2.34	127.89	124.84
1	H	63[A]	CH6	C2-N3-C1	2.32	109.14	108.07
1	C	63[A]	CH6	C3-CA3-N3	-2.32	107.15	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63[B]	NRQ	CB2-CA2-C2	2.28	125.12	122.36
1	G	63[A]	CH6	C3-CA3-N3	-2.23	107.36	112.43
1	D	63[A]	CH6	CE-SD-CG1	-2.22	88.84	100.32
1	D	63[B]	NRQ	CE-SD-CG1	-2.22	88.84	100.32
1	H	63[A]	CH6	CE2-CD2-CG2	-2.21	118.36	121.22
1	H	63[B]	NRQ	CE2-CD2-CG2	-2.21	118.36	121.22
1	F	63[A]	CH6	C3-CA3-N3	-2.20	107.41	112.43
1	B	63[A]	CH6	CD1-CG2-CD2	2.12	120.80	117.65
1	B	63[B]	NRQ	CD1-CG2-CD2	2.12	120.80	117.65
1	E	63[A]	CH6	CE2-CD2-CG2	-2.11	118.50	121.22
1	E	63[B]	NRQ	CE2-CD2-CG2	-2.11	118.50	121.22
1	H	63[A]	CH6	CA1-C1-N3	2.11	127.58	124.84
1	C	63[A]	CH6	CB1-CA1-N1	-2.05	104.77	110.12
1	B	63[B]	NRQ	CD2-CG2-CB2	-2.01	114.32	121.22
1	E	63[A]	CH6	CD1-CG2-CD2	2.01	120.63	117.65
1	E	63[B]	NRQ	CD1-CG2-CD2	2.01	120.63	117.65

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63[A]	CH6	N2-CA2-CB2-CG2
1	A	63[A]	CH6	C2-CA2-CB2-CG2
1	A	63[B]	NRQ	N2-CA2-CB2-CG2
1	A	63[B]	NRQ	C2-CA2-CB2-CG2
1	B	63[A]	CH6	N2-CA2-CB2-CG2
1	B	63[A]	CH6	C2-CA2-CB2-CG2
1	B	63[B]	NRQ	N2-CA2-CB2-CG2
1	B	63[B]	NRQ	C2-CA2-CB2-CG2
1	C	63[A]	CH6	N2-CA2-CB2-CG2
1	C	63[A]	CH6	C2-CA2-CB2-CG2
1	C	63[B]	NRQ	N2-CA2-CB2-CG2
1	C	63[B]	NRQ	C2-CA2-CB2-CG2
1	D	63[A]	CH6	C2-CA2-CB2-CG2
1	D	63[B]	NRQ	N2-CA2-CB2-CG2
1	D	63[B]	NRQ	C2-CA2-CB2-CG2
1	E	63[A]	CH6	N2-CA2-CB2-CG2
1	E	63[A]	CH6	C2-CA2-CB2-CG2
1	E	63[B]	NRQ	N2-CA2-CB2-CG2
1	E	63[B]	NRQ	C2-CA2-CB2-CG2
1	F	63[A]	CH6	N2-CA2-CB2-CG2
1	F	63[A]	CH6	C2-CA2-CB2-CG2

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Mol	Chain	Res	Type	Atoms
1	F	63[B]	NRQ	CA1-CB1-CG1-SD
1	F	63[B]	NRQ	N2-CA2-CB2-CG2
1	F	63[B]	NRQ	C2-CA2-CB2-CG2
1	G	63[A]	CH6	C1-CA1-CB1-CG1
1	G	63[A]	CH6	N2-CA2-CB2-CG2
1	G	63[A]	CH6	C2-CA2-CB2-CG2
1	G	63[B]	NRQ	N2-CA2-CB2-CG2
1	G	63[B]	NRQ	C2-CA2-CB2-CG2
1	H	63[A]	CH6	N2-CA2-CB2-CG2
1	H	63[A]	CH6	C2-CA2-CB2-CG2
1	H	63[B]	NRQ	CA1-CB1-CG1-SD
1	H	63[B]	NRQ	N2-CA2-CB2-CG2
1	H	63[B]	NRQ	C2-CA2-CB2-CG2
1	A	63[A]	CH6	CA2-CB2-CG2-CD2
1	B	63[A]	CH6	CA2-CB2-CG2-CD2
1	C	63[B]	NRQ	CA2-CB2-CG2-CD2
1	E	63[B]	NRQ	CA2-CB2-CG2-CD1
1	A	63[A]	CH6	CA2-CB2-CG2-CD1
1	B	63[B]	NRQ	CA2-CB2-CG2-CD1
1	C	63[A]	CH6	CA2-CB2-CG2-CD2
1	C	63[A]	CH6	CA2-CB2-CG2-CD1
1	A	63[B]	NRQ	CA2-CB2-CG2-CD2
1	A	63[B]	NRQ	CA2-CB2-CG2-CD1
1	B	63[A]	CH6	CA2-CB2-CG2-CD1
1	B	63[B]	NRQ	CA2-CB2-CG2-CD2
1	C	63[B]	NRQ	CA2-CB2-CG2-CD1
1	E	63[A]	CH6	CA2-CB2-CG2-CD2
1	G	63[A]	CH6	CA2-CB2-CG2-CD2
1	E	63[B]	NRQ	CA2-CB2-CG2-CD2
1	G	63[B]	NRQ	CA2-CB2-CG2-CD2
1	D	63[B]	NRQ	CA2-CB2-CG2-CD2
1	D	63[B]	NRQ	CA2-CB2-CG2-CD1
1	E	63[A]	CH6	CA2-CB2-CG2-CD1
1	G	63[A]	CH6	CA2-CB2-CG2-CD1
1	F	63[B]	NRQ	CA2-CB2-CG2-CD2
1	C	63[B]	NRQ	CB1-CG1-SD-CE
1	A	63[A]	CH6	C1-CA1-CB1-CG1
1	C	63[A]	CH6	C1-CA1-CB1-CG1
1	B	63[B]	NRQ	CB1-CG1-SD-CE
1	F	63[A]	CH6	CB1-CG1-SD-CE
1	H	63[A]	CH6	CB1-CG1-SD-CE
1	D	63[A]	CH6	N2-CA2-CB2-CG2

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Mol	Chain	Res	Type	Atoms
1	F	63[B]	NRQ	CA2-CB2-CG2-CD1
1	G	63[B]	NRQ	CB1-CG1-SD-CE
1	G	63[B]	NRQ	CA2-CB2-CG2-CD1
1	A	63[B]	NRQ	CB1-CG1-SD-CE
1	H	63[B]	NRQ	CA2-CB2-CG2-CD2
1	H	63[B]	NRQ	CA2-CB2-CG2-CD1
1	A	63[A]	CH6	CB1-CG1-SD-CE
1	B	63[B]	NRQ	CA1-CB1-CG1-SD
1	D	63[B]	NRQ	CA1-CB1-CG1-SD
1	D	63[A]	CH6	CA2-CB2-CG2-CD2
1	G	63[A]	CH6	N1-CA1-CB1-CG1
1	F	63[A]	CH6	CA2-CB2-CG2-CD2
1	D	63[A]	CH6	CA2-CB2-CG2-CD1
1	F	63[A]	CH6	CA2-CB2-CG2-CD1
1	D	63[B]	NRQ	CB1-CG1-SD-CE
1	E	63[B]	NRQ	CB1-CG1-SD-CE
1	H	63[A]	CH6	CA2-CB2-CG2-CD2
1	H	63[A]	CH6	CA2-CB2-CG2-CD1
1	D	63[A]	CH6	C3-CA3-N3-C1
1	E	63[A]	CH6	C3-CA3-N3-C1
1	A	63[A]	CH6	N1-CA1-CB1-CG1

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	63[A]	CH6	1	0
1	G	63[A]	CH6	3	0
1	H	63[A]	CH6	1	0
1	B	63[A]	CH6	1	0
1	A	63[A]	CH6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	219/238 (92%)	0.24	5 (2%) 61 58	21, 49, 84, 127	4 (1%)
1	B	225/238 (94%)	0.28	4 (1%) 67 64	29, 51, 90, 122	3 (1%)
1	C	221/238 (92%)	0.36	6 (2%) 56 53	34, 57, 87, 115	3 (1%)
1	D	217/238 (91%)	0.26	2 (0%) 81 79	26, 56, 84, 96	4 (1%)
1	E	217/238 (91%)	0.28	3 (1%) 73 71	28, 58, 87, 125	2 (0%)
1	F	225/238 (94%)	0.56	9 (4%) 42 39	36, 66, 101, 132	2 (0%)
1	G	214/238 (89%)	0.67	7 (3%) 49 46	41, 74, 108, 127	2 (0%)
1	H	216/238 (90%)	0.68	10 (4%) 37 34	40, 72, 105, 131	3 (1%)
All	All	1754/1904 (92%)	0.42	46 (2%) 57 54	21, 59, 100, 132	23 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	202	LEU	4.3
1	C	223	ALA	3.5
1	H	4	LEU	3.5
1	G	207	GLY	3.4
1	A	2	ALA	3.4
1	H	204	ALA	3.3
1	A	1	GLY	3.3
1	E	3	PRO	3.3
1	G	3	PRO	3.3
1	H	73	VAL	3.2
1	F	204	ALA	3.1
1	G	209	PHE	3.1
1	H	3	PRO	3.1
1	F	3	PRO	3.0
1	G	75	GLY	2.8
1	A	184	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	228	LEU	2.6
1	H	209	PHE	2.6
1	C	225	PRO	2.5
1	F	5	VAL	2.5
1	B	209	PHE	2.5
1	D	3	PRO	2.4
1	H	220	TYR	2.4
1	D	186	ALA	2.4
1	C	207	GLY	2.4
1	F	213	TYR	2.3
1	G	220	TYR	2.3
1	B	202	LEU	2.3
1	F	185	ASN	2.3
1	A	202	LEU	2.3
1	G	213	TYR	2.3
1	F	230	HIS	2.3
1	B	230	HIS	2.2
1	E	209	PHE	2.2
1	F	50	PRO	2.2
1	C	166	ASP	2.2
1	F	229	GLY	2.2
1	H	113	ASN	2.2
1	F	207	GLY	2.2
1	C	188	ASN	2.2
1	A	3	PRO	2.1
1	C	112	GLY	2.1
1	H	40	VAL	2.1
1	E	202	LEU	2.1
1	H	22[A]	HIS	2.1
1	H	48	GLY	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CH6	C	63[A]	23/24	0.85	0.17	57,67,75,77	23
1	NRQ	A	63[B]	23/24	-	-	47,55,64,71	23
1	CH6	G	63[A]	23/24	0.85	0.16	65,79,83,88	23

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	NRQ	B	63[B]	23/24	-	-	50,54,64,68	23
1	CH6	F	63[A]	23/24	0.87	0.17	66,74,79,90	23
1	NRQ	C	63[B]	23/24	-	-	57,67,75,77	23
1	CH6	E	63[A]	23/24	0.87	0.14	63,67,72,74	23
1	NRQ	D	63[B]	23/24	-	-	62,65,71,72	23
1	CH6	H	63[A]	23/24	0.87	0.13	63,69,76,89	23
1	NRQ	E	63[B]	23/24	-	-	63,67,72,74	23
1	CH6	A	63[A]	23/24	0.89	0.14	47,56,64,71	23
1	NRQ	F	63[B]	23/24	-	-	66,73,79,90	23
1	CH6	D	63[A]	23/24	0.92	0.12	62,65,71,72	0
1	NRQ	G	63[B]	23/24	-	-	65,79,84,88	23
1	CH6	B	63[A]	23/24	0.93	0.11	50,54,64,68	0
1	NRQ	H	63[B]	23/24	-	-	64,69,76,89	23

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	D	301	1/1	0.88	0.12	70,70,70,70	0
2	CL	B	301	1/1	0.89	0.12	74,74,74,74	0
2	CL	C	301	1/1	0.90	0.10	63,63,63,63	0
2	CL	A	301	1/1	0.92	0.09	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.