



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:59 AM UTC

PDB ID : 3D23 / pdb_00003d23
Title : Main protease of HCoV-HKU1
Authors : Zhao, Q.; Chen, C.; Li, S.; Zou, Y.
Deposited on : 2008-05-07
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

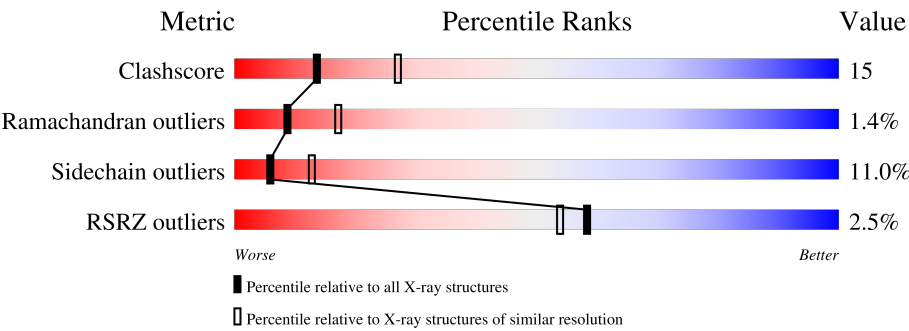
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	302	2% 70% 24% 5%
1	B	302	3% 70% 24% 5%
1	C	302	2% 72% 22%
1	D	302	3% 72% 23%
2	E	6	17% 67% 17%
2	F	6	33% 50% 17%
2	G	6	17% 33% 50%

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Mol	Chain	Length	Quality of chain
2	H	6	33% 50% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	02J	E	1	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9579 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 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	301	Total	C	N	O	S	0	1	0
			2312	1472	377	441	22			
1	A	299	Total	C	N	O	S	0	0	0
			2288	1461	372	433	22			
1	C	298	Total	C	N	O	S	0	0	0
			2285	1457	372	434	22			
1	D	299	Total	C	N	O	S	0	0	0
			2290	1460	372	436	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ALA	-	expression tag	UNP Q5MQD2
B	0	SER	-	expression tag	UNP Q5MQD2
A	-1	ALA	-	expression tag	UNP Q5MQD2
A	0	SER	-	expression tag	UNP Q5MQD2
C	-1	ALA	-	expression tag	UNP Q5MQD2
C	0	SER	-	expression tag	UNP Q5MQD2
D	-1	ALA	-	expression tag	UNP Q5MQD2
D	0	SER	-	expression tag	UNP Q5MQD2

- Molecule 2 is a protein called N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYLOXY)-4-OXO-1-{[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-LEUCINAMIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	F	6	Total	C	N	O	0	0	0
			49	35	6	8			
2	E	6	Total	C	N	O	0	0	0
			49	35	6	8			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	6	Total	C	N	O	0	0	0
			49	35	6	8			

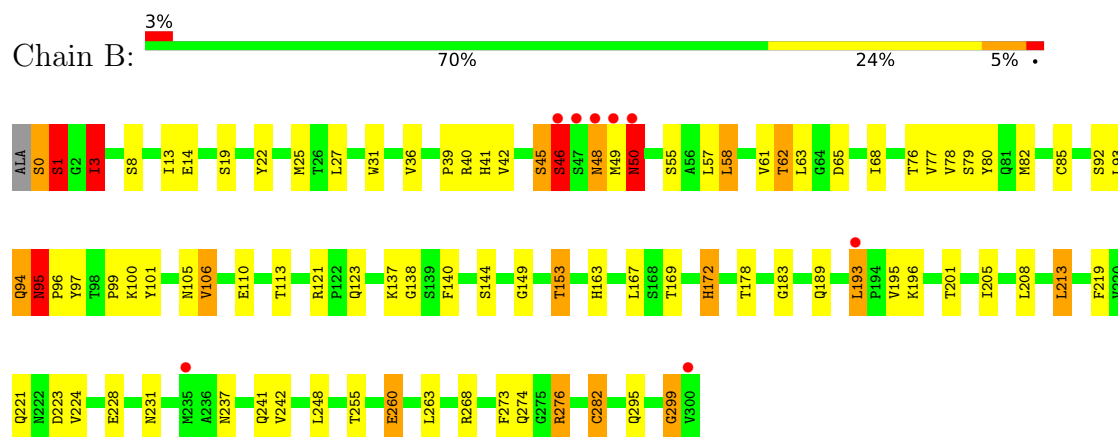
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	56	Total	O	0	0
			56	56		
3	A	56	Total	O	0	0
			56	56		
3	C	41	Total	O	0	0
			41	41		
3	D	55	Total	O	0	0
			55	55		

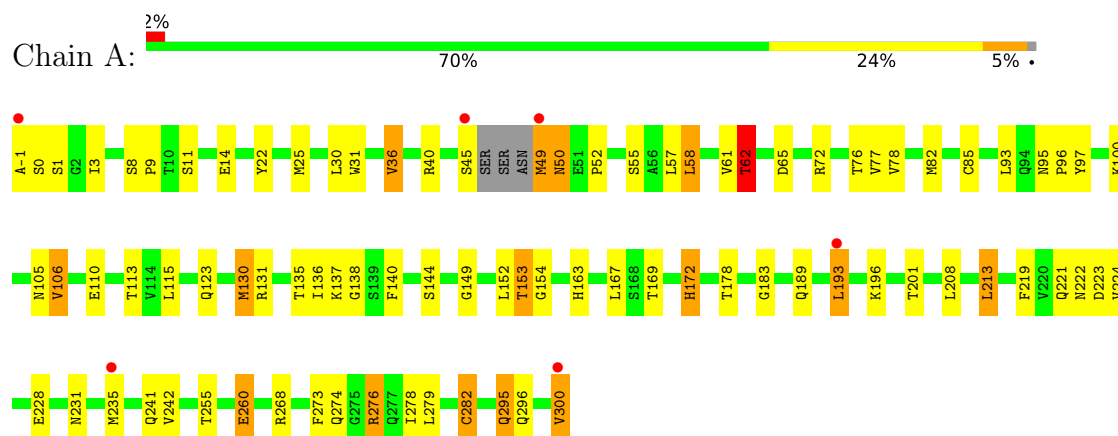
3 Residue-property plots [i](#)

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.

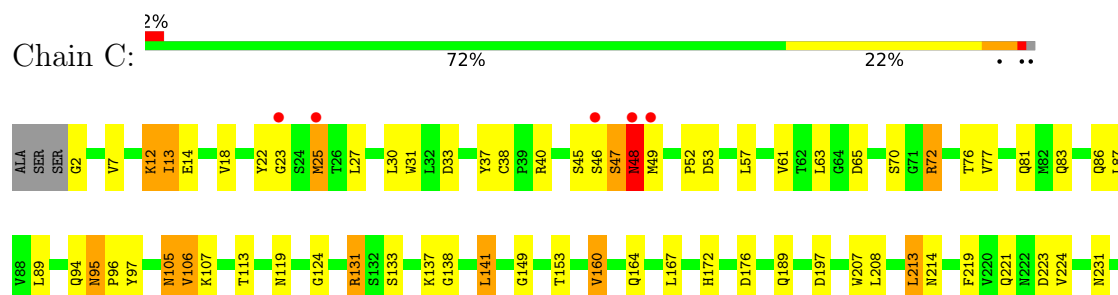
• Molecule 1: 3C-like proteinase



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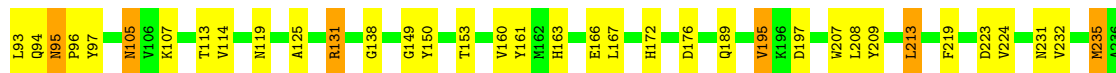
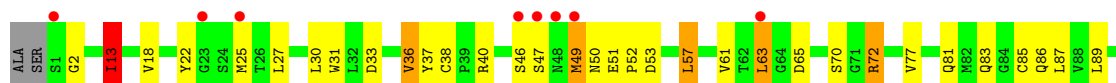


• Molecule 1: 3C-like proteinase





- Molecule 1: 3C-like proteinase



- Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYL OXY)-4-OXO-1-[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-L EUCINAMIDE



- Molecule 2: N-[(5-METHYLISOXAZOL-3-YL)CARBONYL]ALANYL-L-VALYL-N 1 -((1R,2Z)-4-(BENZYL OXY)-4-OXO-1-[(3R)-2-OXOPYRROLIDIN-3-YL]METHYL}BUT-2-ENYL)-L-L EUCINAMIDE

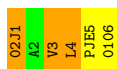


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4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	91.77 Å 91.77 Å 187.91 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.50) 68.2 (50.00-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 1.97 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.285 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9579	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 99.82 % 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 1.0991e-14. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 010, PJE, 02J

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	1.11	2/2338 (0.1%)	1.31	14/3181 (0.4%)
1	B	1.16	2/2363 (0.1%)	1.23	17/3216 (0.5%)
1	C	1.26	4/2336 (0.2%)	1.29	14/3179 (0.4%)
1	D	1.25	4/2341 (0.2%)	1.23	8/3185 (0.3%)
2	E	0.73	0/19	2.33	1/25 (4.0%)
2	F	0.65	0/19	1.65	0/25
2	G	0.79	0/19	2.33	1/25 (4.0%)
2	H	0.76	0/19	1.74	0/25
All	All	1.19	12/9454 (0.1%)	1.27	55/12861 (0.4%)

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	A	1	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	164	GLN	N-CA	8.62	1.57	1.46
1	D	13	ILE	CA-CB	8.55	1.64	1.54
1	B	196	LYS	C-O	6.72	1.32	1.23
1	A	196	LYS	C-O	6.47	1.31	1.23
1	B	3	ILE	CA-CB	-6.09	1.46	1.54
1	C	30	LEU	CA-C	5.89	1.59	1.52
1	C	265	ALA	CA-CB	-5.84	1.44	1.53
1	D	30	LEU	CA-C	5.78	1.59	1.52
1	D	209	TYR	CA-C	5.37	1.59	1.52
1	D	2	GLY	N-CA	5.34	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	THR	CA-CB	5.15	1.61	1.53
1	C	13	ILE	CA-CB	5.13	1.61	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLN	CB-CA-C	26.53	147.41	116.63
1	A	50	ASN	N-CA-C	12.37	128.60	113.38
1	C	164	GLN	N-CA-C	7.81	127.44	110.80
1	C	38	CYS	CA-C-N	-7.58	112.18	119.76
1	C	38	CYS	C-N-CA	-7.58	112.18	119.76
1	B	14	GLU	CA-C-N	-7.34	111.97	120.12
1	B	14	GLU	C-N-CA	-7.34	111.97	120.12
1	C	48	ASN	N-CA-C	-7.30	103.33	112.90
1	C	237	ASN	N-CA-C	7.06	122.90	112.94
1	D	237	ASN	N-CA-C	6.87	121.74	112.88
1	A	50	ASN	CA-C-N	-6.79	115.55	122.74
1	A	50	ASN	C-N-CA	-6.79	115.55	122.74
1	B	178	THR	N-CA-C	-6.49	105.12	113.16
2	E	3	VAL	N-CA-CB	-6.05	102.68	111.52
1	B	299	GLY	CA-C-N	5.92	132.36	121.70
1	B	299	GLY	C-N-CA	5.92	132.36	121.70
1	C	38	CYS	N-CA-C	5.88	113.30	108.07
1	B	183	GLY	CA-C-N	-5.79	114.34	120.94
1	B	183	GLY	C-N-CA	-5.79	114.34	120.94
1	B	63	LEU	N-CA-C	5.76	117.36	111.14
1	B	46	SER	N-CA-C	5.75	123.06	110.80
1	B	48	ASN	CB-CA-C	-5.72	103.41	111.65
1	A	274	GLN	N-CA-C	-5.71	98.43	108.08
1	A	163	HIS	N-CA-C	5.71	118.52	109.96
1	A	178	THR	N-CA-C	-5.70	106.09	113.16
1	D	93	LEU	N-CA-C	5.70	117.50	108.67
1	A	1	SER	N-CA-C	5.68	120.20	113.16
1	A	183	GLY	CA-C-N	-5.65	114.50	120.94
1	A	183	GLY	C-N-CA	-5.65	114.50	120.94
1	A	14	GLU	CA-C-N	-5.59	113.92	120.12
1	A	14	GLU	C-N-CA	-5.59	113.92	120.12
1	A	172	HIS	N-CA-C	5.58	118.31	109.50
1	C	95	ASN	CA-C-N	5.56	125.39	119.28
1	C	95	ASN	C-N-CA	5.56	125.39	119.28
1	C	106	VAL	CB-CA-C	5.55	118.81	110.98
1	C	276	ARG	N-CA-C	-5.55	102.06	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	VAL	N-CA-CB	-5.51	103.47	111.52
1	D	276	ARG	N-CA-C	-5.48	102.17	110.28
1	D	38	CYS	N-CA-C	5.46	113.13	108.22
1	B	95	ASN	CA-C-N	-5.41	114.24	119.87
1	B	95	ASN	C-N-CA	-5.41	114.24	119.87
1	D	95	ASN	CA-C-N	5.31	125.12	119.28
1	D	95	ASN	C-N-CA	5.31	125.12	119.28
1	C	81	GLN	N-CA-C	5.30	117.87	109.50
1	C	12	LYS	CA-C-N	-5.27	117.55	122.66
1	C	12	LYS	C-N-CA	-5.27	117.55	122.66
1	D	36	VAL	N-CA-C	5.22	115.48	108.17
1	C	23	GLY	N-CA-C	-5.21	100.83	113.18
1	B	1	SER	N-CA-C	5.18	121.84	110.80
1	B	172	HIS	N-CA-C	5.17	117.82	109.40
1	A	93	LEU	N-CA-C	5.12	117.42	108.76
1	B	121	ARG	CA-C-N	5.11	125.03	119.76
1	B	121	ARG	C-N-CA	5.11	125.03	119.76
1	D	81	GLN	N-CA-C	5.05	117.06	109.23
1	B	237	ASN	N-CA-C	5.02	120.02	113.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	274	GLN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	MET	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	2288	0	2249	72	0
1	B	2312	0	2269	75	0
1	C	2285	0	2242	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2290	0	2246	61	0
2	E	49	0	41	8	0
2	F	49	0	41	6	0
2	G	49	0	41	8	0
2	H	49	0	41	6	0
3	A	56	0	0	3	0
3	B	56	0	0	2	0
3	C	41	0	0	5	0
3	D	55	0	0	5	0
All	All	9579	0	9170	271	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 15.

All (271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.06	1.15
1:B:276:ARG:HG2	1:B:276:ARG:HH11	1.13	1.07
1:B:189:GLN:HE21	2:H:4:LEU:H	1.08	0.99
1:B:0:SER:O	1:B:1:SER:HB3	1.64	0.97
1:A:189:GLN:HE21	2:F:4:LEU:H	1.12	0.97
1:A:-1:ALA:HB3	1:A:0:SER:HA	1.49	0.95
1:C:2:GLY:HA2	1:C:214:ASN:HD21	1.29	0.95
1:D:189:GLN:HE21	2:G:4:LEU:H	1.03	0.93
1:B:193:LEU:HD22	1:B:193:LEU:H	1.34	0.92
1:C:46:SER:HA	1:C:49:MET:HB2	1.49	0.92
1:A:49:MET:O	1:A:49:MET:HG2	1.69	0.91
1:A:130:MET:HE3	1:A:130:MET:HA	1.52	0.89
1:D:25:MET:SD	2:G:6:010:HA	2.13	0.89
1:C:189:GLN:HE21	2:E:4:LEU:H	0.94	0.88
1:C:189:GLN:NE2	2:E:4:LEU:H	1.70	0.88
1:B:45:SER:H	1:B:48:ASN:ND2	1.72	0.88
1:A:193:LEU:HD22	1:A:193:LEU:H	1.37	0.87
1:B:201:THR:HG21	1:B:242:VAL:HG23	1.57	0.86
1:B:45:SER:H	1:B:48:ASN:HD22	1.24	0.85
1:D:276:ARG:HG2	1:D:276:ARG:HH11	1.40	0.84
1:A:276:ARG:HG2	1:A:276:ARG:NH1	1.87	0.83
1:A:-1:ALA:HB2	1:C:137:LYS:HE3	1.61	0.81
1:B:0:SER:O	1:B:1:SER:CB	2.29	0.80
1:C:138:GLY:H	1:C:172:HIS:HD2	1.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ARG:HG2	1:B:276:ARG:NH1	1.90	0.79
1:B:95:ASN:ND2	1:B:97:TYR:H	1.80	0.78
1:B:80:TYR:H	1:C:221:GLN:HE22	1.29	0.78
1:C:276:ARG:HG2	1:C:276:ARG:HH11	1.47	0.78
1:D:105:ASN:ND2	1:D:176:ASP:OD2	2.16	0.78
1:B:276:ARG:HH11	1:B:276:ARG:CG	1.94	0.78
1:C:72:ARG:HH11	1:C:72:ARG:CG	1.96	0.77
1:A:201:THR:HG21	1:A:242:VAL:HG23	1.64	0.77
1:B:138:GLY:H	1:B:172:HIS:HD2	1.32	0.76
1:D:189:GLN:NE2	2:G:4:LEU:H	1.84	0.76
1:D:25:MET:SD	2:G:6:010:H5	2.27	0.75
1:B:193:LEU:H	1:B:193:LEU:CD2	2.00	0.74
1:B:231:ASN:HD21	1:B:242:VAL:H	1.36	0.74
1:A:231:ASN:HD21	1:A:242:VAL:H	1.37	0.73
1:A:193:LEU:H	1:A:193:LEU:CD2	2.02	0.72
1:B:3:ILE:HG22	1:B:3:ILE:O	1.90	0.72
1:A:276:ARG:HH11	1:A:276:ARG:CG	1.93	0.72
1:C:63:LEU:HD12	1:C:63:LEU:H	1.55	0.71
1:C:25:MET:SD	2:E:6:010:H1	2.30	0.71
1:C:105:ASN:ND2	1:C:176:ASP:OD2	2.24	0.71
1:A:153:THR:HG22	1:A:153:THR:O	1.90	0.71
1:C:189:GLN:HE21	2:E:4:LEU:N	1.79	0.71
1:A:228:GLU:CD	1:A:228:GLU:H	1.99	0.70
1:D:166:GLU:OE1	1:D:172:HIS:HE1	1.75	0.70
1:C:231:ASN:HD21	1:C:242:VAL:H	1.40	0.69
1:A:9:PRO:HD3	1:C:124:GLY:HA2	1.75	0.69
1:A:189:GLN:NE2	2:F:4:LEU:H	1.88	0.68
1:D:189:GLN:HE21	2:G:4:LEU:N	1.86	0.68
1:C:53:ASP:HA	3:C:436:HOH:O	1.93	0.67
1:C:40:ARG:HA	1:C:87:LEU:HG	1.76	0.67
1:B:228:GLU:H	1:B:228:GLU:CD	2.03	0.66
1:B:153:THR:HG22	1:B:153:THR:O	1.94	0.66
1:A:95:ASN:ND2	1:A:97:TYR:H	1.94	0.66
1:C:22:TYR:CE1	1:C:65:ASP:HB2	2.31	0.66
1:C:72:ARG:HH11	1:C:72:ARG:HG2	1.59	0.66
1:D:231:ASN:HD21	1:D:242:VAL:H	1.44	0.66
1:C:52:PRO:O	3:C:436:HOH:O	2.13	0.65
1:C:189:GLN:HE21	2:E:4:LEU:HB2	1.61	0.65
1:D:22:TYR:CE1	1:D:65:ASP:HB2	2.32	0.65
1:C:47:SER:H	1:C:49:MET:H	1.45	0.65
1:D:95:ASN:ND2	3:D:420:HOH:O	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:SER:HA	1:C:49:MET:CB	2.26	0.64
1:A:50:ASN:HB2	1:A:189:GLN:O	1.98	0.64
1:A:189:GLN:HE21	2:F:4:LEU:HB2	1.62	0.63
1:C:72:ARG:HG2	1:C:72:ARG:NH1	2.12	0.63
1:D:63:LEU:H	1:D:63:LEU:CD2	2.10	0.63
1:A:138:GLY:H	1:A:172:HIS:HD2	1.46	0.62
1:B:31:TRP:CE2	1:B:95:ASN:HB2	2.34	0.62
1:B:58:LEU:HG	1:B:82:MET:HE3	1.82	0.61
1:B:224:VAL:HG13	1:B:260:GLU:HB2	1.83	0.61
1:C:95:ASN:ND2	1:C:97:TYR:H	1.99	0.61
1:B:106:VAL:HG13	1:B:110:GLU:HB2	1.83	0.61
1:B:201:THR:CG2	1:B:242:VAL:HG23	2.30	0.61
1:A:130:MET:HA	1:A:130:MET:CE	2.28	0.60
1:C:276:ARG:HH11	1:C:276:ARG:CG	2.15	0.60
1:A:58:LEU:HG	1:A:82:MET:HE3	1.81	0.60
1:C:31:TRP:CE2	1:C:95:ASN:HB2	2.37	0.60
1:B:45:SER:N	1:B:48:ASN:HD22	1.97	0.59
1:B:221:GLN:NE2	3:B:427:HOH:O	2.34	0.59
1:C:72:ARG:CG	1:C:72:ARG:NH1	2.62	0.59
1:D:276:ARG:HG2	1:D:276:ARG:NH1	2.12	0.59
1:A:113:THR:O	1:A:149:GLY:HA2	2.02	0.59
1:D:46:SER:HA	1:D:49:MET:HB3	1.84	0.59
1:A:-1:ALA:CB	1:C:137:LYS:HE3	2.31	0.59
1:D:53:ASP:HA	3:D:445:HOH:O	2.01	0.59
1:A:140:PHE:HB3	1:A:144:SER:OG	2.03	0.58
1:A:221:GLN:NE2	3:A:447:HOH:O	2.36	0.58
1:C:213:LEU:HD13	1:C:255:THR:HG22	1.84	0.58
1:D:95:ASN:HD22	1:D:96:PRO:HD2	1.68	0.58
1:C:95:ASN:ND2	3:C:415:HOH:O	2.36	0.58
1:A:95:ASN:C	1:A:95:ASN:HD22	2.12	0.57
1:D:95:ASN:HD22	1:D:96:PRO:CD	2.17	0.57
1:D:213:LEU:HD13	1:D:255:THR:HG22	1.85	0.57
1:A:-1:ALA:CB	1:A:0:SER:HA	2.30	0.57
1:D:33:ASP:HA	1:D:94:GLN:NE2	2.19	0.57
1:B:201:THR:HG21	1:B:242:VAL:CG2	2.33	0.57
1:A:130:MET:HE3	1:A:136:ILE:HG23	1.88	0.56
1:A:213:LEU:HD13	1:A:255:THR:HG22	1.87	0.56
1:D:276:ARG:HH11	1:D:276:ARG:CG	2.14	0.56
1:B:213:LEU:HD13	1:B:255:THR:HG22	1.88	0.56
1:A:189:GLN:HE21	2:F:4:LEU:N	1.94	0.56
1:B:95:ASN:C	1:B:95:ASN:HD22	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LEU:HG	1:B:82:MET:CE	2.37	0.55
1:D:31:TRP:CE2	1:D:95:ASN:HB2	2.40	0.55
1:A:201:THR:HG21	1:A:242:VAL:CG2	2.34	0.55
1:D:95:ASN:ND2	1:D:97:TYR:H	2.05	0.55
1:C:189:GLN:NE2	2:E:4:LEU:HB2	2.22	0.55
1:A:222:ASN:H	1:A:222:ASN:ND2	2.05	0.54
1:B:189:GLN:NE2	2:H:4:LEU:H	1.91	0.54
1:A:130:MET:HE2	1:A:135:THR:O	2.08	0.54
1:C:63:LEU:H	1:C:63:LEU:CD1	2.21	0.54
1:C:231:ASN:ND2	1:C:242:VAL:H	2.02	0.54
1:A:106:VAL:HG13	1:A:110:GLU:HB2	1.89	0.53
1:A:201:THR:CG2	1:A:242:VAL:HG23	2.36	0.53
1:D:13:ILE:CD1	1:D:13:ILE:N	2.72	0.53
1:C:25:MET:SD	2:E:6:010:HA	2.49	0.53
1:C:95:ASN:HD22	1:C:96:PRO:CD	2.21	0.53
1:B:138:GLY:H	1:B:172:HIS:CD2	2.20	0.52
1:D:63:LEU:H	1:D:63:LEU:HD22	1.72	0.52
1:A:95:ASN:HD22	1:A:96:PRO:HD2	1.74	0.52
1:B:189:GLN:HE21	2:H:4:LEU:N	1.91	0.52
1:C:276:ARG:HG2	1:C:276:ARG:NH1	2.17	0.52
1:A:40:ARG:HD3	1:A:85:CYS:HA	1.92	0.52
1:C:7:VAL:HG13	1:C:113:THR:HG23	1.92	0.52
1:A:95:ASN:HD22	1:A:96:PRO:N	2.08	0.51
1:D:40:ARG:HA	1:D:87:LEU:HG	1.91	0.51
1:A:95:ASN:HD22	1:A:96:PRO:CD	2.24	0.51
1:D:231:ASN:ND2	1:D:242:VAL:H	2.06	0.51
1:A:295:GLN:HA	1:A:300:VAL:HG23	1.93	0.51
2:F:4:LEU:O	2:F:6:010:H1	2.10	0.51
1:B:97:TYR:CD1	2:G:1:02J:H6A	2.46	0.51
1:B:113:THR:O	1:B:149:GLY:HA2	2.11	0.51
1:C:45:SER:H	1:C:48:ASN:ND2	2.08	0.51
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.46	0.51
1:B:46:SER:HA	1:B:49:MET:HG3	1.91	0.51
1:A:8:SER:HB3	1:A:152:LEU:HD22	1.93	0.50
1:B:189:GLN:HE21	2:H:4:LEU:HB2	1.75	0.50
1:A:201:THR:CG2	1:A:242:VAL:CG2	2.90	0.50
1:A:58:LEU:HG	1:A:82:MET:CE	2.42	0.50
1:A:131:ARG:HG2	1:A:135:THR:O	2.11	0.50
1:C:33:ASP:HA	1:C:94:GLN:NE2	2.27	0.50
1:C:138:GLY:H	1:C:172:HIS:CD2	2.19	0.50
2:H:4:LEU:O	2:H:6:010:H1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:TYR:OH	1:C:61:VAL:HA	2.12	0.49
1:B:13:ILE:HD12	1:B:13:ILE:N	2.28	0.49
1:B:19:SER:O	1:B:68:ILE:HA	2.13	0.49
1:A:130:MET:CE	1:A:135:THR:O	2.60	0.49
1:A:130:MET:CE	1:A:136:ILE:HG23	2.42	0.49
1:D:52:PRO:O	3:D:445:HOH:O	2.20	0.49
1:D:131:ARG:HD3	3:D:450:HOH:O	2.12	0.49
1:C:12:LYS:C	1:C:13:ILE:HD12	2.37	0.48
1:D:72:ARG:HH11	1:D:72:ARG:HB3	1.76	0.48
1:A:189:GLN:NE2	2:F:4:LEU:HB2	2.28	0.48
1:B:201:THR:CG2	1:B:242:VAL:CG2	2.90	0.48
1:B:40:ARG:C	1:B:42:VAL:H	2.22	0.48
1:B:49:MET:O	1:B:50[B]:ASN:HB2	2.13	0.48
1:B:62:THR:O	1:B:65:ASP:HB2	2.13	0.48
1:B:95:ASN:HD22	1:B:96:PRO:N	2.11	0.48
1:C:18:VAL:HG12	1:C:70:SER:HB2	1.95	0.48
1:C:95:ASN:HD22	1:C:96:PRO:HD2	1.79	0.48
1:B:27:LEU:HD22	1:B:39:PRO:HG2	1.95	0.48
1:D:37:TYR:N	1:D:37:TYR:CD2	2.81	0.48
1:B:140:PHE:HB3	1:B:144:SER:OG	2.14	0.48
1:A:76:THR:CG2	3:A:456:HOH:O	2.61	0.48
1:C:131:ARG:HD3	3:C:434:HOH:O	2.14	0.47
1:D:166:GLU:OE1	1:D:172:HIS:CE1	2.61	0.47
1:B:40:ARG:C	1:B:42:VAL:N	2.71	0.47
1:A:58:LEU:O	1:A:61:VAL:HB	2.14	0.47
1:B:22:TYR:CE1	1:B:65:ASP:HB3	2.48	0.47
1:A:95:ASN:ND2	1:A:95:ASN:C	2.70	0.47
1:C:95:ASN:HD22	1:C:96:PRO:N	2.12	0.47
1:D:114:VAL:O	1:D:125:ALA:HA	2.15	0.47
1:A:62:THR:O	1:A:65:ASP:HB2	2.15	0.47
1:B:223:ASP:OD1	1:B:268:ARG:NH1	2.48	0.47
1:A:76:THR:HG23	3:A:456:HOH:O	2.14	0.47
1:C:53:ASP:OD1	3:C:421:HOH:O	2.20	0.47
1:A:49:MET:HA	1:A:52:PRO:HG3	1.96	0.46
1:D:22:TYR:OH	1:D:61:VAL:HA	2.15	0.46
1:A:296:GLN:O	1:C:141:LEU:HD21	2.15	0.46
1:B:95:ASN:ND2	1:B:95:ASN:C	2.73	0.46
1:A:50:ASN:CB	1:A:189:GLN:HB2	2.45	0.46
1:C:131:ARG:NH2	1:C:286:ASP:OD2	2.41	0.46
1:A:224:VAL:HG13	1:A:260:GLU:HB2	1.97	0.46
1:D:83:GLN:O	1:D:86:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:PHE:O	1:D:268:ARG:NH2	2.41	0.46
1:C:213:LEU:HD23	1:C:297:LEU:HD12	1.97	0.46
1:C:72:ARG:HH11	1:C:72:ARG:HG3	1.77	0.46
1:B:94:GLN:HB2	1:D:46:SER:OG	2.16	0.45
1:B:231:ASN:HB3	1:B:241:GLN:HE22	1.81	0.45
1:D:207:TRP:CD2	1:D:285:GLU:HB3	2.52	0.45
1:B:49:MET:O	1:B:50[A]:ASN:HB2	2.16	0.45
1:A:219:PHE:O	1:A:268:ARG:NH2	2.49	0.45
1:B:93:LEU:HD11	1:D:189:GLN:HE22	1.81	0.45
1:C:207:TRP:CD2	1:C:285:GLU:HB3	2.52	0.45
1:B:96:PRO:HB3	1:D:189:GLN:HB3	1.97	0.45
1:A:231:ASN:HB3	1:A:241:GLN:HE22	1.82	0.45
1:C:219:PHE:O	1:C:268:ARG:NH2	2.41	0.45
1:B:58:LEU:O	1:B:61:VAL:HB	2.17	0.45
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.52	0.45
1:C:95:ASN:ND2	1:C:95:ASN:C	2.75	0.44
1:C:31:TRP:CD2	1:C:95:ASN:HB2	2.53	0.44
1:A:49:MET:O	1:A:49:MET:CG	2.45	0.44
1:B:189:GLN:NE2	2:H:4:LEU:HB2	2.32	0.44
1:C:2:GLY:CA	1:C:214:ASN:HD21	2.14	0.44
1:D:95:ASN:HD22	1:D:96:PRO:N	2.15	0.44
1:B:76:THR:OG1	1:B:92:SER:HB3	2.17	0.44
1:D:95:ASN:ND2	1:D:95:ASN:C	2.76	0.44
1:A:130:MET:CE	1:A:135:THR:C	2.91	0.44
1:B:50[A]:ASN:ND2	3:B:455:HOH:O	2.50	0.44
1:B:219:PHE:O	1:B:268:ARG:NH2	2.51	0.43
1:D:50:ASN:HD22	1:D:50:ASN:HA	1.60	0.43
1:A:82:MET:HE3	1:A:82:MET:HB2	1.88	0.43
1:A:223:ASP:OD1	1:A:268:ARG:NH1	2.51	0.43
1:D:223:ASP:OD2	1:D:223:ASP:N	2.46	0.43
1:A:153:THR:O	1:A:153:THR:CG2	2.62	0.43
1:C:46:SER:O	1:C:46:SER:OG	2.32	0.43
1:C:95:ASN:HD22	1:C:95:ASN:C	2.27	0.43
1:C:223:ASP:OD2	1:C:223:ASP:N	2.46	0.43
1:B:45:SER:O	1:B:48:ASN:ND2	2.52	0.43
1:B:82:MET:HE3	1:B:82:MET:HB2	1.75	0.43
1:C:27:LEU:C	1:C:27:LEU:HD12	2.44	0.43
1:D:231:ASN:HB3	1:D:241:GLN:HE22	1.83	0.43
1:C:83:GLN:O	1:C:86:GLN:HG2	2.18	0.43
1:D:13:ILE:N	1:D:13:ILE:HD12	2.33	0.43
1:D:95:ASN:HD22	1:D:95:ASN:C	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:HIS:HE1	1:B:172:HIS:HB3	1.84	0.43
1:C:95:ASN:HA	1:C:96:PRO:HD2	1.83	0.43
1:D:40:ARG:HD3	1:D:85:CYS:HA	2.01	0.43
1:B:40:ARG:HD3	1:B:85:CYS:HA	2.01	0.43
1:D:150:TYR:CD2	1:D:150:TYR:C	2.96	0.42
1:D:285:GLU:OE2	1:D:287:GLU:HB2	2.19	0.42
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.53	0.42
1:C:7:VAL:HG13	1:C:113:THR:CG2	2.48	0.42
1:A:11:SER:HB3	1:C:14:GLU:CD	2.45	0.42
1:B:153:THR:O	1:B:153:THR:CG2	2.66	0.42
1:D:195:VAL:HB	3:D:436:HOH:O	2.20	0.42
1:D:138:GLY:H	1:D:172:HIS:HD2	1.66	0.42
1:B:273:PHE:CD1	1:B:282:CYS:HA	2.55	0.42
1:A:22:TYR:CE1	1:A:65:ASP:HB3	2.55	0.42
1:D:113:THR:O	1:D:149:GLY:HA2	2.20	0.42
1:D:213:LEU:HD23	1:D:297:LEU:HD12	2.02	0.42
1:A:11:SER:HB3	1:C:14:GLU:OE1	2.19	0.42
1:B:79:SER:HA	1:C:221:GLN:NE2	2.35	0.42
1:B:49:MET:O	1:B:50[B]:ASN:CB	2.67	0.42
1:B:99:PRO:O	1:B:101:TYR:HD1	2.03	0.42
1:D:18:VAL:HG12	1:D:70:SER:HB2	2.02	0.42
1:B:205:ILE:HG22	1:B:248:LEU:HD22	2.02	0.41
1:C:46:SER:O	1:C:47:SER:HB2	2.20	0.41
1:B:231:ASN:HD21	1:B:242:VAL:N	2.10	0.41
1:A:130:MET:HE3	1:A:136:ILE:CG2	2.49	0.41
1:D:31:TRP:CD2	1:D:95:ASN:HB2	2.55	0.41
1:B:242:VAL:HG21	1:B:263:LEU:HD21	2.02	0.41
1:C:113:THR:O	1:C:149:GLY:HA2	2.20	0.41
1:D:231:ASN:HD21	1:D:242:VAL:HG23	1.85	0.41
1:A:273:PHE:CD1	1:A:282:CYS:HA	2.55	0.41
1:C:138:GLY:N	1:C:172:HIS:HD2	2.07	0.41
1:C:37:TYR:CD2	1:C:37:TYR:N	2.88	0.41
1:D:25:MET:SD	2:G:6:010:C	2.97	0.41
1:D:53:ASP:O	1:D:57:LEU:HD22	2.21	0.41
1:B:231:ASN:HB3	1:B:241:GLN:NE2	2.36	0.41
1:A:30:LEU:O	1:A:36:VAL:HA	2.21	0.41
1:B:231:ASN:ND2	1:B:242:VAL:H	2.12	0.40
1:D:25:MET:HA	2:G:6:010:C4	2.52	0.40
1:C:25:MET:HA	2:E:6:010:C2	2.52	0.40
1:D:161:TYR:OH	1:D:163:HIS:HD2	2.05	0.40
1:A:278:ILE:O	1:A:279:LEU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ASN:HA	1:D:96:PRO:HD2	1.89	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	295/302 (98%)	280 (95%)	12 (4%)	3 (1%)	12	24
1	B	300/302 (99%)	276 (92%)	15 (5%)	9 (3%)	3	5
1	C	296/302 (98%)	272 (92%)	22 (7%)	2 (1%)	18	34
1	D	297/302 (98%)	272 (92%)	21 (7%)	4 (1%)	9	18
2	E	3/6 (50%)	3 (100%)	0	0	100	100
2	F	3/6 (50%)	3 (100%)	0	0	100	100
2	G	3/6 (50%)	3 (100%)	0	0	100	100
2	H	3/6 (50%)	3 (100%)	0	0	100	100
All	All	1200/1232 (97%)	1112 (93%)	70 (6%)	18 (2%)	9	16

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	SER
1	B	50[A]	ASN
1	B	50[B]	ASN
1	B	299	GLY
1	C	47	SER
1	D	235	MET
1	B	1	SER
1	D	47	SER
1	B	41	HIS

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Mol	Chain	Res	Type
1	A	154	GLY
1	B	153	THR
1	A	153	THR
1	B	274	GLN
1	A	235	MET
1	B	195	VAL
1	D	275	GLY
1	C	160	VAL
1	D	232	VAL

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	254/258 (98%)	226 (89%)	28 (11%)	6	13
1	B	259/258 (100%)	229 (88%)	30 (12%)	5	11
1	C	255/258 (99%)	230 (90%)	25 (10%)	7	16
1	D	255/258 (99%)	229 (90%)	26 (10%)	7	15
2	E	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	F	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	G	2/2 (100%)	0	2 (100%)	0	0
2	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	1031/1040 (99%)	917 (89%)	114 (11%)	6	12

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	SER
1	B	3	ILE
1	B	8	SER
1	B	25	MET
1	B	36	VAL
1	B	45	SER

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Mol	Chain	Res	Type
1	B	50[A]	ASN
1	B	50[B]	ASN
1	B	55	SER
1	B	57	LEU
1	B	58	LEU
1	B	62	THR
1	B	77	VAL
1	B	78	VAL
1	B	94	GLN
1	B	95	ASN
1	B	100	LYS
1	B	105	ASN
1	B	106	VAL
1	B	123	GLN
1	B	137	LYS
1	B	167	LEU
1	B	169	THR
1	B	193	LEU
1	B	208	LEU
1	B	213	LEU
1	B	260	GLU
1	B	276	ARG
1	B	282	CYS
1	B	295	GLN
1	A	3	ILE
1	A	25	MET
1	A	36	VAL
1	A	45	SER
1	A	55	SER
1	A	57	LEU
1	A	58	LEU
1	A	62	THR
1	A	72	ARG
1	A	77	VAL
1	A	78	VAL
1	A	100	LYS
1	A	105	ASN
1	A	106	VAL
1	A	115	LEU
1	A	123	GLN
1	A	130	MET
1	A	137	LYS

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Mol	Chain	Res	Type
1	A	167	LEU
1	A	169	THR
1	A	193	LEU
1	A	208	LEU
1	A	213	LEU
1	A	260	GLU
1	A	276	ARG
1	A	282	CYS
1	A	295	GLN
1	A	300	VAL
1	C	25	MET
1	C	48	ASN
1	C	57	LEU
1	C	72	ARG
1	C	76	THR
1	C	77	VAL
1	C	89	LEU
1	C	105	ASN
1	C	106	VAL
1	C	107	LYS
1	C	119	ASN
1	C	131	ARG
1	C	133	SER
1	C	141	LEU
1	C	153	THR
1	C	160	VAL
1	C	167	LEU
1	C	197	ASP
1	C	208	LEU
1	C	213	LEU
1	C	224	VAL
1	C	235	MET
1	C	253	SER
1	C	276	ARG
1	C	295	GLN
1	D	13	ILE
1	D	27	LEU
1	D	36	VAL
1	D	49	MET
1	D	51	GLU
1	D	57	LEU
1	D	63	LEU

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Mol	Chain	Res	Type
1	D	72	ARG
1	D	77	VAL
1	D	89	LEU
1	D	105	ASN
1	D	107	LYS
1	D	119	ASN
1	D	131	ARG
1	D	153	THR
1	D	160	VAL
1	D	167	LEU
1	D	195	VAL
1	D	197	ASP
1	D	208	LEU
1	D	213	LEU
1	D	224	VAL
1	D	235	MET
1	D	253	SER
1	D	276	ARG
1	D	295	GLN
2	H	4	LEU
2	F	4	LEU
2	E	4	LEU
2	G	3	VAL
2	G	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	ASN
1	B	81	GLN
1	B	86	GLN
1	B	94	GLN
1	B	95	ASN
1	B	123	GLN
1	B	127	HIS
1	B	172	HIS
1	B	189	GLN
1	B	214	ASN
1	B	221	GLN
1	B	231	ASN
1	B	237	ASN
1	B	241	GLN

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Mol	Chain	Res	Type
1	B	277	GLN
1	B	295	GLN
1	A	86	GLN
1	A	95	ASN
1	A	123	GLN
1	A	127	HIS
1	A	172	HIS
1	A	189	GLN
1	A	221	GLN
1	A	222	ASN
1	A	231	ASN
1	A	237	ASN
1	A	241	GLN
1	A	277	GLN
1	A	295	GLN
1	C	41	HIS
1	C	48	ASN
1	C	86	GLN
1	C	95	ASN
1	C	105	ASN
1	C	119	ASN
1	C	172	HIS
1	C	189	GLN
1	C	214	ASN
1	C	215	ASN
1	C	221	GLN
1	C	222	ASN
1	C	231	ASN
1	C	237	ASN
1	C	241	GLN
1	C	277	GLN
1	D	48	ASN
1	D	50	ASN
1	D	95	ASN
1	D	105	ASN
1	D	123	GLN
1	D	163	HIS
1	D	172	HIS
1	D	189	GLN
1	D	214	ASN
1	D	221	GLN
1	D	222	ASN

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Mol	Chain	Res	Type
1	D	231	ASN
1	D	237	ASN
1	D	241	GLN
1	D	277	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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$
2	02J	E	1	2	8,8,9	2.39	4 (50%)	9,10,12	3.96	7 (77%)
2	02J	F	1	2	8,8,9	1.99	2 (25%)	9,10,12	3.00	2 (22%)
2	PJE	F	5	2	11,13,14	2.89	3 (27%)	11,16,18	2.49	3 (27%)
2	PJE	G	5	2	11,13,14	2.23	3 (27%)	11,16,18	4.08	6 (54%)
2	PJE	H	5	2	11,13,14	3.31	4 (36%)	11,16,18	3.06	5 (45%)
2	02J	H	1	2	8,8,9	1.86	2 (25%)	9,10,12	2.86	2 (22%)
2	02J	G	1	2	8,8,9	2.15	2 (25%)	9,10,12	2.45	5 (55%)
2	PJE	E	5	2	11,13,14	4.61	6 (54%)	11,16,18	3.53	5 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	02J	E	1	2	-	1/1/2/4	0/1/1/1
2	02J	F	1	2	-	1/1/2/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PJE	F	5	2	-	3/7/18/19	0/1/1/1
2	PJE	G	5	2	-	3/7/18/19	0/1/1/1
2	PJE	H	5	2	-	3/7/18/19	0/1/1/1
2	02J	H	1	2	-	1/1/2/4	0/1/1/1
2	02J	G	1	2	-	0/1/2/4	0/1/1/1
2	PJE	E	5	2	-	3/7/18/19	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	PJE	C27-C28	9.45	1.66	1.53
2	E	5	PJE	C28-N6	8.35	1.63	1.46
2	H	5	PJE	C27-C28	8.27	1.65	1.53
2	F	5	PJE	C27-C28	6.68	1.62	1.53
2	G	5	PJE	C21-C20	6.07	1.55	1.33
2	E	5	PJE	C21-C20	5.84	1.55	1.33
2	E	5	PJE	C29-N6	5.37	1.39	1.33
2	H	5	PJE	C21-C20	5.12	1.52	1.33
2	F	5	PJE	C21-C20	5.03	1.52	1.33
2	F	1	02J	CA-N	4.54	1.38	1.31
2	E	1	02J	CA-N	4.54	1.38	1.31
2	H	1	02J	CA-N	4.37	1.38	1.31
2	G	1	02J	CA-N	4.11	1.37	1.31
2	H	5	PJE	C28-N6	3.89	1.54	1.46
2	G	1	02J	C4-C5	3.80	1.41	1.34
2	F	5	PJE	C29-N6	3.47	1.37	1.33
2	E	1	02J	C4-C5	3.45	1.41	1.34
2	E	1	02J	O1-N	2.48	1.46	1.42
2	E	5	PJE	C25-C26	2.40	1.59	1.53
2	F	1	02J	C4-C5	2.34	1.38	1.34
2	G	5	PJE	O8-C29	2.29	1.27	1.23
2	H	1	02J	C4-C5	2.20	1.38	1.34
2	E	1	02J	C-CA	2.16	1.53	1.45
2	E	5	PJE	C21-C	2.15	1.50	1.44
2	G	5	PJE	C21-C	2.15	1.50	1.44
2	H	5	PJE	C21-C	2.01	1.50	1.44

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	PJE	CA-C20-C21	-10.68	108.08	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	PJE	CA-C20-C21	-9.12	110.47	124.42
2	H	5	PJE	CA-C20-C21	-7.64	112.73	124.42
2	F	5	PJE	CA-C20-C21	-7.18	113.43	124.42
2	F	1	02J	O1-C5-C6	6.27	124.52	115.89
2	H	1	02J	O1-C5-C6	6.02	124.17	115.89
2	E	1	02J	O1-C5-C6	5.80	123.87	115.89
2	E	1	02J	C4-CA-N	-5.77	105.92	111.19
2	F	1	02J	C6-C5-C4	-5.65	124.28	134.05
2	G	5	PJE	O8-C29-C26	-5.41	119.96	126.21
2	H	1	02J	C6-C5-C4	-5.26	124.96	134.05
2	E	5	PJE	C28-C27-C26	4.81	112.79	105.69
2	E	1	02J	O1-N-CA	4.62	109.28	105.65
2	G	1	02J	O1-N-CA	4.59	109.26	105.65
2	E	1	02J	C-CA-N	4.50	126.78	118.78
2	E	1	02J	C6-C5-C4	-4.35	126.54	134.05
2	H	5	PJE	C28-C27-C26	-4.17	99.53	105.69
2	G	1	02J	C4-CA-N	-3.90	107.63	111.19
2	G	5	PJE	O8-C29-N6	3.73	130.98	125.76
2	E	5	PJE	C28-N6-C29	3.57	121.37	113.79
2	H	5	PJE	O8-C29-N6	3.11	130.12	125.76
2	H	5	PJE	O8-C29-C26	-3.02	122.72	126.21
2	G	5	PJE	C25-CA-C20	2.95	115.51	110.99
2	E	1	02J	CA-C4-C5	2.94	108.83	105.23
2	G	1	02J	C5-O1-N	-2.81	105.61	108.47
2	E	5	PJE	O-C-C21	-2.60	117.33	125.61
2	G	5	PJE	C27-C26-C29	2.40	106.17	102.87
2	G	5	PJE	O-C-C21	-2.39	117.98	125.61
2	H	5	PJE	O-C-C21	-2.26	118.39	125.61
2	F	5	PJE	O-C-C21	-2.14	118.78	125.61
2	E	1	02J	C5-O1-N	-2.11	106.32	108.47
2	G	1	02J	O1-C5-C4	2.11	112.25	109.88
2	E	5	PJE	O8-C29-N6	2.05	128.64	125.76
2	G	1	02J	C6-C5-C4	-2.03	130.54	134.05
2	F	5	PJE	C27-C26-C29	2.00	105.62	102.87

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	02J	O-C-CA-C4
2	F	1	02J	O-C-CA-C4
2	E	1	02J	O-C-CA-C4

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Mol	Chain	Res	Type	Atoms
2	H	5	PJE	O-C-C21-C20
2	F	5	PJE	O-C-C21-C20
2	E	5	PJE	O-C-C21-C20
2	G	5	PJE	O-C-C21-C20
2	H	5	PJE	CA-C20-C21-C
2	F	5	PJE	CA-C20-C21-C
2	E	5	PJE	CA-C20-C21-C
2	G	5	PJE	CA-C20-C21-C
2	H	5	PJE	C21-C20-CA-C25
2	F	5	PJE	C21-C20-CA-C25
2	E	5	PJE	C21-C20-CA-C25
2	G	5	PJE	C21-C20-CA-C25

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	02J	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/302 (99%)	0.12	6 (2%) 65 61	22, 36, 60, 82	0
1	B	301/302 (99%)	0.16	8 (2%) 56 51	21, 36, 60, 84	1 (0%)
1	C	298/302 (98%)	0.13	6 (2%) 65 61	19, 36, 61, 72	0
1	D	299/302 (99%)	0.16	10 (3%) 49 45	21, 36, 62, 72	0
2	E	3/6 (50%)	-0.23	0 100 100	27, 27, 28, 35	0
2	F	3/6 (50%)	-0.36	0 100 100	36, 36, 37, 42	0
2	G	3/6 (50%)	-0.04	0 100 100	26, 26, 27, 31	0
2	H	3/6 (50%)	-0.30	0 100 100	38, 38, 39, 42	0
All	All	1209/1232 (98%)	0.14	30 (2%) 58 54	19, 36, 61, 84	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	48	ASN	4.8
1	A	49	MET	4.6
1	D	25	MET	4.1
1	D	46	SER	3.8
1	C	25	MET	3.7
1	C	23	GLY	3.6
1	D	23	GLY	3.4
1	D	1	SER	3.4
1	A	300	VAL	3.3
1	B	300	VAL	3.2
1	B	49	MET	3.1
1	C	46	SER	3.0
1	B	46	SER	2.8
1	B	47	SER	2.8
1	A	-1	ALA	2.8
1	C	299	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	235	MET	2.6
1	A	45	SER	2.6
1	D	299	GLY	2.5
1	D	49	MET	2.5
1	C	49	MET	2.4
1	D	47	SER	2.4
1	B	193	LEU	2.2
1	C	48	ASN	2.2
1	B	50[A]	ASN	2.2
1	A	235	MET	2.2
1	D	271	MET	2.2
1	D	63	LEU	2.1
1	A	193	LEU	2.1
1	D	48	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	02J	E	1	8/9	0.85	0.15	51,55,58,59	0
2	02J	G	1	8/9	0.87	0.14	49,53,56,57	0
2	PJE	F	5	13/14	0.88	0.12	30,36,62,65	0
2	02J	H	1	8/9	0.89	0.14	46,57,60,61	0
2	PJE	E	5	13/14	0.89	0.14	30,37,50,52	0
2	02J	F	1	8/9	0.91	0.12	47,57,60,62	0
2	PJE	G	5	13/14	0.92	0.11	19,25,50,50	0
2	PJE	H	5	13/14	0.93	0.11	30,38,64,66	0

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.