



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 08:03 PM EST

PDB ID : 3D23  
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](mailto: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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

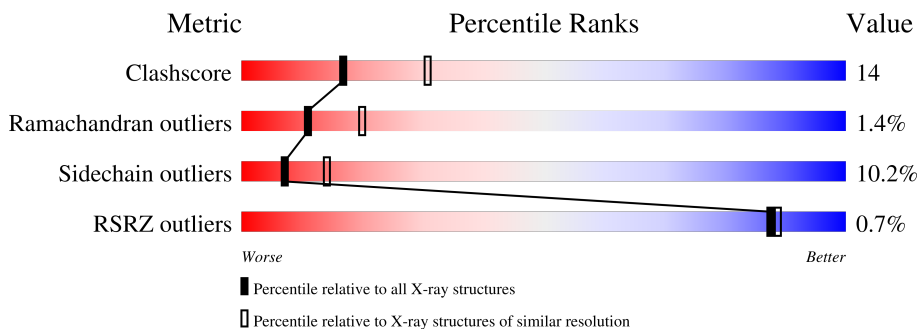
# 1 Overall quality at a glance i

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">73%      21%      5%</p>
1	B	302	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="text-align: center;">71%      23%      6%</p>
1	C	302	<div style="display: flex; align-items: center;"> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="text-align: center;">72%      23%</p>
1	D	302	<div style="display: flex; align-items: center;"> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="text-align: center;">75%      20%</p>
2	E	6	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="text-align: center;">33%      50%      17%</p>
2	F	6	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="text-align: center;">33%      50%      17%</p>
2	G	6	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="text-align: center;">33%      33%      33%</p>

Continued on next page...

*Continued from previous page...*

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

## 2 Entry composition i

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

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
			Total	C	N	O			
2	H	6	49	35	6	8	0	0	0
2	F	6	49	35	6	8	0	0	0
2	E	6	49	35	6	8	0	0	0

*Continued on next page...*

*Continued from previous page...*

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

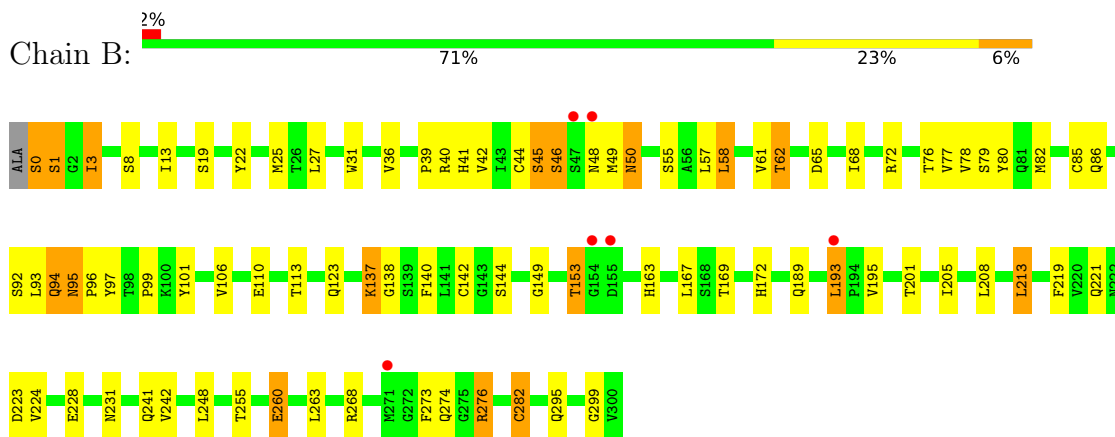
- Molecule 3 is water.

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		

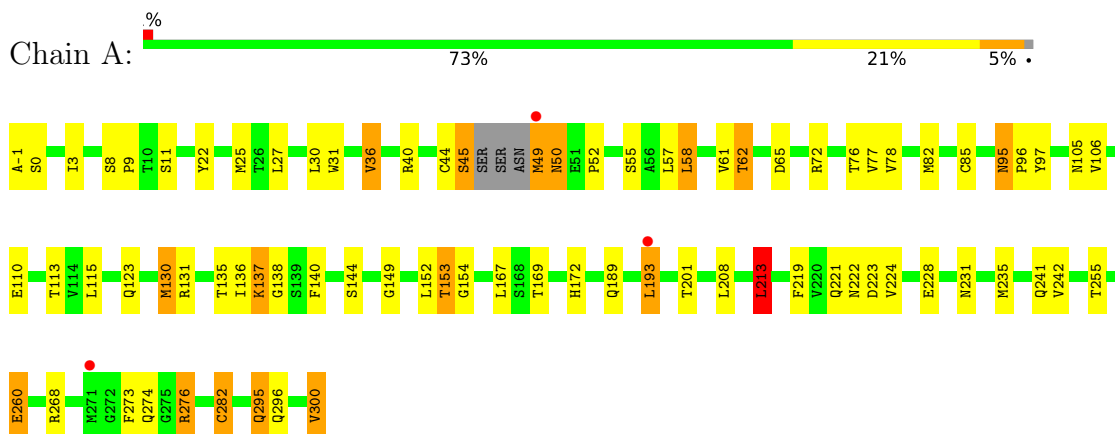
### 3 Residue-property plots [i](#)

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.

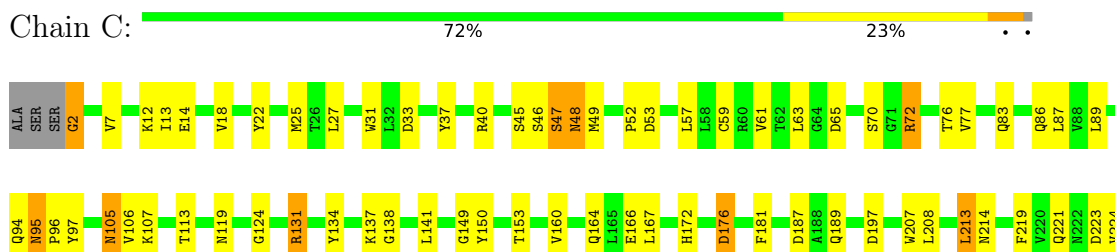
- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



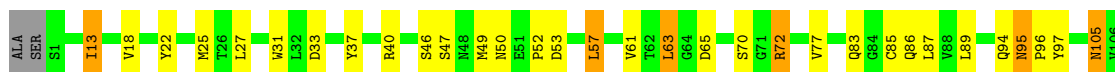
- Molecule 1: 3C-like proteinase





- Molecule 1: 3C-like proteinase

Chain D: 75% 20%



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

Chain H: 33% 50% 17%



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

Chain F: 33% 50% 17%



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

Chain E: 33% 50% 17%



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

Chain G: 33% 33% 33%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.77Å 91.77Å 187.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 41.04 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.50) 63.2 (41.04-1.97)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.77 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.229 , 0.285 0.211 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PJE, 010, 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	0.99	2/2338 (0.1%)	0.99	4/3181 (0.1%)
1	B	1.02	3/2363 (0.1%)	0.94	0/3216
1	C	1.07	6/2336 (0.3%)	1.01	7/3179 (0.2%)
1	D	1.03	0/2341	0.99	5/3185 (0.2%)
2	E	0.65	0/19	1.99	0/25
2	F	0.59	0/19	1.38	0/25
2	G	0.70	0/19	1.82	0/25
2	H	0.65	0/19	1.50	0/25
All	All	1.03	11/9454 (0.1%)	0.99	16/12861 (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	A	1	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	TYR	CD1-CE1	7.23	1.50	1.39
1	A	44	CYS	CB-SG	-6.63	1.71	1.82
1	C	166	GLU	CB-CG	6.38	1.64	1.52
1	B	44	CYS	CB-SG	-5.58	1.72	1.81
1	B	137	LYS	CE-NZ	5.56	1.62	1.49
1	B	142	CYS	CB-SG	-5.55	1.72	1.81
1	C	164	GLN	N-CA	5.48	1.57	1.46
1	C	181	PHE	CE2-CZ	5.29	1.47	1.37
1	C	59	CYS	CB-SG	-5.25	1.73	1.81
1	A	137	LYS	CD-CE	5.17	1.64	1.51

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	TYR	CD1-CE1	5.01	1.46	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLN	CB-CA-C	18.50	147.41	110.40
1	A	50	ASN	N-CA-C	6.52	128.60	111.00
1	D	268	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	164	GLN	N-CA-C	6.09	127.44	111.00
1	D	268	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	D	187	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	2	GLY	N-CA-C	-5.65	98.98	113.10
1	D	176	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	176	ASP	CB-CG-OD1	5.59	123.34	118.30
1	A	213	LEU	CB-CG-CD1	5.37	120.13	111.00
1	C	286	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	268	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	187	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	286	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	268	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	45	SER	N-CA-C	-5.12	97.19	111.00

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	68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2312	0	2269	75	0
1	C	2285	0	2242	68	0
1	D	2290	0	2246	58	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	261	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 14.

All (261) 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:130:MET:HE3	1:A:130:MET:HA	1.46	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: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

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:58:LEU:HG	1:B:82:MET:HE3	1.68	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: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: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:A:228:GLU:CD	1:A:228:GLU:H	1.99	0.65
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:58:LEU:HG	1:A:82:MET:HE3	1.79	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:228:GLU:H	1:B:228:GLU:CD	2.03	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: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: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: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:58:LEU:HG	1:B:82:MET:CE	2.37	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:95:ASN:C	1:A:95:ASN:HD22	2.12	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:A:130:MET:HE2	1:A:135:THR:O	2.08	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:95:ASN:C	1:B:95:ASN:HD22	2.14	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:130:MET:CE	1:A:136:ILE:HG23	2.42	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:72:ARG:HH11	1:D:72:ARG:HB3	1.76	0.48
1:A:130:MET:HE3	1:A:136:ILE:HG23	1.95	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: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: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: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: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
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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:50[A]:ASN:ND2	3:B:455:HOH:O	2.50	0.44
1:C:12:LYS:C	1:C:13:ILE:HD12	2.37	0.44
1:B:40:ARG:C	1:B:42:VAL:N	2.71	0.43
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:B:40:ARG:C	1:B:42:VAL:H	2.22	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: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:D:231:ASN:HB3	1:D:241:GLN:HE22	1.83	0.43
1:A:95:ASN:ND2	1:A:95:ASN:C	2.70	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: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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:MET:HE3	1:B:82:MET:HB2	1.87	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:95:ASN:ND2	1:B:95:ASN:C	2.73	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:A:82:MET:HE3	1:A:82:MET:HB2	1.90	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: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: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%)	15	28
1	B	300/302 (99%)	276 (92%)	15 (5%)	9 (3%)	4	6
1	C	296/302 (98%)	272 (92%)	22 (7%)	2 (1%)	22	39
1	D	297/302 (98%)	272 (92%)	21 (7%)	4 (1%)	12	21
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%)	11	18

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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	232	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/258 (98%)	226 (89%)	28 (11%)	6	12
1	B	259/258 (100%)	232 (90%)	27 (10%)	7	13
1	C	255/258 (99%)	232 (91%)	23 (9%)	9	19
1	D	255/258 (99%)	232 (91%)	23 (9%)	9	19
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%)	1 (50%)	1 (50%)	0	0
2	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	1031/1040 (99%)	926 (90%)	105 (10%)	7	14

All (105) 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
1	B	55	SER
1	B	57	LEU
1	B	58	LEU
1	B	62	THR
1	B	72	ARG
1	B	77	VAL
1	B	78	VAL
1	B	86	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	94	GLN
1	B	95	ASN
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	27	LEU
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	95	ASN
1	A	105	ASN
1	A	115	LEU
1	A	123	GLN
1	A	130	MET
1	A	137	LYS
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	27	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	95	ASN
1	C	105	ASN
1	C	106	VAL
1	C	107	LYS
1	C	119	ASN
1	C	131	ARG
1	C	153	THR
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	57	LEU
1	D	63	LEU
1	D	72	ARG
1	D	77	VAL
1	D	89	LEU
1	D	95	ASN
1	D	105	ASN
1	D	107	LYS
1	D	119	ASN
1	D	131	ARG
1	D	153	THR
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	ASN
1	B	86	GLN
1	B	94	GLN
1	B	95	ASN
1	B	123	GLN
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
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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	C	105	ASN
1	C	172	HIS
1	C	189	GLN
1	C	214	ASN
1	C	221	GLN
1	C	222	ASN
1	C	231	ASN
1	C	241	GLN
1	C	277	GLN
1	D	41	HIS
1	D	50	ASN
1	D	95	ASN
1	D	105	ASN
1	D	163	HIS
1	D	172	HIS
1	D	189	GLN
1	D	214	ASN
1	D	221	GLN
1	D	222	ASN
1	D	231	ASN
1	D	241	GLN
1	D	277	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	G	1	2	6,8,9	1.91	3 (50%)	4,10,12	0.94	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PJE	E	5	2	12,13,14	4.37	7 (58%)	12,16,18	4.46	6 (50%)
2	02J	F	1	2	6,8,9	1.54	2 (33%)	4,10,12	2.39	1 (25%)
2	PJE	G	5	2	12,13,14	2.36	5 (41%)	12,16,18	4.03	5 (41%)
2	PJE	H	5	2	12,13,14	3.08	4 (33%)	12,16,18	3.54	6 (50%)
2	PJE	F	5	2	12,13,14	2.67	3 (25%)	12,16,18	2.60	3 (25%)
2	02J	E	1	2	6,8,9	2.87	3 (50%)	4,10,12	1.88	2 (50%)
2	02J	H	1	2	6,8,9	1.51	2 (33%)	4,10,12	2.74	1 (25%)

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	G	1	2	-	0/0/2/4	0/1/1/1
2	PJE	E	5	2	-	3/7/18/19	0/1/1/1
2	02J	F	1	2	-	0/0/2/4	0/1/1/1
2	PJE	G	5	2	-	3/7/18/19	0/1/1/1
2	PJE	H	5	2	-	5/7/18/19	0/1/1/1
2	PJE	F	5	2	-	3/7/18/19	0/1/1/1
2	02J	E	1	2	-	0/0/2/4	0/1/1/1
2	02J	H	1	2	-	0/0/2/4	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	PJE	C27-C28	8.89	1.66	1.53
2	E	5	PJE	C28-N6	8.36	1.63	1.46
2	H	5	PJE	C27-C28	7.79	1.65	1.53
2	F	5	PJE	C27-C28	6.29	1.62	1.53
2	G	5	PJE	C21-C20	5.64	1.55	1.33
2	E	5	PJE	C21-C20	5.42	1.55	1.33
2	E	5	PJE	C29-N6	5.29	1.39	1.33
2	H	5	PJE	C21-C20	4.75	1.52	1.33
2	F	5	PJE	C21-C20	4.67	1.52	1.33
2	E	1	02J	CA-C	4.62	1.53	1.48
2	E	1	02J	C6-C5	4.20	1.53	1.48
2	G	5	PJE	CA-C20	3.89	1.55	1.50
2	H	5	PJE	C28-N6	3.88	1.54	1.46
2	E	5	PJE	CA-C20	3.46	1.54	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	PJE	C29-N6	3.40	1.37	1.33
2	F	1	02J	CA-N	2.69	1.38	1.33
2	E	1	02J	CA-N	2.68	1.38	1.33
2	G	1	02J	CA-C	2.62	1.51	1.48
2	H	1	02J	CA-N	2.55	1.38	1.33
2	G	1	02J	CA-N	2.35	1.37	1.33
2	F	1	02J	C6-C5	2.32	1.51	1.48
2	H	1	02J	C6-C5	2.31	1.51	1.48
2	E	5	PJE	C25-C26	2.30	1.59	1.53
2	G	1	02J	C6-C5	2.29	1.51	1.48
2	H	5	PJE	CA-C20	2.22	1.53	1.50
2	G	5	PJE	O8-C29	2.22	1.27	1.23
2	E	5	PJE	C21-C	2.05	1.50	1.44
2	G	5	PJE	C21-C	2.05	1.50	1.44
2	G	5	PJE	C26-C29	-2.04	1.49	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	PJE	CA-C20-C21	-11.43	108.08	124.41
2	E	5	PJE	CA-C20-C21	-9.75	110.47	124.41
2	E	5	PJE	C27-C28-N6	-9.57	89.40	103.43
2	H	5	PJE	CA-C20-C21	-8.17	112.73	124.41
2	F	5	PJE	CA-C20-C21	-7.68	113.43	124.41
2	H	5	PJE	C27-C28-N6	-6.46	93.96	103.43
2	G	5	PJE	O8-C29-C26	-5.34	119.96	126.23
2	H	1	02J	O-C-CA	-4.99	119.50	124.22
2	E	5	PJE	C28-C27-C26	4.34	112.79	105.75
2	F	1	02J	O-C-CA	-4.04	120.40	124.22
2	G	5	PJE	O8-C29-N6	3.92	130.98	125.54
2	H	5	PJE	C28-C27-C26	-3.84	99.53	105.75
2	E	5	PJE	C28-N6-C29	3.83	121.37	113.84
2	H	5	PJE	O8-C29-N6	3.30	130.12	125.54
2	H	5	PJE	O8-C29-C26	-2.99	122.72	126.23
2	G	5	PJE	C27-C26-C29	2.53	106.17	102.88
2	E	5	PJE	O-C-C21	-2.44	117.33	125.67
2	G	5	PJE	O-C-C21	-2.25	117.98	125.67
2	E	5	PJE	O8-C29-N6	2.23	128.64	125.54
2	E	1	02J	C4-CA-N	-2.22	105.92	109.94
2	E	1	02J	CA-C4-C5	2.16	108.83	106.06
2	H	5	PJE	O-C-C21	-2.13	118.39	125.67
2	F	5	PJE	C27-C26-C29	2.11	105.62	102.88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	PJE	O-C-C21	-2.02	118.78	125.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

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	C26-C25-CA-C20
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
2	H	5	PJE	C26-C25-CA-N

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 monosaccharides 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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	299/302 (99%)	-0.40	3 (1%) 82 84	22, 36, 60, 82	0
1	B	301/302 (99%)	-0.37	6 (1%) 65 68	21, 36, 61, 84	0
1	C	298/302 (98%)	-0.56	0 100 100	19, 36, 61, 72	0
1	D	299/302 (99%)	-0.56	0 100 100	21, 36, 62, 72	0
2	E	3/6 (50%)	-0.37	0 100 100	27, 27, 28, 35	0
2	F	3/6 (50%)	-0.98	0 100 100	36, 36, 37, 42	0
2	G	3/6 (50%)	-0.61	0 100 100	26, 26, 27, 31	0
2	H	3/6 (50%)	-0.79	0 100 100	38, 38, 39, 42	0
All	All	1209/1232 (98%)	-0.47	9 (0%) 87 89	19, 36, 61, 84	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	SER	3.8
1	A	271	MET	3.6
1	B	48	ASN	3.2
1	B	155	ASP	2.7
1	B	271	MET	2.6
1	A	193	LEU	2.5
1	A	49	MET	2.4
1	B	193	LEU	2.1
1	B	154	GLY	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, 95<sup>th</sup> 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	02J	F	1	8/9	0.89	0.23	47,57,60,62	0
2	02J	E	1	8/9	0.89	0.18	51,55,58,59	0
2	02J	G	1	8/9	0.89	0.16	49,53,56,57	0
2	02J	H	1	8/9	0.90	0.22	46,57,60,61	0
2	PJE	E	5	13/14	0.91	0.24	30,37,50,52	0
2	PJE	G	5	13/14	0.91	0.19	19,25,50,50	0
2	PJE	H	5	13/14	0.92	0.14	30,38,64,66	0
2	PJE	F	5	13/14	0.92	0.12	30,36,62,65	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.