



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 01:33 AM EDT

PDB ID : 1JC1  
Title : CRYSTAL STRUCTURE ANALYSIS OF A REDOX-SENSITIVE GREEN FLUORESCENT PROTEIN VARIANT IN A OXIDIZED FORM  
Authors : Hanson, G.T.; Aggeler, R.; Oglesbee, D.; Cannon, M.; Capaldi, R.A.; Tsien, R.Y.; Remington, S.J.  
Deposited on : 2001-06-07  
Resolution : 1.90 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>.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

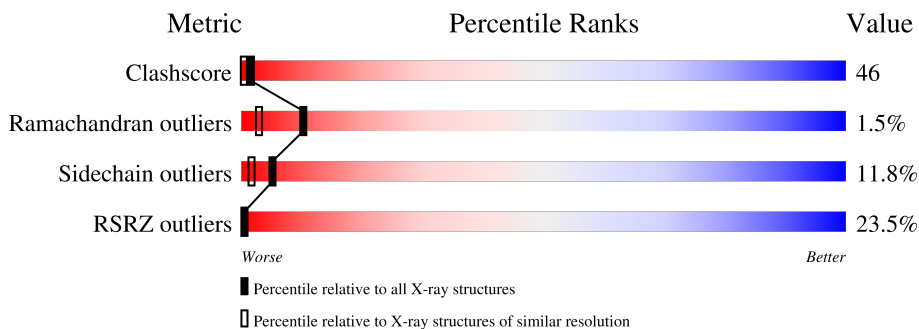
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	236	
1	B	236	
1	C	236	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5394 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 GREEN FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	Total 1782	C 1133	N 298	O 343	S 8	0	0	0
1	B	226	Total 1760	C 1119	N 293	O 340	S 8	0	0	0
1	C	226	Total 1678	C 1067	N 276	O 328	S 7	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	SER	CYS	engineered mutation	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	147	CYS	SER	engineered mutation	UNP P42212
A	204	CYS	GLN	engineered mutation	UNP P42212
B	48	SER	CYS	engineered mutation	UNP P42212
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	CRO	SER	chromophore	UNP P42212
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
B	147	CYS	SER	engineered mutation	UNP P42212
B	204	CYS	GLN	engineered mutation	UNP P42212
C	48	SER	CYS	engineered mutation	UNP P42212
C	64	LEU	PHE	engineered mutation	UNP P42212
C	66	CRO	SER	chromophore	UNP P42212
C	66	CRO	TYR	chromophore	UNP P42212
C	66	CRO	GLY	chromophore	UNP P42212
C	80	ARG	GLN	engineered mutation	UNP P42212
C	147	CYS	SER	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	204	CYS	GLN	engineered mutation	UNP P42212

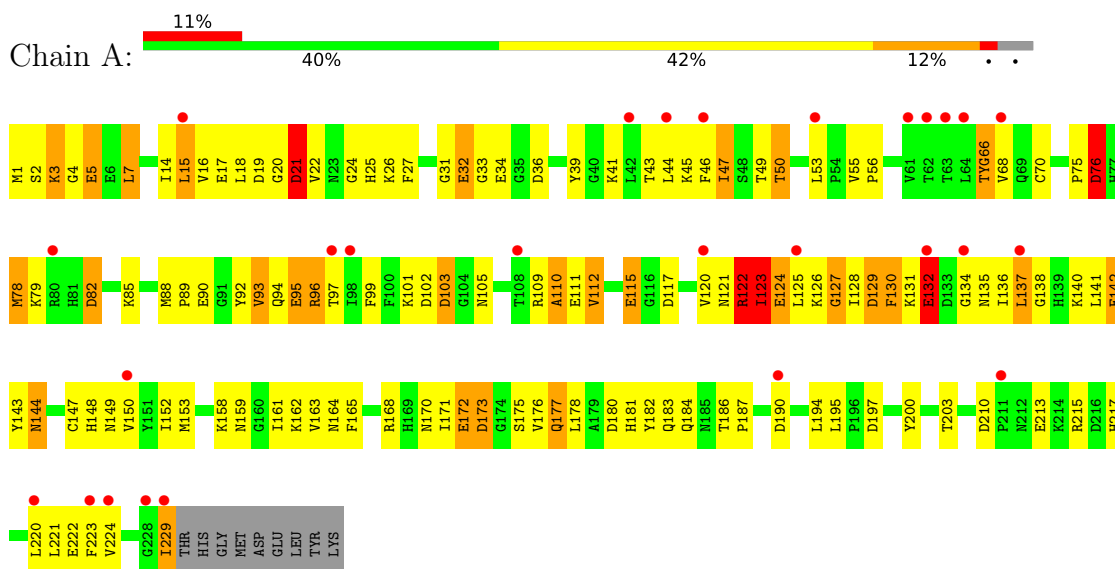
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	93	Total O 93 93	0	0
2	B	58	Total O 58 58	0	0
2	C	23	Total O 23 23	0	0

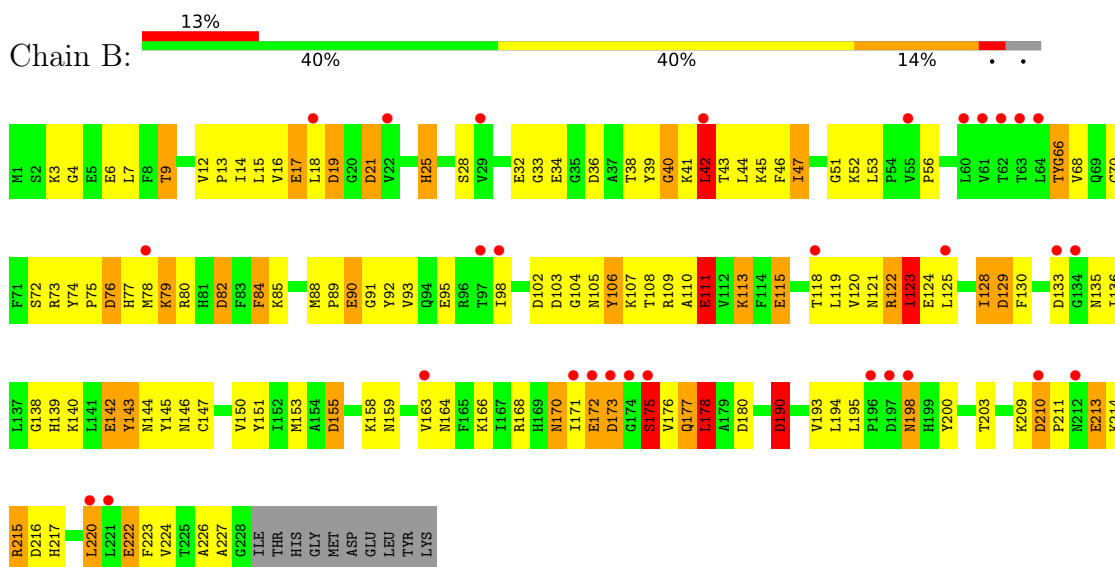
### 3 Residue-property plots [i](#)

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: GREEN FLUORESCENT PROTEIN



- Molecule 1: GREEN FLUORESCENT PROTEIN



- Molecule 1: GREEN FLUORESCENT PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.84Å 67.61Å 56.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.71 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.90) 99.7 (29.71-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 1.91Å)	Xtrriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.229 , (Not available) 0.241 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtrriage
Anisotropy	0.378	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 125.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5394	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CRO

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	1.38	14/1800 (0.8%)	1.78	39/2437 (1.6%)
1	B	1.28	13/1778 (0.7%)	1.82	42/2411 (1.7%)
1	C	1.26	11/1695 (0.6%)	1.81	39/2303 (1.7%)
All	All	1.31	38/5273 (0.7%)	1.80	120/7151 (1.7%)

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	3	0
1	B	4	2
1	C	8	0
All	All	15	2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLU	CD-OE2	11.45	1.38	1.25
1	B	222	GLU	CD-OE2	8.48	1.34	1.25
1	A	132	GLU	CD-OE2	8.05	1.34	1.25
1	C	213	GLU	CD-OE2	8.02	1.34	1.25
1	A	115	GLU	CD-OE2	7.89	1.34	1.25
1	B	142	GLU	CD-OE2	7.60	1.34	1.25
1	A	17	GLU	CD-OE2	7.59	1.33	1.25
1	C	5	GLU	CD-OE2	7.43	1.33	1.25
1	C	115	GLU	CD-OE2	7.42	1.33	1.25
1	A	5	GLU	CD-OE2	7.34	1.33	1.25
1	A	95	GLU	CD-OE2	7.32	1.33	1.25
1	B	172	GLU	CD-OE2	7.25	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	GLU	CD-OE2	7.01	1.33	1.25
1	B	34	GLU	CD-OE2	6.90	1.33	1.25
1	C	6	GLU	CD-OE2	6.84	1.33	1.25
1	B	32	GLU	CD-OE2	6.78	1.33	1.25
1	C	222	GLU	CD-OE2	6.54	1.32	1.25
1	C	142	GLU	CD-OE2	6.51	1.32	1.25
1	B	17	GLU	CD-OE2	6.46	1.32	1.25
1	A	111	GLU	CD-OE2	6.32	1.32	1.25
1	A	24	GLY	CA-C	-5.87	1.42	1.51
1	C	95	GLU	CD-OE2	5.85	1.32	1.25
1	B	111	GLU	CD-OE2	5.83	1.32	1.25
1	A	3	LYS	C-N	5.83	1.43	1.33
1	B	115	GLU	CD-OE2	5.82	1.32	1.25
1	C	17	GLU	CD-OE2	5.81	1.32	1.25
1	A	124	GLU	CD-OE2	5.54	1.31	1.25
1	B	6	GLU	CD-OE2	5.52	1.31	1.25
1	B	90	GLU	CD-OE2	5.44	1.31	1.25
1	B	95	GLU	CD-OE2	5.42	1.31	1.25
1	C	111	GLU	CD-OE1	-5.37	1.19	1.25
1	B	40	GLY	CA-C	5.34	1.60	1.51
1	A	34	GLU	CD-OE2	5.30	1.31	1.25
1	C	168	ARG	CZ-NH1	5.28	1.40	1.33
1	C	34	GLU	CD-OE2	5.08	1.31	1.25
1	A	142	GLU	CD-OE2	5.08	1.31	1.25
1	A	127	GLY	CA-C	5.05	1.59	1.51
1	B	53	LEU	C-N	-5.03	1.24	1.34

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	ASP	CB-CG-OD2	-11.19	108.23	118.30
1	B	180	ASP	CB-CG-OD2	-10.87	108.52	118.30
1	A	36	ASP	CB-CG-OD1	10.24	127.52	118.30
1	C	180	ASP	CB-CG-OD2	-10.22	109.10	118.30
1	A	180	ASP	CB-CG-OD2	-9.60	109.66	118.30
1	C	216	ASP	CB-CG-OD1	9.46	126.82	118.30
1	B	21	ASP	CB-CG-OD1	9.42	126.78	118.30
1	A	21	ASP	CB-CG-OD1	9.37	126.73	118.30
1	C	82	ASP	CB-CG-OD2	-9.30	109.93	118.30
1	B	216	ASP	CB-CG-OD2	-9.19	110.03	118.30
1	A	102	ASP	CB-CG-OD1	8.97	126.37	118.30
1	A	190	ASP	CB-CG-OD2	-8.83	110.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	B	155	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	C	216	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	C	19	ASP	CB-CG-OD1	8.43	125.89	118.30
1	C	82	ASP	CB-CG-OD1	8.41	125.87	118.30
1	B	216	ASP	CB-CG-OD1	8.31	125.78	118.30
1	C	19	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	B	129	ASP	CB-CG-OD1	8.07	125.56	118.30
1	B	129	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	102	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	C	210	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	A	190	ASP	CB-CG-OD1	7.76	125.28	118.30
1	B	92	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	B	168	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	C	210	ASP	CB-CG-OD1	7.72	125.25	118.30
1	B	102	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	A	210	ASP	CB-CG-OD1	7.58	125.12	118.30
1	A	76	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	B	36	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	B	36	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	103	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	36	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	A	173	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	C	102	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	B	190	ASP	CB-CG-OD2	-7.29	111.73	118.30
1	C	168	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	9	THR	CA-CB-CG2	-7.21	102.31	112.40
1	A	168	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	21	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	C	36	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	B	82	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	C	191	GLY	C-N-CD	-7.07	105.04	120.60
1	A	129	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	C	173	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	180	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	180	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	103	ASP	CB-CG-OD1	6.97	124.57	118.30
1	B	76	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	B	213	GLU	N-CA-CB	6.91	123.04	110.60
1	B	180	ASP	CB-CG-OD1	6.85	124.47	118.30
1	C	76	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	B	111	GLU	N-CA-CB	6.82	122.88	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	B	210	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	82	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	173	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	129	ASP	CB-CG-OD1	6.61	124.25	118.30
1	B	122	ARG	CB-CA-C	6.53	123.46	110.40
1	C	168	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	103	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	A	76	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	129	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	197	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	143	TYR	CB-CG-CD1	6.27	124.76	121.00
1	A	50	THR	CA-CB-CG2	-6.24	103.66	112.40
1	B	222	GLU	CG-CD-OE2	-6.21	105.88	118.30
1	C	2	SER	N-CA-C	6.19	127.72	111.00
1	B	222	GLU	OE1-CD-OE2	6.17	130.70	123.30
1	B	19	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	96	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	76	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	130	PHE	CA-CB-CG	-5.99	99.52	113.90
1	A	122	ARG	N-CA-CB	5.95	121.31	110.60
1	B	84	PHE	N-CA-CB	5.88	121.18	110.60
1	C	173	ASP	CB-CG-OD1	5.87	123.59	118.30
1	B	42	LEU	CB-CA-C	-5.86	99.06	110.20
1	C	95	GLU	CB-CA-C	5.84	122.09	110.40
1	A	93	VAL	CA-CB-CG1	-5.78	102.23	110.90
1	B	178	LEU	CA-CB-CG	-5.76	102.06	115.30
1	C	102	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	143	TYR	CB-CG-CD2	5.67	124.40	121.00
1	B	222	GLU	CB-CA-C	-5.64	99.12	110.40
1	B	175	SER	N-CA-CB	5.60	118.90	110.50
1	B	133	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	179	ALA	CB-CA-C	5.55	118.42	110.10
1	A	117	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	B	173	ASP	CB-CA-C	-5.49	99.42	110.40
1	B	106	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	B	107	LYS	N-CA-CB	5.44	120.40	110.60
1	A	210	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	161	ILE	N-CA-CB	-5.41	98.37	110.80
1	A	68	VAL	CA-CB-CG1	-5.37	102.84	110.90
1	B	123	ILE	CB-CA-C	-5.36	100.87	111.60
1	C	155	ASP	CB-CG-OD2	-5.36	113.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	GLU	N-CA-CB	5.35	120.23	110.60
1	C	106	TYR	CB-CA-C	-5.34	99.72	110.40
1	C	158	LYS	C-N-CA	-5.33	108.39	121.70
1	C	179	ALA	N-CA-CB	5.30	117.52	110.10
1	C	11	VAL	CA-CB-CG2	-5.30	102.95	110.90
1	C	225	THR	N-CA-CB	5.26	120.30	110.30
1	A	82	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	21	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	128	ILE	CB-CA-C	-5.25	101.09	111.60
1	B	210	ASP	C-N-CD	-5.25	109.06	120.60
1	A	110	ALA	O-C-N	5.19	131.00	122.70
1	A	49	THR	CA-CB-CG2	-5.14	105.20	112.40
1	C	93	VAL	CA-CB-CG1	-5.09	103.27	110.90
1	A	123	ILE	CB-CA-C	-5.08	101.44	111.60
1	C	21	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	39	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	C	95	GLU	N-CA-CB	5.05	119.70	110.60
1	A	176	VAL	CB-CA-C	-5.04	101.83	111.40
1	C	114	PHE	CB-CA-C	-5.04	100.33	110.40
1	A	117	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	39	TYR	CA-CB-CG	-5.02	103.86	113.40
1	B	102	ASP	N-CA-CB	5.02	119.64	110.60
1	A	122	ARG	CB-CA-C	5.00	120.41	110.40
1	B	106	TYR	CB-CG-CD1	5.00	124.00	121.00

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	9	THR	CB
1	A	15	LEU	CA
1	A	229	ILE	CB
1	B	9	THR	CB
1	B	128	ILE	CB
1	B	155	ASP	CA
1	B	213	GLU	CA
1	C	46	PHE	CA
1	C	79	LYS	CA
1	C	95	GLU	CA
1	C	122	ARG	CA
1	C	159	ASN	CA
1	C	161	ILE	CB
1	C	198	ASN	CA

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Mol	Chain	Res	Type	Atom
1	C	213	GLU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	190	ASP	Sidechain
1	B	198	ASN	Sidechain

## 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	1782	0	1685	112	0
1	B	1760	0	1647	127	0
1	C	1678	0	1488	223	0
2	A	93	0	0	4	1
2	B	58	0	0	8	0
2	C	23	0	0	1	0
All	All	5394	0	4820	460	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (460) 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:C:96:ARG:HG3	1:C:183:GLN:HB2	1.31	1.10
1:B:42:LEU:HD12	1:B:222:GLU:HB3	1.33	1.10
1:B:171:ILE:HD11	1:B:177:GLN:HB2	1.30	1.09
1:C:18:LEU:HD12	1:C:123:ILE:HB	1.33	1.08
1:C:13:PRO:HG2	1:C:118:THR:HA	1.39	1.04
1:B:203:THR:HG23	1:B:224:VAL:HG22	1.42	1.01
1:C:16:VAL:HG13	1:C:121:ASN:HB3	1.42	0.99
1:C:152:ILE:HD11	1:C:201:LEU:HG	1.46	0.98
1:B:47:ILE:HD11	1:B:213:GLU:HG2	1.47	0.97
1:C:8:PHE:CE2	1:C:85:LYS:HG2	2.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ILE:HD11	1:C:177:GLN:HB3	1.52	0.91
1:C:20:GLY:HA3	1:C:27:PHE:CE2	2.05	0.91
1:C:48:SER:HB2	1:C:216:ASP:HB3	1.53	0.91
1:A:75:PRO:HG2	1:A:78:MET:HG3	1.51	0.90
1:B:203:THR:HG23	1:B:224:VAL:CG2	2.02	0.89
1:B:171:ILE:HD11	1:B:177:GLN:CB	2.03	0.88
1:C:161:ILE:CG1	1:C:185:ASN:HB2	2.02	0.88
1:C:41:LYS:HD3	1:C:223:PHE:CE1	2.09	0.87
1:C:41:LYS:HB2	1:C:223:PHE:CE1	2.10	0.87
1:C:130:PHE:HB2	1:C:137:LEU:HD11	1.59	0.84
1:C:93:VAL:HG13	1:C:110:ALA:O	1.77	0.84
1:B:135:ASN:HA	1:B:140:LYS:HG3	1.57	0.84
1:C:96:ARG:CG	1:C:183:GLN:HB2	2.07	0.84
1:A:21:ASP:HB2	1:A:26:LYS:HG2	1.58	0.83
1:A:130:PHE:CB	1:A:137:LEU:HD11	2.09	0.82
1:B:18:LEU:HD12	1:B:19:ASP:N	1.95	0.82
1:B:142:GLU:HG3	1:B:144:ASN:HD21	1.44	0.82
1:B:166:LYS:CG	1:B:178:LEU:HD23	2.11	0.81
1:B:170:ASN:ND2	1:B:170:ASN:H	1.78	0.81
1:C:30:SER:O	1:C:46:PHE:HB3	1.81	0.81
1:C:93:VAL:CG2	1:C:111:GLU:HG2	2.11	0.81
1:A:115:GLU:OE2	1:A:120:VAL:HG11	1.81	0.80
1:B:41:LYS:HE3	1:C:204:CYS:HB3	1.63	0.80
1:A:43:THR:HG22	1:A:221:LEU:CD1	2.13	0.78
1:C:154:ALA:HB2	1:C:196:PRO:HD2	1.64	0.78
1:B:193:VAL:HG23	1:B:195:LEU:HD21	1.65	0.77
1:C:8:PHE:CD2	1:C:85:LYS:HG2	2.20	0.76
1:A:4:GLY:O	1:A:7:LEU:HB2	1.85	0.76
1:A:132:GLU:HA	1:A:137:LEU:HD13	1.65	0.76
1:A:130:PHE:HB3	1:A:137:LEU:HD11	1.69	0.75
1:C:81:HIS:HD2	1:C:229:ILE:HD13	1.52	0.75
1:A:2:SER:O	1:A:5:GLU:HB3	1.86	0.74
1:A:15:LEU:HB2	1:A:31:GLY:O	1.87	0.74
1:B:38:THR:O	1:B:73:ARG:HD2	1.86	0.74
1:B:41:LYS:HG3	1:B:223:PHE:CE1	2.21	0.74
1:C:31:GLY:HA2	1:C:45:LYS:O	1.87	0.74
1:A:70:CYS:O	1:A:85:LYS:HE3	1.88	0.74
1:B:25:HIS:ND1	1:B:25:HIS:N	2.32	0.73
1:A:43:THR:HG22	1:A:221:LEU:HD12	1.69	0.72
1:C:22:VAL:HG13	1:C:127:GLY:HA3	1.71	0.72
1:C:103:ASP:OD1	1:C:104:GLY:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:THR:HG22	2:B:287:HOH:O	1.88	0.72
1:B:210:ASP:OD1	1:B:211:PRO:HD2	1.89	0.72
1:A:41:LYS:HG3	1:A:223:PHE:CE1	2.24	0.72
1:C:88:MET:HE1	1:C:112:VAL:O	1.90	0.71
1:C:4:GLY:O	1:C:5:GLU:C	2.27	0.71
1:C:110:ALA:HB2	1:C:123:ILE:HG23	1.71	0.71
1:A:95:GLU:HG2	1:A:109:ARG:HB2	1.73	0.71
1:C:97:THR:HG23	1:C:182:TYR:HB2	1.73	0.70
1:C:88:MET:HB3	1:C:89:PRO:HA	1.73	0.70
1:C:161:ILE:HG12	1:C:185:ASN:HB2	1.74	0.70
1:A:140:LYS:O	1:A:172:GLU:HG3	1.91	0.70
1:B:47:ILE:HD12	1:B:217:HIS:HB2	1.74	0.70
1:A:66:CRO:N2	1:A:66:CRO:HG12	2.05	0.70
1:B:153:MET:HE2	2:B:258:HOH:O	1.90	0.70
1:C:95:GLU:OE2	1:C:184:GLN:HB3	1.92	0.69
1:C:12:VAL:HG13	1:C:13:PRO:HD2	1.74	0.69
1:C:93:VAL:HG22	1:C:111:GLU:HG2	1.73	0.69
1:C:199:HIS:HB3	1:C:229:ILE:CD1	2.23	0.69
1:C:153:MET:HB2	1:C:198:ASN:OD1	1.93	0.69
1:A:153:MET:HE2	1:A:162:LYS:HE2	1.75	0.69
1:B:213:GLU:OE2	1:B:215:ARG:HD2	1.93	0.69
1:B:13:PRO:O	1:B:118:THR:HG23	1.94	0.68
1:C:194:LEU:N	1:C:194:LEU:HD23	2.09	0.68
1:A:171:ILE:HD12	1:A:171:ILE:N	2.07	0.68
1:A:172:GLU:HG2	2:A:253:HOH:O	1.93	0.68
1:A:142:GLU:HG2	2:A:253:HOH:O	1.93	0.67
1:B:173:ASP:CG	1:B:175:SER:H	1.97	0.67
1:C:199:HIS:HB3	1:C:229:ILE:HD12	1.76	0.67
1:C:210:ASP:H	1:C:217:HIS:CD2	2.11	0.67
1:B:135:ASN:ND2	1:B:171:ILE:HD12	2.10	0.66
1:B:210:ASP:O	1:B:213:GLU:N	2.28	0.66
1:C:153:MET:O	1:C:162:LYS:N	2.25	0.66
1:C:108:THR:CG2	1:C:125:LEU:HD12	2.26	0.66
1:A:149:ASN:HB3	1:A:200:TYR:CD1	2.31	0.66
1:A:153:MET:CE	1:A:162:LYS:HE2	2.25	0.66
1:C:128:ILE:HD12	1:C:128:ILE:O	1.95	0.66
1:B:142:GLU:HG3	1:B:144:ASN:ND2	2.12	0.65
1:C:213:GLU:OE2	1:C:215:ARG:N	2.30	0.65
1:A:131:LYS:C	1:A:137:LEU:HD12	2.17	0.65
1:B:103:ASP:OD1	1:B:104:GLY:N	2.29	0.65
1:A:21:ASP:HB2	1:A:26:LYS:CG	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:THR:O	1:C:44:LEU:HG	1.97	0.64
1:C:91:GLY:HA3	1:C:112:VAL:O	1.96	0.64
1:B:110:ALA:HB2	1:B:123:ILE:HG23	1.80	0.64
1:A:161:ILE:O	1:A:184:GLN:NE2	2.30	0.64
1:C:141:LEU:N	1:C:141:LEU:HD23	2.13	0.64
1:C:41:LYS:HD3	1:C:223:PHE:HE1	1.62	0.64
1:B:173:ASP:OD1	1:B:175:SER:N	2.26	0.64
1:C:130:PHE:HB2	1:C:137:LEU:CD1	2.27	0.63
1:C:88:MET:CE	1:C:91:GLY:HA2	2.28	0.63
1:B:41:LYS:HE2	1:B:223:PHE:CZ	2.34	0.63
1:C:4:GLY:O	1:C:7:LEU:N	2.29	0.63
1:B:40:GLY:O	1:B:223:PHE:HA	1.99	0.63
1:B:140:LYS:O	1:B:172:GLU:HG3	1.99	0.62
1:C:77:HIS:CE1	1:C:78:MET:HG3	2.35	0.62
1:B:47:ILE:HD12	1:B:217:HIS:CB	2.29	0.62
1:B:143:TYR:CZ	1:B:209:LYS:HE2	2.34	0.62
1:C:22:VAL:HA	1:C:127:GLY:O	2.00	0.62
1:C:99:PHE:HE1	1:C:182:TYR:CE2	2.17	0.62
1:C:131:LYS:O	1:C:137:LEU:HD12	1.99	0.62
1:A:103:ASP:OD1	1:A:131:LYS:N	2.29	0.62
1:C:48:SER:HB2	1:C:216:ASP:CB	2.29	0.61
1:C:152:ILE:HD11	1:C:201:LEU:CG	2.25	0.61
1:B:193:VAL:HG23	1:B:195:LEU:CD2	2.29	0.61
1:C:173:ASP:OD1	1:C:175:SER:N	2.33	0.61
1:B:66:CRO:HG12	1:B:66:CRO:N2	2.15	0.61
1:C:199:HIS:CB	1:C:229:ILE:HD12	2.29	0.61
1:B:128:ILE:HG22	1:B:129:ASP:N	2.15	0.61
1:B:47:ILE:HD11	1:B:213:GLU:CG	2.28	0.61
1:B:143:TYR:CE2	1:B:209:LYS:HE2	2.35	0.61
1:A:131:LYS:O	1:A:134:GLY:N	2.27	0.60
1:A:221:LEU:HD21	1:A:223:PHE:HE2	1.66	0.60
1:A:221:LEU:HD21	1:A:223:PHE:CE2	2.35	0.60
1:C:146:ASN:ND2	1:C:168:ARG:O	2.34	0.60
1:C:164:ASN:HB2	2:C:249:HOH:O	2.02	0.60
1:C:18:LEU:O	1:C:28:SER:HA	2.00	0.60
1:C:41:LYS:HD3	1:C:223:PHE:CZ	2.36	0.60
1:A:132:GLU:HA	1:A:137:LEU:CD1	2.31	0.60
1:B:194:LEU:C	1:B:195:LEU:HD23	2.21	0.60
1:C:56:PRO:HD2	1:C:136:ILE:HG23	1.84	0.60
1:A:85:LYS:O	1:A:88:MET:HB2	2.01	0.60
1:B:18:LEU:HD12	1:B:19:ASP:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:PHE:O	1:C:84:PHE:C	2.40	0.59
1:C:210:ASP:N	1:C:217:HIS:NE2	2.44	0.59
1:B:16:VAL:HG13	1:B:121:ASN:HB3	1.83	0.59
1:B:153:MET:HB2	1:B:198:ASN:OD1	2.01	0.59
1:B:171:ILE:HB	1:B:173:ASP:OD1	2.02	0.59
1:C:23:ASN:N	1:C:127:GLY:O	2.36	0.59
1:C:55:VAL:HB	1:C:56:PRO:HD2	1.85	0.59
1:C:152:ILE:HG23	1:C:163:VAL:HG22	1.84	0.59
1:A:31:GLY:HA2	1:A:45:LYS:O	2.03	0.59
1:C:171:ILE:HG22	1:C:172:GLU:N	2.17	0.59
1:C:161:ILE:CD1	1:C:185:ASN:HB2	2.32	0.59
1:C:66:CRO:N2	1:C:66:CRO:HG12	2.18	0.59
1:C:99:PHE:HE1	1:C:182:TYR:CD2	2.20	0.58
1:C:53:LEU:HD12	1:C:57:TRP:CE2	2.38	0.58
1:A:97:THR:HG22	1:A:99:PHE:CE1	2.38	0.58
1:A:213:GLU:OE1	1:A:215:ARG:HG3	2.03	0.58
1:C:87:ALA:CB	1:C:92:TYR:HD2	2.15	0.58
1:C:165:PHE:O	1:C:181:HIS:HB2	2.04	0.58
1:B:93:VAL:HG22	1:B:111:GLU:HG2	1.85	0.58
1:A:142:GLU:HA	2:A:253:HOH:O	2.03	0.58
1:B:42:LEU:HD12	1:B:222:GLU:CB	2.22	0.58
1:B:128:ILE:HD13	2:B:279:HOH:O	2.03	0.58
1:C:221:LEU:HD21	1:C:223:PHE:CE2	2.39	0.57
1:C:221:LEU:HD21	1:C:223:PHE:HE2	1.68	0.57
1:A:165:PHE:O	1:A:181:HIS:HB2	2.04	0.57
1:B:17:GLU:OE1	1:B:17:GLU:HA	2.05	0.57
1:C:88:MET:HE2	1:C:91:GLY:HA2	1.87	0.57
1:B:125:LEU:HD23	1:B:125:LEU:O	2.04	0.56
1:B:15:LEU:HB3	1:B:120:VAL:HG12	1.87	0.56
1:C:152:ILE:HG22	1:C:161:ILE:CG2	2.34	0.56
1:A:130:PHE:HB3	1:A:137:LEU:CD1	2.35	0.56
1:B:75:PRO:O	1:B:79:LYS:HG2	2.06	0.56
1:C:23:ASN:HD21	1:C:130:PHE:H	1.51	0.56
1:C:92:TYR:CE1	1:C:112:VAL:HG21	2.40	0.56
1:A:82:ASP:OD2	1:A:85:LYS:NZ	2.30	0.56
1:C:7:LEU:HD21	1:C:89:PRO:HB3	1.88	0.56
1:C:171:ILE:N	1:C:175:SER:O	2.29	0.56
1:C:22:VAL:HG13	1:C:127:GLY:CA	2.35	0.56
1:C:161:ILE:HD11	1:C:185:ASN:HB2	1.86	0.56
1:C:92:TYR:HA	1:C:188:ILE:H	1.70	0.55
1:C:16:VAL:CG1	1:C:121:ASN:HB3	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:CD1	1:A:217:HIS:HB3	2.35	0.55
1:A:170:ASN:C	1:A:171:ILE:HD12	2.27	0.55
1:C:59:THR:HG21	1:C:136:ILE:HG12	1.88	0.55
1:B:213:GLU:HG3	1:B:214:LYS:N	2.21	0.55
1:B:33:GLY:HA3	1:B:44:LEU:HD23	1.89	0.55
1:B:98:ILE:HB	1:B:106:TYR:HB2	1.89	0.55
1:C:7:LEU:CD2	1:C:89:PRO:HB3	2.37	0.55
1:B:42:LEU:CD1	1:B:222:GLU:HB3	2.22	0.55
1:C:31:GLY:HA3	1:C:46:PHE:CD2	2.42	0.55
1:C:155:ASP:O	1:C:156:LYS:C	2.45	0.54
1:B:39:TYR:HE1	1:C:202:SER:HG	1.55	0.54
1:C:95:GLU:OE2	1:C:95:GLU:HA	2.08	0.54
1:C:154:ALA:HB1	1:C:195:LEU:HD13	1.90	0.54
1:C:133:ASP:OD1	1:C:133:ASP:N	2.36	0.54
1:C:221:LEU:HD11	1:C:223:PHE:CZ	2.42	0.54
1:B:12:VAL:HG13	1:B:13:PRO:HD2	1.90	0.54
1:B:21:ASP:HA	1:B:25:HIS:O	2.07	0.54
1:C:112:VAL:O	1:C:112:VAL:HG23	2.08	0.54
1:A:171:ILE:HD11	1:A:177:GLN:HB3	1.88	0.54
1:C:20:GLY:O	1:C:26:LYS:HA	2.07	0.54
1:C:156:LYS:O	1:C:159:ASN:N	2.29	0.54
1:C:7:LEU:HD23	1:C:114:PHE:CE2	2.43	0.54
1:C:42:LEU:O	1:C:221:LEU:HD12	2.08	0.54
1:A:152:ILE:HG12	1:A:163:VAL:HG22	1.90	0.54
1:C:74:TYR:O	1:C:75:PRO:O	2.26	0.54
1:B:138:GLY:O	1:B:140:LYS:HG2	2.08	0.53
1:B:93:VAL:CG2	1:B:111:GLU:HG2	2.39	0.53
1:C:178:LEU:HD12	1:C:179:ALA:N	2.24	0.53
1:C:13:PRO:HG2	1:C:117:ASP:O	2.08	0.53
1:C:41:LYS:HG3	1:C:42:LEU:N	2.24	0.53
1:B:4:GLY:O	1:B:7:LEU:HB2	2.08	0.53
1:C:207:LEU:N	1:C:207:LEU:HD23	2.22	0.53
1:A:134:GLY:O	1:A:138:GLY:N	2.42	0.53
1:B:115:GLU:OE2	1:B:122:ARG:NH1	2.41	0.53
1:C:151:TYR:O	1:C:163:VAL:HG13	2.09	0.53
1:A:112:VAL:HA	1:A:120:VAL:O	2.09	0.52
1:A:131:LYS:O	1:A:137:LEU:HD12	2.09	0.52
1:C:178:LEU:HD12	1:C:179:ALA:H	1.73	0.52
1:C:97:THR:HG23	1:C:182:TYR:CB	2.40	0.52
1:A:55:VAL:HG12	1:A:136:ILE:CG2	2.39	0.52
1:A:78:MET:HE3	1:A:229:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:THR:HG22	1:A:221:LEU:HD13	1.91	0.52
1:B:41:LYS:HE2	1:B:223:PHE:HZ	1.74	0.52
1:C:41:LYS:HB2	1:C:223:PHE:CD1	2.44	0.52
1:C:81:HIS:HD2	1:C:229:ILE:CD1	2.20	0.52
1:C:147:CYS:HA	1:C:203:THR:O	2.10	0.52
1:A:144:ASN:HD21	1:A:170:ASN:HB2	1.75	0.52
1:B:56:PRO:HG3	1:B:139:HIS:HA	1.92	0.52
1:B:74:TYR:O	1:B:79:LYS:HD3	2.10	0.52
1:B:125:LEU:HD23	1:B:125:LEU:C	2.29	0.52
1:C:57:TRP:N	1:C:58:PRO:HD2	2.24	0.52
1:A:21:ASP:HA	1:A:25:HIS:O	2.09	0.51
1:C:163:VAL:HG21	1:C:183:GLN:NE2	2.25	0.51
1:A:115:GLU:OE1	1:A:122:ARG:NH1	2.43	0.51
1:B:220:LEU:C	1:B:220:LEU:HD23	2.31	0.51
1:C:74:TYR:O	1:C:75:PRO:C	2.42	0.51
1:B:78:MET:SD	1:B:227:ALA:HA	2.51	0.51
1:C:69:GLN:HE22	1:C:183:GLN:HE22	1.57	0.51
1:A:103:ASP:OD1	1:A:130:PHE:HA	2.11	0.51
1:A:149:ASN:HB3	1:A:200:TYR:HD1	1.72	0.51
1:B:93:VAL:HG22	1:B:111:GLU:CG	2.41	0.51
1:C:46:PHE:O	1:C:217:HIS:HA	2.11	0.51
1:C:136:ILE:O	1:C:139:HIS:N	2.40	0.51
1:B:43:THR:HG23	1:B:43:THR:O	2.11	0.51
1:B:45:LYS:HZ1	1:B:213:GLU:HB2	1.76	0.50
1:C:87:ALA:O	1:C:91:GLY:N	2.43	0.50
1:A:93:VAL:HG13	1:A:110:ALA:O	2.12	0.50
1:A:33:GLY:HA3	1:A:44:LEU:HD23	1.93	0.50
1:C:156:LYS:O	1:C:157:GLN:C	2.50	0.50
1:A:197:ASP:HB3	2:A:278:HOH:O	2.11	0.50
1:C:98:ILE:O	1:C:106:TYR:N	2.31	0.50
1:C:150:VAL:HB	1:C:201:LEU:HB2	1.93	0.50
1:C:52:LYS:O	1:C:53:LEU:C	2.49	0.49
1:C:86:SER:OG	1:C:193:VAL:HB	2.13	0.49
1:A:130:PHE:HB2	1:A:137:LEU:HD11	1.90	0.49
1:B:70:CYS:HA	1:B:84:PHE:HB2	1.93	0.49
1:C:57:TRP:N	1:C:58:PRO:CD	2.76	0.49
1:C:92:TYR:CE1	1:C:112:VAL:CG2	2.95	0.49
1:A:22:VAL:O	1:A:25:HIS:N	2.40	0.49
1:A:171:ILE:HG22	1:A:173:ASP:H	1.78	0.49
1:A:171:ILE:HB	1:A:175:SER:O	2.13	0.49
1:C:29:VAL:CG1	1:C:46:PHE:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TYR:CZ	1:C:209:LYS:HE2	2.48	0.49
1:C:163:VAL:HG21	1:C:183:GLN:HE21	1.78	0.49
1:A:16:VAL:HG22	1:A:121:ASN:HB3	1.93	0.49
1:B:203:THR:CG2	1:B:224:VAL:HG22	2.30	0.49
1:C:87:ALA:HB3	1:C:92:TYR:HD2	1.77	0.49
1:C:93:VAL:HG22	1:C:111:GLU:CG	2.40	0.49
1:B:147:CYS:HA	1:B:203:THR:O	2.12	0.49
1:C:171:ILE:HD11	1:C:177:GLN:CB	2.35	0.49
1:B:45:LYS:HE3	1:B:47:ILE:CD1	2.43	0.49
1:C:108:THR:HG22	1:C:125:LEU:HD12	1.94	0.49
1:C:199:HIS:HB3	1:C:229:ILE:HD11	1.93	0.49
1:A:128:ILE:O	1:A:129:ASP:HB2	2.13	0.49
1:B:15:LEU:CB	1:B:120:VAL:HG12	2.42	0.49
1:C:18:LEU:HG	1:C:19:ASP:N	2.27	0.49
1:C:166:LYS:HG2	1:C:178:LEU:HD11	1.93	0.49
1:A:147:CYS:HA	1:A:203:THR:O	2.12	0.48
1:B:51:GLY:O	1:B:52:LYS:C	2.52	0.48
1:C:23:ASN:HD21	1:C:130:PHE:N	2.10	0.48
1:C:98:ILE:HD12	1:C:181:HIS:CD2	2.48	0.48
1:C:155:ASP:CG	1:C:158:LYS:H	2.16	0.48
1:C:22:VAL:HG22	1:C:127:GLY:HA3	1.94	0.48
1:B:98:ILE:O	1:B:105:ASN:HB2	2.12	0.48
1:C:12:VAL:CG1	1:C:13:PRO:HD2	2.44	0.48
1:C:197:ASP:O	1:C:198:ASN:HB3	2.13	0.48
1:C:89:PRO:CB	1:C:114:PHE:CD2	2.97	0.48
1:A:89:PRO:HD2	1:A:90:GLU:OE2	2.14	0.48
1:C:33:GLY:HA3	1:C:43:THR:O	2.13	0.48
1:C:105:ASN:OD1	1:C:128:ILE:HD11	2.14	0.48
1:A:14:ILE:O	1:A:15:LEU:HB3	2.14	0.48
1:C:94:GLN:CG	1:C:185:ASN:HD21	2.26	0.48
1:A:66:CRO:N2	1:A:66:CRO:CG1	2.76	0.48
1:A:5:GLU:OE1	1:A:79:LYS:HE2	2.14	0.48
1:A:76:ASP:HA	1:A:79:LYS:HG2	1.95	0.47
1:A:96:ARG:HG2	1:A:183:GLN:HB2	1.96	0.47
1:A:130:PHE:CD1	1:A:130:PHE:N	2.81	0.47
1:C:81:HIS:CD2	1:C:229:ILE:HD13	2.41	0.47
1:B:103:ASP:CG	1:B:104:GLY:H	2.17	0.47
1:C:47:ILE:O	1:C:49:THR:N	2.47	0.47
1:A:203:THR:HG23	1:A:224:VAL:HG22	1.96	0.47
1:A:27:PHE:HA	1:A:50:THR:OG1	2.13	0.47
1:B:128:ILE:HG22	1:B:129:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:PHE:CE1	1:C:182:TYR:CD2	3.02	0.47
1:C:210:ASP:OD1	1:C:211:PRO:N	2.46	0.47
1:A:144:ASN:C	1:A:144:ASN:HD22	2.18	0.47
1:B:72:SER:O	1:B:85:LYS:NZ	2.38	0.47
1:C:93:VAL:HG12	1:C:94:GLN:N	2.29	0.47
1:C:43:THR:C	1:C:44:LEU:HG	2.34	0.47
1:C:93:VAL:N	1:C:186:THR:O	2.28	0.47
1:C:110:ALA:HB2	1:C:123:ILE:CG2	2.42	0.47
1:C:133:ASP:OD1	1:C:134:GLY:N	2.45	0.47
1:C:210:ASP:HA	1:C:211:PRO:HD2	1.65	0.47
1:B:43:THR:N	2:B:287:HOH:O	2.47	0.47
1:B:115:GLU:OE2	1:B:120:VAL:HG21	2.14	0.47
1:C:20:GLY:O	1:C:27:PHE:N	2.47	0.47
1:C:4:GLY:O	1:C:7:LEU:HB2	2.14	0.47
1:C:16:VAL:HG13	1:C:121:ASN:O	2.15	0.47
1:C:70:CYS:HA	1:C:84:PHE:CB	2.44	0.46
1:C:85:LYS:O	1:C:88:MET:N	2.43	0.46
1:C:100:PHE:CD1	1:C:130:PHE:HE2	2.33	0.46
1:C:93:VAL:HG21	1:C:111:GLU:HG2	1.96	0.46
1:C:209:LYS:NZ	1:C:217:HIS:O	2.48	0.46
1:A:105:ASN:O	1:A:127:GLY:HA2	2.15	0.46
1:B:193:VAL:CG2	1:B:195:LEU:HD21	2.43	0.46
1:C:70:CYS:HA	1:C:84:PHE:HB2	1.97	0.46
1:C:143:TYR:CE2	1:C:209:LYS:HE2	2.50	0.46
1:B:90:GLU:OE1	1:B:90:GLU:N	2.27	0.46
1:C:93:VAL:CG1	1:C:94:GLN:N	2.78	0.46
1:C:156:LYS:O	1:C:159:ASN:OD1	2.33	0.46
1:A:92:TYR:CZ	1:A:112:VAL:CG2	2.99	0.46
1:A:105:ASN:N	1:A:130:PHE:CZ	2.84	0.46
1:A:148:HIS:N	1:A:203:THR:O	2.47	0.46
1:A:46:PHE:O	1:A:217:HIS:HB2	2.15	0.46
1:A:194:LEU:O	1:A:195:LEU:HD23	2.16	0.45
1:B:46:PHE:O	1:B:217:HIS:HB2	2.16	0.45
1:B:128:ILE:CG2	1:B:129:ASP:N	2.77	0.45
1:C:14:ILE:HG13	1:C:34:GLU:HA	1.97	0.45
1:A:93:VAL:HG12	1:A:94:GLN:N	2.30	0.45
1:B:78:MET:O	1:B:80:ARG:N	2.50	0.45
1:C:13:PRO:CG	1:C:118:THR:HA	2.28	0.45
1:B:158:LYS:O	1:B:159:ASN:HB3	2.17	0.45
1:C:118:THR:CG2	1:C:119:LEU:N	2.79	0.45
1:B:108:THR:HA	1:B:124:GLU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:TRP:HZ2	1:C:216:ASP:O	1.99	0.45
1:C:80:ARG:O	1:C:194:LEU:HB3	2.17	0.45
1:C:81:HIS:CD2	1:C:229:ILE:CD1	2.99	0.45
1:C:221:LEU:CD2	1:C:223:PHE:HE2	2.30	0.45
1:B:14:ILE:CG2	1:B:15:LEU:N	2.79	0.45
1:C:83:PHE:CE2	1:C:92:TYR:CD2	3.05	0.45
1:C:88:MET:CB	1:C:89:PRO:HA	2.40	0.45
1:C:161:ILE:HG13	1:C:185:ASN:HB2	1.95	0.45
1:C:100:PHE:CD2	1:C:136:ILE:HD11	2.51	0.45
1:B:89:PRO:HD2	1:B:90:GLU:OE1	2.16	0.45
1:B:213:GLU:CG	1:B:214:LYS:N	2.79	0.45
1:C:118:THR:HG22	1:C:119:LEU:N	2.31	0.44
1:B:106:TYR:CD1	1:B:130:PHE:CZ	3.05	0.44
1:B:198:ASN:ND2	1:B:198:ASN:H	2.15	0.44
1:B:110:ALA:HA	1:B:122:ARG:O	2.18	0.44
1:B:195:LEU:HD23	1:B:195:LEU:N	2.33	0.44
1:C:96:ARG:NH2	1:C:183:GLN:OE1	2.47	0.44
1:C:143:TYR:OH	1:C:218:MET:HG3	2.17	0.44
1:B:79:LYS:HG2	1:B:79:LYS:H	1.63	0.44
1:C:57:TRP:O	1:C:58:PRO:C	2.54	0.44
1:A:75:PRO:CG	1:A:78:MET:HG3	2.34	0.44
1:A:171:ILE:N	1:A:171:ILE:CD1	2.79	0.44
1:C:186:THR:HA	1:C:187:PRO:HD3	1.65	0.44
1:B:104:GLY:HA3	1:B:130:PHE:CD2	2.53	0.44
1:B:170:ASN:ND2	1:B:170:ASN:N	2.53	0.44
1:C:32:GLU:O	1:C:44:LEU:HA	2.17	0.44
1:C:96:ARG:HD3	1:C:98:ILE:HD11	1.99	0.44
1:B:88:MET:CE	1:B:91:GLY:HA2	2.47	0.44
1:B:136:ILE:O	1:B:139:HIS:N	2.46	0.44
1:C:3:LYS:O	1:C:6:GLU:HB2	2.18	0.44
1:B:72:SER:HB2	2:B:246:HOH:O	2.18	0.43
1:C:164:ASN:HB2	1:C:181:HIS:O	2.17	0.43
1:A:186:THR:HA	1:A:187:PRO:HD3	1.61	0.43
1:B:145:TYR:HD2	1:B:146:ASN:O	2.01	0.43
1:A:153:MET:HE1	1:A:162:LYS:HE2	1.99	0.43
1:B:150:VAL:O	1:B:200:TYR:HA	2.18	0.43
1:C:103:ASP:CG	1:C:104:GLY:H	2.15	0.43
1:B:109:ARG:HG2	1:B:110:ALA:N	2.34	0.43
1:C:97:THR:C	1:C:98:ILE:HD13	2.38	0.43
1:A:220:LEU:HD21	1:A:222:GLU:HB2	2.01	0.43
1:A:97:THR:CG2	1:A:99:PHE:CE1	3.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ILE:HG22	1:C:124:GLU:N	2.34	0.43
1:C:200:TYR:O	1:C:201:LEU:HD23	2.19	0.43
1:A:18:LEU:HD12	1:A:19:ASP:N	2.34	0.43
1:A:79:LYS:HD2	1:A:79:LYS:HA	1.69	0.43
1:C:23:ASN:OD1	1:C:128:ILE:HA	2.19	0.43
1:C:89:PRO:HB3	1:C:114:PHE:CD2	2.53	0.43
1:C:95:GLU:N	1:C:184:GLN:O	2.28	0.43
1:B:106:TYR:CE1	1:B:130:PHE:CZ	3.07	0.43
1:C:98:ILE:HB	1:C:106:TYR:HB2	2.00	0.43
1:C:22:VAL:O	1:C:23:ASN:HB2	2.19	0.43
1:A:164:ASN:O	1:A:165:PHE:HB3	2.19	0.43
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.71	0.43
1:B:135:ASN:ND2	1:B:171:ILE:CD1	2.79	0.43
1:C:5:GLU:O	1:C:8:PHE:N	2.38	0.43
1:C:99:PHE:HD2	1:C:105:ASN:HD22	1.66	0.43
1:C:71:PHE:CE2	1:C:119:LEU:HD22	2.54	0.42
1:C:98:ILE:O	1:C:105:ASN:HB2	2.18	0.42
1:A:15:LEU:HB2	1:A:16:VAL:H	1.48	0.42
1:B:215:ARG:H	1:B:215:ARG:HG3	1.60	0.42
1:A:20:GLY:HA2	1:A:125:LEU:O	2.19	0.42
1:B:66:CRO:N2	1:B:66:CRO:HD1	2.34	0.42
1:B:151:TYR:O	1:B:163:VAL:HA	2.19	0.42
1:C:14:ILE:HG22	1:C:15:LEU:N	2.33	0.42
1:C:100:PHE:O	1:C:101:LYS:C	2.56	0.42
1:A:158:LYS:O	1:A:159:ASN:HB3	2.18	0.42
1:C:23:ASN:ND2	1:C:130:PHE:H	2.17	0.42
1:C:99:PHE:CE1	1:C:182:TYR:CE2	3.05	0.42
1:A:55:VAL:HG12	1:A:136:ILE:HG22	2.01	0.42
1:B:45:LYS:HE3	1:B:47:ILE:HD13	2.02	0.42
1:C:161:ILE:HG13	1:C:161:ILE:O	2.18	0.42
1:A:92:TYR:CZ	1:A:112:VAL:HG22	2.54	0.42
1:A:18:LEU:HD13	1:A:123:ILE:HB	2.01	0.42
1:B:78:MET:CE	1:B:226:ALA:HB1	2.49	0.42
1:A:55:VAL:HB	1:A:56:PRO:HD2	2.01	0.42
1:A:101:LYS:HB3	1:A:177:GLN:NE2	2.35	0.42
1:A:97:THR:HG21	1:A:99:PHE:CZ	2.55	0.42
1:B:51:GLY:HA2	2:B:278:HOH:O	2.19	0.42
1:C:35:GLY:HA2	1:C:42:LEU:HB3	2.01	0.42
1:C:62:THR:HG22	1:C:66:CRO:CG2	2.50	0.42
1:C:84:PHE:HA	1:C:92:TYR:CE2	2.55	0.42
1:B:45:LYS:NZ	1:B:213:GLU:HB2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HB3	1:A:177:GLN:HE22	1.85	0.41
1:B:19:ASP:OD1	1:B:28:SER:OG	2.30	0.41
1:A:150:VAL:O	1:A:200:TYR:HB2	2.19	0.41
1:A:150:VAL:O	1:A:200:TYR:HA	2.20	0.41
1:C:80:ARG:HA	1:C:194:LEU:HD13	2.01	0.41
1:B:41:LYS:HE2	1:B:223:PHE:CE1	2.54	0.41
1:B:90:GLU:H	1:B:90:GLU:CD	2.18	0.41
1:C:110:ALA:HB2	1:C:123:ILE:CG1	2.50	0.41
1:B:9:THR:HG21	2:B:263:HOH:O	2.20	0.41
1:C:92:TYR:HB2	1:C:186:THR:O	2.20	0.41
1:A:66:CRO:CZ	1:A:203:THR:HG21	2.51	0.41
1:C:5:GLU:O	1:C:7:LEU:N	2.54	0.41
1:C:152:ILE:HD12	1:C:199:HIS:NE2	2.34	0.41
1:A:78:MET:CE	1:A:229:ILE:HG13	2.51	0.41
1:B:106:TYR:CD1	1:B:130:PHE:HZ	2.38	0.41
1:C:86:SER:C	1:C:88:MET:H	2.24	0.41
1:C:199:HIS:HB2	1:C:229:ILE:HD12	2.01	0.41
1:B:74:TYR:CG	1:B:82:ASP:HB2	2.56	0.41
1:B:111:GLU:OE1	1:B:113:LYS:NZ	2.54	0.41
1:B:194:LEU:O	1:B:195:LEU:HD23	2.21	0.41
1:C:152:ILE:CG2	1:C:161:ILE:CG2	2.99	0.41
1:A:123:ILE:HG22	1:A:124:GLU:N	2.36	0.41
1:C:104:GLY:HA3	1:C:130:PHE:CG	2.56	0.41
1:C:110:ALA:HA	1:C:122:ARG:O	2.21	0.41
1:C:171:ILE:HG23	1:C:171:ILE:HD12	1.78	0.41
1:B:77:HIS:NE2	1:B:78:MET:HG3	2.37	0.40
1:A:171:ILE:HD13	1:A:177:GLN:N	2.36	0.40
1:C:155:ASP:O	1:C:156:LYS:O	2.40	0.40
1:A:22:VAL:HG22	1:A:127:GLY:HA3	2.03	0.40
1:A:165:PHE:O	1:A:181:HIS:N	2.45	0.40
1:B:42:LEU:HD21	1:B:68:VAL:HG23	2.02	0.40
1:A:96:ARG:HA	1:A:182:TYR:O	2.21	0.40
1:A:135:ASN:HA	1:A:140:LYS:HG3	2.01	0.40
1:A:153:MET:HE2	1:A:162:LYS:CE	2.49	0.40
1:B:18:LEU:HD12	1:B:123:ILE:O	2.21	0.40
1:C:8:PHE:CD2	1:C:85:LYS:CG	2.99	0.40
1:A:112:VAL:HG12	1:A:121:ASN:OD1	2.22	0.40
1:B:12:VAL:HG13	2:B:292:HOH:O	2.22	0.40
1:C:11:VAL:HG11	1:C:34:GLU:OE1	2.21	0.40
1:C:22:VAL:HG13	1:C:127:GLY:C	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:312:HOH:O	2:A:312:HOH:O[2_755]	1.63	0.57

## 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	222/236 (94%)	214 (96%)	7 (3%)	1 (0%)	29	18
1	B	221/236 (94%)	205 (93%)	15 (7%)	1 (0%)	29	18
1	C	221/236 (94%)	189 (86%)	24 (11%)	8 (4%)	3	0
All	All	664/708 (94%)	608 (92%)	46 (7%)	10 (2%)	10	3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	135	ASN
1	C	192	PRO
1	B	79	LYS
1	C	75	PRO
1	A	132	GLU
1	C	48	SER
1	C	157	GLN
1	C	215	ARG
1	C	9	THR
1	C	156	LYS

### 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	188/206 (91%)	169 (90%)	19 (10%)	7	2
1	B	184/206 (89%)	164 (89%)	20 (11%)	6	2
1	C	164/206 (80%)	140 (85%)	24 (15%)	3	1
All	All	536/618 (87%)	473 (88%)	63 (12%)	5	2

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LYS
1	A	7	LEU
1	A	15	LEU
1	A	21	ASP
1	A	32	GLU
1	A	47	ILE
1	A	53	LEU
1	A	76	ASP
1	A	78	MET
1	A	112	VAL
1	A	122	ARG
1	A	123	ILE
1	A	126	LYS
1	A	137	LEU
1	A	141	LEU
1	A	144	ASN
1	A	177	GLN
1	A	229	ILE
1	B	3	LYS
1	B	25	HIS
1	B	42	LEU
1	B	47	ILE
1	B	76	ASP
1	B	111	GLU
1	B	113	LYS
1	B	119	LEU
1	B	123	ILE
1	B	128	ILE
1	B	155	ASP
1	B	164	ASN

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Mol	Chain	Res	Type
1	B	170	ASN
1	B	175	SER
1	B	176	VAL
1	B	177	GLN
1	B	178	LEU
1	B	190	ASP
1	B	215	ARG
1	B	220	LEU
1	C	18	LEU
1	C	41	LYS
1	C	42	LEU
1	C	46	PHE
1	C	47	ILE
1	C	83	PHE
1	C	95	GLU
1	C	99	PHE
1	C	105	ASN
1	C	117	ASP
1	C	119	LEU
1	C	123	ILE
1	C	125	LEU
1	C	133	ASP
1	C	141	LEU
1	C	177	GLN
1	C	183	GLN
1	C	186	THR
1	C	194	LEU
1	C	195	LEU
1	C	213	GLU
1	C	222	GLU
1	C	225	THR
1	C	229	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	135	ASN
1	A	144	ASN
1	A	170	ASN
1	A	177	GLN
1	A	184	GLN

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Mol	Chain	Res	Type
1	B	144	ASN
1	B	146	ASN
1	B	149	ASN
1	B	164	ASN
1	B	170	ASN
1	C	69	GLN
1	C	146	ASN
1	C	149	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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	CRO	A	66	1	23,23,24	2.64	11 (47%)	30,32,34	1.92	9 (30%)
1	CRO	C	66	1	23,23,24	2.52	7 (30%)	30,32,34	2.14	9 (30%)
1	CRO	B	66	1	23,23,24	2.46	9 (39%)	30,32,34	1.97	8 (26%)

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	CRO	A	66	1	-	0/12/31/32	0/2/2/2
1	CRO	C	66	1	-	2/12/31/32	0/2/2/2
1	CRO	B	66	1	-	0/12/31/32	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CRO	CE1-CZ	6.71	1.51	1.38
1	B	66	CRO	CE1-CZ	6.54	1.51	1.38
1	A	66	CRO	CB2-CA2	6.09	1.40	1.35
1	A	66	CRO	CE1-CZ	5.18	1.48	1.38
1	C	66	CRO	C1-N3	4.41	1.44	1.37
1	C	66	CRO	CE2-CZ	4.34	1.47	1.38
1	B	66	CRO	CE2-CZ	4.32	1.47	1.38
1	A	66	CRO	CA3-N3	-4.24	1.38	1.47
1	B	66	CRO	CG2-CB2	-4.22	1.38	1.46
1	A	66	CRO	CE2-CZ	3.91	1.46	1.38
1	C	66	CRO	CD1-CG2	3.89	1.47	1.39
1	A	66	CRO	CD1-CG2	3.72	1.46	1.39
1	C	66	CRO	CG2-CB2	-3.65	1.39	1.46
1	B	66	CRO	CD1-CG2	3.26	1.45	1.39
1	B	66	CRO	OH-CZ	-3.18	1.29	1.37
1	A	66	CRO	C1-N3	3.10	1.42	1.37
1	B	66	CRO	C1-N2	3.00	1.36	1.32
1	B	66	CRO	C1-N3	2.92	1.42	1.37
1	B	66	CRO	CD2-CG2	2.75	1.44	1.39
1	C	66	CRO	CB2-CA2	2.65	1.37	1.35
1	C	66	CRO	OH-CZ	-2.60	1.30	1.37
1	A	66	CRO	CD2-CG2	2.39	1.44	1.39
1	A	66	CRO	CA1-C1	2.35	1.54	1.51
1	A	66	CRO	CE1-CD1	-2.05	1.35	1.38
1	A	66	CRO	CA2-N2	2.04	1.42	1.38
1	B	66	CRO	CA3-N3	-2.03	1.43	1.47
1	A	66	CRO	CA2-C2	2.02	1.50	1.48

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	CA1-C1-N3	-4.89	118.89	124.75
1	C	66	CRO	N3-C1-N2	4.84	114.80	111.45
1	C	66	CRO	C2-N3-C1	-4.59	105.64	107.97
1	C	66	CRO	CA1-C1-N3	-4.50	119.35	124.75
1	A	66	CRO	O2-C2-CA2	4.14	133.29	130.96
1	B	66	CRO	CA1-C1-N2	4.12	129.65	123.89
1	B	66	CRO	O2-C2-CA2	4.09	133.26	130.96
1	A	66	CRO	CG2-CB2-CA2	4.03	134.89	129.94
1	A	66	CRO	CE2-CZ-CE1	-3.75	113.44	119.77
1	C	66	CRO	CE2-CZ-CE1	-3.43	113.98	119.77
1	C	66	CRO	C1-CA1-N1	-3.40	104.45	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CRO	CD2-CE2-CZ	3.31	123.50	119.88
1	B	66	CRO	CE2-CZ-CE1	-3.19	114.39	119.77
1	B	66	CRO	CD1-CE1-CZ	3.15	123.33	119.88
1	C	66	CRO	CG2-CB2-CA2	3.01	133.64	129.94
1	C	66	CRO	CA2-C2-N3	3.00	104.79	103.37
1	A	66	CRO	O3-C3-CA3	-2.86	117.76	126.39
1	C	66	CRO	CD2-CE2-CZ	2.72	122.86	119.88
1	B	66	CRO	CA2-C2-N3	2.70	104.65	103.37
1	A	66	CRO	CA2-N2-C1	2.52	107.63	105.77
1	A	66	CRO	CD1-CE1-CZ	2.46	122.57	119.88
1	A	66	CRO	C1-CA1-N1	-2.37	106.12	109.96
1	B	66	CRO	O3-C3-CA3	-2.32	119.40	126.39
1	A	66	CRO	CA1-C1-N3	-2.23	122.07	124.75
1	B	66	CRO	CA2-N2-C1	2.21	107.40	105.77
1	C	66	CRO	O2-C2-CA2	2.15	132.17	130.96

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	66	CRO	C3-CA3-N3-C2
1	C	66	CRO	N1-CA1-CB1-OG1

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRO	3	0
1	C	66	CRO	2	0
1	B	66	CRO	2	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 [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, 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	226/236 (95%)	1.07	27 (11%) 4 5	22, 37, 60, 84	0
1	B	225/236 (95%)	1.15	30 (13%) 3 3	24, 41, 62, 81	0
1	C	225/236 (95%)	2.14	102 (45%) 0 0	31, 57, 88, 98	0
All	All	676/708 (95%)	1.45	159 (23%) 0 0	22, 44, 77, 98	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	ILE	6.7
1	C	55	VAL	6.7
1	C	91	GLY	6.2
1	C	48	SER	5.9
1	C	76	ASP	5.6
1	B	173	ASP	5.6
1	C	133	ASP	5.4
1	C	195	LEU	5.3
1	C	63	THR	5.1
1	C	211	PRO	5.1
1	C	116	GLY	5.0
1	A	229	ILE	4.8
1	C	47	ILE	4.7
1	C	215	ARG	4.6
1	C	198	ASN	4.5
1	C	174	GLY	4.5
1	C	98	ILE	4.5
1	C	214	LYS	4.5
1	C	128	ILE	4.5
1	C	89	PRO	4.4
1	C	27	PHE	4.4
1	B	171	ILE	4.3
1	C	134	GLY	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	216	ASP	4.2
1	C	192	PRO	4.1
1	C	212	ASN	4.0
1	C	22	VAL	4.0
1	A	98	ILE	4.0
1	B	98	ILE	4.0
1	C	130	PHE	3.9
1	C	155	ASP	3.9
1	C	175	SER	3.9
1	C	77	HIS	3.9
1	B	175	SER	3.9
1	C	153	MET	3.8
1	C	213	GLU	3.8
1	C	53	LEU	3.7
1	C	118	THR	3.7
1	C	80	ARG	3.7
1	C	119	LEU	3.7
1	C	49	THR	3.6
1	C	108	THR	3.6
1	C	125	LEU	3.6
1	C	191	GLY	3.6
1	A	211	PRO	3.6
1	C	54	PRO	3.6
1	C	137	LEU	3.6
1	C	51	GLY	3.5
1	C	29	VAL	3.5
1	C	138	GLY	3.5
1	C	117	ASP	3.5
1	C	154	ALA	3.5
1	C	64	LEU	3.5
1	C	50	THR	3.3
1	C	115	GLU	3.3
1	C	113	LYS	3.3
1	C	189	GLY	3.3
1	A	64	LEU	3.3
1	C	141	LEU	3.2
1	C	107	LYS	3.2
1	C	217	HIS	3.1
1	B	64	LEU	3.1
1	C	161	ILE	3.0
1	B	60	LEU	3.0
1	C	14	ILE	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	13	PRO	3.0
1	C	60	LEU	3.0
1	C	194	LEU	3.0
1	C	196	PRO	3.0
1	B	212	ASN	3.0
1	C	156	LYS	2.9
1	C	61	VAL	2.9
1	A	15	LEU	2.9
1	B	134	GLY	2.9
1	B	133	ASP	2.9
1	B	172	GLU	2.9
1	B	78	MET	2.9
1	C	193	VAL	2.9
1	C	23	ASN	2.9
1	B	220	LEU	2.9
1	C	8	PHE	2.8
1	B	55	VAL	2.8
1	C	92	TYR	2.8
1	A	223	PHE	2.8
1	A	137	LEU	2.7
1	C	52	LYS	2.7
1	A	228	GLY	2.7
1	B	174	GLY	2.7
1	C	43	THR	2.7
1	A	53	LEU	2.7
1	C	28	SER	2.7
1	B	61	VAL	2.7
1	C	24	GLY	2.6
1	C	42	LEU	2.6
1	C	190	ASP	2.6
1	C	12	VAL	2.6
1	B	63	THR	2.6
1	A	220	LEU	2.6
1	C	87	ALA	2.6
1	C	139	HIS	2.6
1	B	163	VAL	2.6
1	C	46	PHE	2.6
1	A	120	VAL	2.6
1	B	42	LEU	2.5
1	B	125	LEU	2.5
1	C	223	PHE	2.5
1	A	132	GLU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	18	LEU	2.5
1	C	159	ASN	2.5
1	C	90	GLU	2.5
1	C	2	SER	2.4
1	C	33	GLY	2.4
1	C	121	ASN	2.4
1	C	152	ILE	2.4
1	A	42	LEU	2.4
1	A	46	PHE	2.4
1	A	134	GLY	2.4
1	C	129	ASP	2.4
1	B	18	LEU	2.4
1	C	197	ASP	2.4
1	B	22	VAL	2.4
1	C	114	PHE	2.3
1	A	68	VAL	2.3
1	C	163	VAL	2.3
1	C	44	LEU	2.3
1	B	197	ASP	2.3
1	B	210	ASP	2.3
1	B	198	ASN	2.3
1	C	188	ILE	2.3
1	C	7	LEU	2.3
1	C	220	LEU	2.3
1	A	63	THR	2.3
1	C	9	THR	2.3
1	C	186	THR	2.3
1	A	125	LEU	2.3
1	C	97	THR	2.2
1	B	196	PRO	2.2
1	A	108	THR	2.2
1	C	228	GLY	2.2
1	A	224	VAL	2.2
1	A	62	THR	2.2
1	A	97	THR	2.2
1	B	62	THR	2.2
1	C	30	SER	2.1
1	C	123	ILE	2.1
1	A	80	ARG	2.1
1	A	150	VAL	2.1
1	B	97	THR	2.1
1	C	84	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	100	PHE	2.1
1	B	29	VAL	2.1
1	C	62	THR	2.1
1	B	221	LEU	2.1
1	A	61	VAL	2.1
1	C	219	VAL	2.1
1	A	190	ASP	2.0
1	C	15	LEU	2.0
1	A	44	LEU	2.0
1	B	118	THR	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(Å <sup>2</sup> )	Q<0.9
1	CRO	C	66	22/23	0.86	0.22	22,41,56,60	0
1	CRO	A	66	22/23	0.91	0.21	14,28,38,70	0
1	CRO	B	66	22/23	0.93	0.20	19,25,33,52	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.