



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:14 PM UTC

PDB ID : 1JC1 / pdb_00001jc1
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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

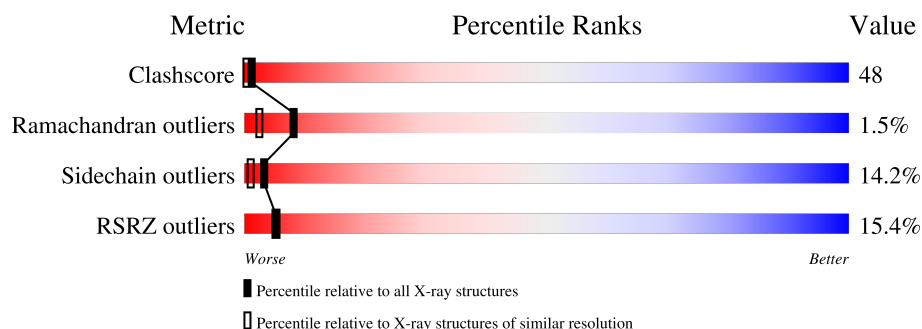
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 ≥ 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	3% 36% 40% 15% . .
1	B	236	4% 32% 41% 18% . .
1	C	236	37% 19% 44% 25% 6% .

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
1	A	227	Total	C	N	O	S	0	0	0
			1782	1133	298	343	8			
1	B	226	Total	C	N	O	S	0	0	0
			1760	1119	293	340	8			
1	C	226	Total	C	N	O	S	0	0	0
			1678	1067	276	328	7			

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

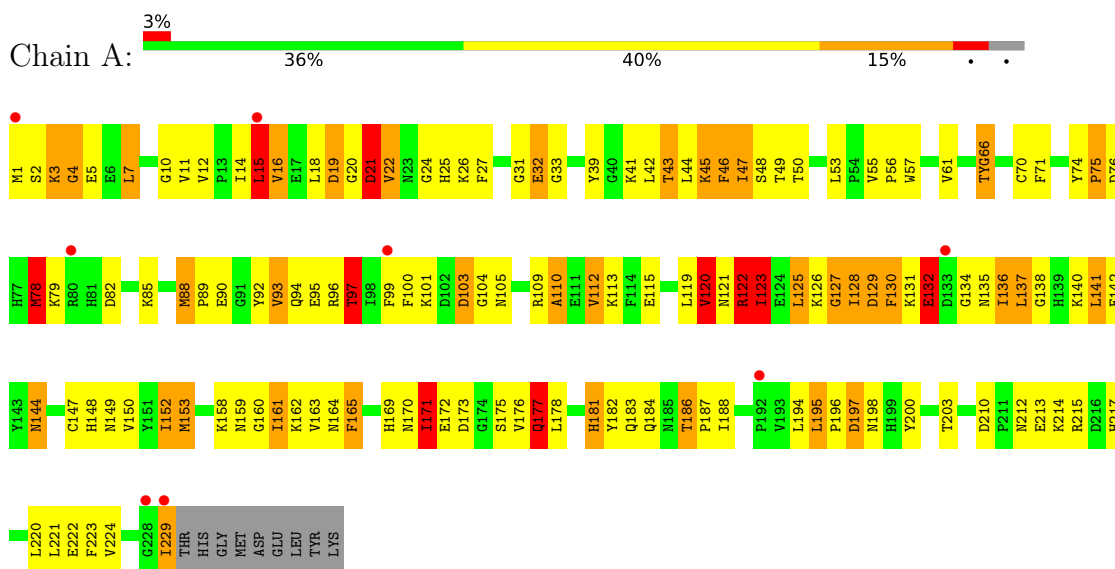
- Molecule 2 is water.

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

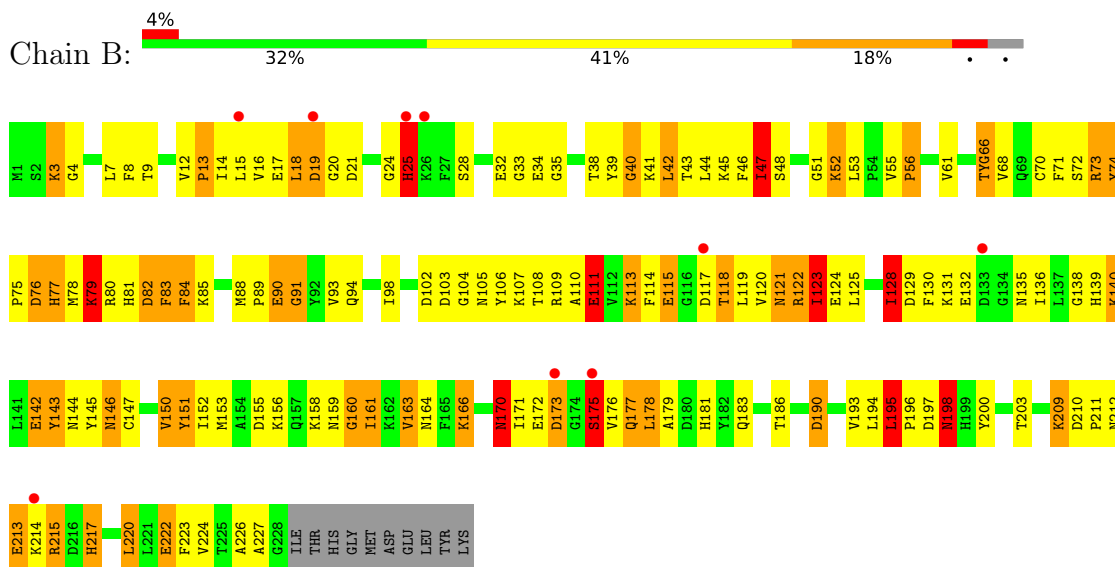
3 Residue-property plots

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.

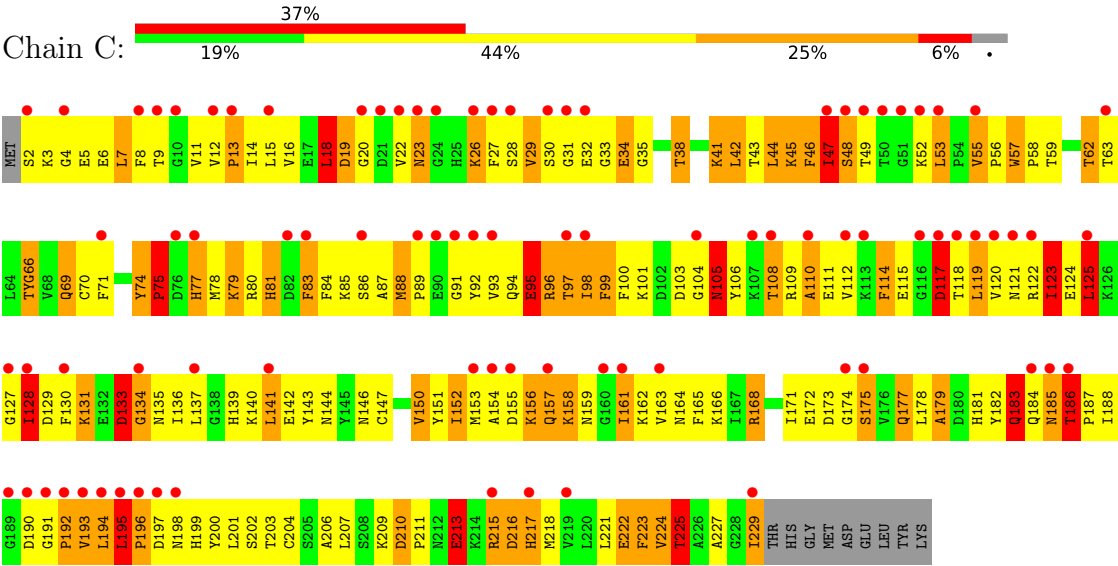
• Molecule 1: GREEN FLUORESCENT PROTEIN



• 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, α , β , γ	186.84Å 67.61Å 56.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.90) 99.6 (30.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.91Å)	Xtriage
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 ²)	28.3	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 95.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5394	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.75	20/1800 (1.1%)	2.16	66/2437 (2.7%)
1	B	1.63	17/1778 (1.0%)	2.17	81/2411 (3.4%)
1	C	1.62	13/1695 (0.8%)	2.25	91/2303 (4.0%)
All	All	1.67	50/5273 (0.9%)	2.19	238/7151 (3.3%)

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 (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	GLY	CA-C	10.46	1.59	1.52
1	B	181	HIS	CE1-NE2	7.55	1.40	1.32
1	B	53	LEU	C-N	-7.48	1.24	1.34
1	A	24	GLY	CA-C	-7.06	1.42	1.51
1	B	179	ALA	C-O	6.84	1.32	1.23
1	A	3	LYS	C-N	6.81	1.43	1.33
1	A	32	GLU	CD-OE2	6.78	1.38	1.25
1	A	110	ALA	N-CA	-6.78	1.37	1.45
1	C	109	ARG	C-O	6.60	1.31	1.24
1	B	47	ILE	C-O	6.49	1.30	1.23
1	C	38	THR	CA-C	-6.43	1.44	1.52
1	A	152	ILE	CA-CB	-6.31	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	74	TYR	C-O	-6.26	1.16	1.24
1	A	78	MET	CA-C	-6.23	1.44	1.52
1	B	40	GLY	CA-C	6.16	1.60	1.51
1	A	128	ILE	CA-CB	-6.09	1.44	1.55
1	C	223	PHE	CA-CB	6.00	1.62	1.53
1	B	32	GLU	CA-C	-5.96	1.45	1.52
1	A	10	GLY	N-CA	5.92	1.49	1.44
1	C	142	GLU	CA-C	-5.83	1.45	1.53
1	C	117	ASP	CG-OD2	5.78	1.36	1.25
1	C	192	PRO	C-N	5.63	1.38	1.33
1	C	57	TRP	C-N	-5.57	1.25	1.33
1	A	11	VAL	C-N	-5.56	1.27	1.33
1	B	161	ILE	N-CA	-5.53	1.40	1.46
1	B	83	PHE	N-CA	-5.51	1.39	1.46
1	B	8	PHE	CA-C	-5.49	1.45	1.52
1	C	97	THR	CA-C	5.49	1.59	1.52
1	B	56	PRO	CA-C	5.47	1.59	1.52
1	B	186	THR	C-N	-5.47	1.26	1.33
1	A	12	VAL	N-CA	-5.47	1.39	1.46
1	B	166	LYS	N-CA	-5.47	1.39	1.46
1	A	43	THR	N-CA	-5.45	1.40	1.46
1	B	107	LYS	C-O	5.42	1.30	1.23
1	A	74	TYR	CA-CB	5.37	1.61	1.53
1	B	35	GLY	CA-C	5.33	1.56	1.52
1	B	143	TYR	C-N	-5.23	1.26	1.33
1	A	171	ILE	CA-CB	-5.22	1.48	1.54
1	C	183	GLN	C-O	5.21	1.30	1.23
1	A	188	ILE	CA-CB	-5.20	1.46	1.54
1	A	42	LEU	CA-C	-5.16	1.46	1.52
1	A	103	ASP	CG-OD2	5.15	1.35	1.25
1	C	168	ARG	CZ-NH1	5.12	1.40	1.32
1	A	75	PRO	N-CA	-5.10	1.40	1.47
1	C	81	HIS	CA-C	-5.10	1.45	1.52
1	B	222	GLU	CD-OE2	5.07	1.34	1.25
1	A	61	VAL	N-CA	5.07	1.52	1.46
1	B	82	ASP	CG-OD2	5.05	1.34	1.25
1	A	43	THR	CB-OG1	-5.03	1.35	1.43
1	C	193	VAL	CA-CB	-5.01	1.50	1.55

All (238) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	PHE	CA-CB-CG	-14.28	99.52	113.80
1	C	133	ASP	CA-C-N	9.60	130.60	120.43
1	C	133	ASP	C-N-CA	9.60	130.60	120.43
1	A	123	ILE	N-CA-C	9.26	121.81	108.48
1	B	114	PHE	CA-CB-CG	-9.21	104.59	113.80
1	B	196	PRO	CB-CA-C	-9.14	99.53	111.23
1	B	19	ASP	CA-C-N	-8.80	112.29	121.35
1	B	19	ASP	C-N-CA	-8.80	112.29	121.35
1	A	196	PRO	CB-CA-C	-8.73	100.05	111.23
1	C	57	TRP	CA-C-O	8.66	126.59	118.63
1	B	213	GLU	N-CA-CB	8.56	123.04	109.51
1	B	196	PRO	N-CA-C	8.49	124.70	111.21
1	C	134	GLY	N-CA-C	8.44	122.84	111.03
1	B	122	ARG	CB-CA-C	8.09	123.46	110.19
1	C	123	ILE	N-CA-C	7.92	120.26	108.46
1	A	129	ASP	CA-C-N	-7.75	109.87	120.87
1	A	129	ASP	C-N-CA	-7.75	109.87	120.87
1	C	190	ASP	N-CA-C	7.72	122.46	112.89
1	A	181	HIS	N-CA-C	7.64	121.70	109.24
1	C	216	ASP	CA-CB-CG	7.59	120.19	112.60
1	B	55	VAL	N-CA-CB	-7.58	106.60	111.83
1	C	47	ILE	N-CA-C	7.50	118.70	107.75
1	B	84	PHE	N-CA-CB	7.47	121.18	109.82
1	A	160	GLY	CA-C-N	-7.45	112.19	122.92
1	A	160	GLY	C-N-CA	-7.45	112.19	122.92
1	A	186	THR	O-C-N	7.40	127.13	121.88
1	C	18	LEU	N-CA-C	7.38	121.56	109.24
1	C	222	GLU	N-CA-C	7.34	121.53	109.06
1	C	120	VAL	N-CA-C	7.32	118.42	108.17
1	B	123	ILE	N-CA-C	7.29	119.32	108.46
1	A	48	SER	CA-C-N	-7.27	111.23	122.49
1	A	48	SER	C-N-CA	-7.27	111.23	122.49
1	B	111	GLU	N-CA-CB	7.26	122.88	110.68
1	C	161	ILE	N-CA-CB	-7.25	98.37	111.92
1	C	134	GLY	O-C-N	7.24	129.14	122.77
1	C	95	GLU	CB-CA-C	7.15	122.09	109.72
1	B	150	VAL	N-CA-CB	-7.13	102.48	111.46
1	B	195	LEU	CA-C-N	7.12	127.12	119.78
1	B	195	LEU	C-N-CA	7.12	127.12	119.78
1	C	186	THR	CA-C-N	7.08	128.69	119.84
1	C	186	THR	C-N-CA	7.08	128.69	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	144	ASN	CA-CB-CG	-7.05	105.55	112.60
1	C	196	PRO	CB-CA-C	-6.95	101.85	110.95
1	B	217	HIS	CA-CB-CG	-6.91	106.89	113.80
1	C	158	LYS	CA-C-N	-6.89	108.39	121.54
1	C	158	LYS	C-N-CA	-6.89	108.39	121.54
1	B	71	PHE	CA-CB-CG	-6.88	106.92	113.80
1	C	210	ASP	CA-C-O	6.88	125.30	119.66
1	A	49	THR	CA-C-N	-6.86	111.61	122.79
1	A	49	THR	C-N-CA	-6.86	111.61	122.79
1	A	110	ALA	O-C-N	6.80	131.00	123.25
1	B	170	ASN	CA-CB-CG	-6.78	105.83	112.60
1	A	21	ASP	CA-CB-CG	6.75	119.35	112.60
1	C	88	MET	N-CA-C	6.67	119.14	110.40
1	B	94	GLN	CA-C-N	-6.62	112.29	122.62
1	B	94	GLN	C-N-CA	-6.62	112.29	122.62
1	A	186	THR	CA-C-N	6.61	126.57	119.76
1	A	186	THR	C-N-CA	6.61	126.57	119.76
1	C	79	LYS	N-CA-C	6.60	118.13	111.07
1	C	225	THR	CB-CA-C	6.58	120.27	110.14
1	B	142	GLU	N-CA-CB	6.54	120.23	110.29
1	A	122	ARG	N-CA-CB	6.53	121.31	110.47
1	B	48	SER	CA-C-N	-6.53	112.29	122.67
1	B	48	SER	C-N-CA	-6.53	112.29	122.67
1	C	213	GLU	N-CA-C	6.49	119.47	107.99
1	C	193	VAL	N-CA-C	6.46	116.93	107.75
1	B	18	LEU	CA-C-N	-6.43	113.94	123.00
1	B	18	LEU	C-N-CA	-6.43	113.94	123.00
1	A	113	LYS	CA-C-N	-6.42	110.73	121.39
1	A	113	LYS	C-N-CA	-6.42	110.73	121.39
1	B	160	GLY	CA-C-N	-6.40	113.60	122.69
1	B	160	GLY	C-N-CA	-6.40	113.60	122.69
1	C	29	VAL	O-C-N	6.39	129.66	123.14
1	A	210	ASP	CA-C-O	6.37	123.43	119.29
1	A	46	PHE	CA-CB-CG	-6.37	107.44	113.80
1	C	191	GLY	CA-C-N	6.36	127.79	119.84
1	C	191	GLY	C-N-CA	6.36	127.79	119.84
1	A	43	THR	CB-CA-C	6.36	119.90	110.62
1	B	73	ARG	CB-CA-C	-6.35	100.62	110.78
1	A	120	VAL	N-CA-CB	-6.34	102.66	111.41
1	C	69	GLN	CA-C-O	6.26	126.99	119.10
1	C	13	PRO	CA-C-N	-6.26	114.43	123.06
1	C	13	PRO	C-N-CA	-6.26	114.43	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ILE	CB-CA-C	-6.25	100.87	110.50
1	C	134	GLY	CA-C-N	6.24	133.46	121.54
1	C	134	GLY	C-N-CA	6.24	133.46	121.54
1	B	76	ASP	N-CA-CB	6.24	119.23	109.94
1	C	133	ASP	N-CA-C	-6.22	104.75	112.90
1	B	3	LYS	CA-C-N	6.21	127.90	120.14
1	B	3	LYS	C-N-CA	6.21	127.90	120.14
1	A	161	ILE	N-CA-C	6.18	117.83	108.80
1	A	123	ILE	CB-CA-C	-6.16	101.44	110.62
1	A	165	PHE	CA-CB-CG	-6.15	107.65	113.80
1	C	88	MET	CB-CA-C	6.14	118.36	109.09
1	C	19	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	15	LEU	N-CA-C	6.10	118.35	108.41
1	C	110	ALA	CA-C-N	-6.09	114.09	122.93
1	C	110	ALA	C-N-CA	-6.09	114.09	122.93
1	C	105	ASN	CA-CB-CG	6.09	118.69	112.60
1	B	117	ASP	CA-C-N	-6.01	113.37	122.81
1	B	117	ASP	C-N-CA	-6.01	113.37	122.81
1	B	102	ASP	CA-CB-CG	6.01	118.61	112.60
1	C	128	ILE	CB-CA-C	-6.01	101.09	110.52
1	B	152	ILE	N-CA-C	6.00	117.24	108.53
1	A	152	ILE	N-CA-C	6.00	117.12	108.48
1	C	125	LEU	N-CA-C	6.00	118.67	108.90
1	B	212	ASN	CA-CB-CG	-5.99	106.61	112.60
1	B	13	PRO	CB-CA-C	-5.98	103.25	111.21
1	C	2	SER	N-CA-C	5.97	127.72	111.00
1	A	176	VAL	CB-CA-C	-5.95	101.83	110.63
1	B	77	HIS	CA-CB-CG	-5.95	107.85	113.80
1	C	150	VAL	N-CA-CB	-5.95	104.52	111.83
1	C	131	LYS	CA-C-N	-5.94	112.73	122.54
1	C	131	LYS	C-N-CA	-5.94	112.73	122.54
1	A	214	LYS	N-CA-C	5.94	117.84	111.36
1	B	123	ILE	O-C-N	5.94	129.46	123.10
1	C	96	ARG	N-CA-C	5.94	118.43	109.23
1	B	179	ALA	CA-C-O	5.93	128.47	120.47
1	A	71	PHE	CA-CB-CG	-5.92	107.88	113.80
1	C	55	VAL	CA-C-N	5.92	126.11	119.90
1	C	55	VAL	C-N-CA	5.92	126.11	119.90
1	B	107	LYS	N-CA-CB	5.91	120.40	110.77
1	A	122	ARG	CB-CA-C	5.90	120.41	110.79
1	A	42	LEU	CA-C-N	-5.89	113.89	122.44
1	A	42	LEU	C-N-CA	-5.89	113.89	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	LYS	CB-CA-C	-5.89	101.53	111.02
1	A	75	PRO	N-CA-CB	5.88	108.92	103.39
1	A	169	HIS	CA-CB-CG	5.88	119.68	113.80
1	B	213	GLU	N-CA-C	5.87	118.70	109.96
1	A	15	LEU	CA-C-N	-5.86	114.84	122.99
1	A	15	LEU	C-N-CA	-5.86	114.84	122.99
1	C	97	THR	CB-CA-C	5.86	120.17	110.74
1	B	25	HIS	CA-CB-CG	-5.86	107.94	113.80
1	C	225	THR	N-CA-CB	5.85	120.30	110.77
1	C	193	VAL	CB-CA-C	-5.83	103.18	111.40
1	C	95	GLU	N-CA-CB	5.81	119.70	110.57
1	A	93	VAL	N-CA-CB	5.81	117.96	110.99
1	C	217	HIS	N-CA-C	5.77	118.63	110.14
1	A	88	MET	N-CA-CB	-5.77	101.82	109.78
1	A	3	LYS	CA-C-N	5.77	126.49	120.03
1	A	3	LYS	C-N-CA	5.77	126.49	120.03
1	A	171	ILE	CB-CG1-CD1	-5.75	101.74	113.80
1	A	141	LEU	N-CA-CB	5.74	119.77	110.41
1	A	19	ASP	CA-C-N	-5.67	115.47	121.48
1	A	19	ASP	C-N-CA	-5.67	115.47	121.48
1	C	185	ASN	N-CA-CB	5.66	119.44	110.55
1	A	212	ASN	CA-C-N	-5.65	115.14	123.05
1	A	212	ASN	C-N-CA	-5.65	115.14	123.05
1	C	119	LEU	N-CA-CB	5.64	119.40	110.55
1	C	23	ASN	CA-CB-CG	5.62	118.22	112.60
1	B	24	GLY	N-CA-C	-5.61	108.01	114.69
1	B	213	GLU	CB-CA-C	5.61	118.24	110.16
1	A	49	THR	N-CA-C	-5.61	105.78	113.30
1	A	125	LEU	O-C-N	5.61	129.77	123.27
1	C	227	ALA	CA-C-N	-5.60	116.81	123.08
1	C	227	ALA	C-N-CA	-5.60	116.81	123.08
1	B	24	GLY	CA-C-N	-5.59	114.75	122.30
1	B	24	GLY	C-N-CA	-5.59	114.75	122.30
1	B	173	ASP	CB-CA-C	-5.59	99.42	110.27
1	C	140	LYS	N-CA-C	5.59	120.21	113.17
1	A	39	TYR	CA-CB-CG	-5.58	103.86	113.90
1	B	175	SER	N-CA-CB	5.58	118.90	110.42
1	B	151	TYR	N-CA-C	5.58	117.83	108.96
1	B	156	LYS	N-CA-CB	5.57	119.18	109.72
1	C	183	GLN	N-CA-C	5.53	118.48	109.24
1	A	22	VAL	O-C-N	5.51	129.04	123.20
1	A	196	PRO	N-CA-C	5.50	119.95	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	GLN	N-CA-CB	-5.49	101.97	110.65
1	C	117	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	45	LYS	CA-C-N	5.46	129.69	122.42
1	C	45	LYS	C-N-CA	5.46	129.69	122.42
1	C	114	PHE	CB-CA-C	-5.45	100.33	109.53
1	B	222	GLU	CG-CD-OE2	-5.45	105.88	118.40
1	C	168	ARG	CA-C-N	-5.45	115.20	122.72
1	C	168	ARG	C-N-CA	-5.45	115.20	122.72
1	C	120	VAL	CA-C-O	5.44	126.25	120.48
1	C	195	LEU	N-CA-CB	5.44	118.88	110.12
1	C	34	GLU	N-CA-C	5.43	117.52	108.99
1	C	55	VAL	O-C-N	5.43	125.91	121.40
1	C	55	VAL	N-CA-CB	5.43	115.58	111.83
1	C	174	GLY	CA-C-N	-5.42	111.13	122.03
1	C	174	GLY	C-N-CA	-5.42	111.13	122.03
1	B	47	ILE	CA-CB-CG2	5.41	119.69	110.50
1	B	217	HIS	N-CA-C	5.41	116.49	108.60
1	B	115	GLU	N-CA-CB	5.40	119.60	110.69
1	A	177	GLN	CB-CG-CD	-5.39	103.43	112.60
1	B	198	ASN	CA-CB-CG	-5.36	107.24	112.60
1	B	52	LYS	N-CA-CB	5.36	119.54	110.49
1	B	61	VAL	N-CA-C	5.33	115.77	110.23
1	A	4	GLY	CA-C-N	5.32	127.41	120.28
1	A	4	GLY	C-N-CA	5.32	127.41	120.28
1	C	44	LEU	CB-CA-C	-5.30	101.45	109.99
1	B	94	GLN	O-C-N	-5.30	117.12	123.27
1	A	16	VAL	N-CA-C	5.29	115.73	108.12
1	B	91	GLY	N-CA-C	5.26	121.80	112.53
1	A	57	TRP	O-C-N	5.25	125.54	120.55
1	A	198	ASN	CA-CB-CG	-5.25	107.35	112.60
1	C	95	GLU	N-CA-C	5.23	117.49	109.07
1	A	197	ASP	N-CA-C	-5.22	103.14	110.35
1	A	195	LEU	CA-C-N	5.22	125.16	119.78
1	A	195	LEU	C-N-CA	5.22	125.16	119.78
1	B	111	GLU	CB-CG-CD	-5.22	103.73	112.60
1	C	175	SER	N-CA-C	-5.22	103.02	110.59
1	C	174	GLY	N-CA-C	-5.20	108.09	115.43
1	B	42	LEU	CB-CA-C	-5.20	99.06	109.35
1	B	197	ASP	N-CA-C	-5.18	103.69	110.53
1	C	174	GLY	CA-C-O	5.18	125.01	119.06
1	B	47	ILE	O-C-N	5.17	128.89	123.00
1	C	109	ARG	CA-C-O	5.17	125.72	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	TYR	CB-CA-C	-5.16	105.06	110.17
1	C	129	ASP	CA-C-N	-5.16	114.91	122.19
1	C	129	ASP	C-N-CA	-5.16	114.91	122.19
1	B	163	VAL	CA-C-N	-5.16	112.72	121.85
1	B	163	VAL	C-N-CA	-5.16	112.72	121.85
1	B	81	HIS	N-CA-C	5.16	119.11	112.41
1	B	128	ILE	N-CA-C	5.13	117.42	108.95
1	A	132	GLU	CB-CG-CD	5.13	121.32	112.60
1	B	118	THR	CA-CB-OG1	-5.13	101.91	109.60
1	B	146	ASN	O-C-N	5.13	128.68	122.68
1	B	209	LYS	N-CA-C	5.12	118.09	109.95
1	C	161	ILE	N-CA-C	5.12	117.10	108.81
1	B	8	PHE	CA-CB-CG	-5.10	108.70	113.80
1	C	108	THR	O-C-N	5.09	129.08	123.33
1	C	26	LYS	N-CA-C	5.08	118.02	109.95
1	A	100	PHE	CA-CB-CG	-5.07	108.73	113.80
1	C	75	PRO	CB-CA-C	-5.07	103.19	111.56
1	C	179	ALA	CB-CA-C	5.06	118.42	111.23
1	B	20	GLY	N-CA-C	5.04	118.47	110.96
1	C	53	LEU	CA-C-N	5.04	126.14	119.84
1	C	53	LEU	C-N-CA	5.04	126.14	119.84
1	B	121	ASN	CA-C-N	-5.03	116.00	123.05
1	B	121	ASN	C-N-CA	-5.03	116.00	123.05
1	B	48	SER	CB-CA-C	-5.03	101.64	109.84
1	C	115	GLU	CB-CA-C	5.03	119.41	111.72
1	A	97	THR	CA-CB-OG1	-5.01	102.08	109.60
1	B	183	GLN	N-CA-C	5.01	117.00	109.23
1	B	102	ASP	N-CA-CB	5.00	119.64	112.08
1	C	63	THR	O-C-N	5.00	128.73	122.23

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

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Mol	Chain	Res	Type	Atom
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
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	116	0
1	B	1760	0	1647	134	0
1	C	1678	0	1488	233	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	481	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 48.

All (481) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:88:MET:HE2	1:C:91:GLY:HA2	1.45	0.98
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
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:C:4:GLY:O	1:C:5:GLU:C	2.27	0.76
1:A:153:MET:HE2	1:A:162:LYS:HE2	1.68	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:173:ASP:CG	1:B:175:SER:H	1.97	0.72
1:A:41:LYS:HG3	1:A:223:PHE:CE1	2.24	0.72
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:131:LYS:C	1:A:137:LEU:HD12	2.17	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: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:C:88:MET:HE2	1:C:91:GLY:CA	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:194:LEU:C	1:B:195:LEU:HD23	2.21	0.65
1:C:213:GLU:OE2	1:C:215:ARG:N	2.30	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
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:C:83:PHE:O	1:C:84:PHE:C	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:170:ASN:C	1:A:171:ILE:HD12	2.27	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:A:82:ASP:OD2	1:A:85:LYS:NZ	2.30	0.59
1:B:18:LEU:HD12	1:B:19:ASP:H	1.67	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:155:ASP:O	1:C:156:LYS:C	2.45	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: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:B:17:GLU:OE1	1:B:17:GLU:HA	2.05	0.56
1:B:125:LEU:HD23	1:B:125:LEU:C	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:TYR:CE1	1:C:112:VAL:HG21	2.40	0.56
1:B:220:LEU:C	1:B:220:LEU:HD23	2.31	0.56
1:C:74:TYR:O	1:C:75:PRO:C	2.42	0.56
1:C:7:LEU:HD21	1:C:89:PRO:HB3	1.88	0.56
1:C:88:MET:CE	1:C:91:GLY:HA2	2.28	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
1:A:47:ILE:CD1	1:A:217:HIS:HB3	2.35	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:C:156:LYS:O	1:C:157:GLN:C	2.50	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:B:39:TYR:HE1	1:C:202:SER:HG	1.55	0.54
1:C:52:LYS:O	1:C:53:LEU:C	2.49	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:51:GLY:O	1:B:52:LYS:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ASP:CG	1:C:158:LYS:H	2.16	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:B:103:ASP:CG	1:B:104:GLY:H	2.17	0.52
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:A:144:ASN:C	1:A:144:ASN:HD22	2.18	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:C:78:MET:HE3	1:C:229:ILE:HD13	1.91	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: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:43:THR:C	1:C:44:LEU:HG	2.34	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:VAL:HB	1:C:201:LEU:HB2	1.93	0.50
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
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:A:78:MET:HE3	1:A:229:ILE:HG13	1.94	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:78:MET:HE1	1:B:226:ALA:HB1	1.95	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: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:103:ASP:CG	1:C:104:GLY:H	2.15	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:97:THR:C	1:C:98:ILE:HD13	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:93:VAL:HG12	1:C:94:GLN:N	2.29	0.47
1:C:100:PHE:O	1:C:101:LYS:C	2.56	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:88:MET:HE1	1:C:112:VAL:O	2.14	0.47
1:C:57:TRP:O	1:C:58:PRO:C	2.54	0.46
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:A:153:MET:HE2	1:A:162:LYS:CE	2.44	0.46
1:B:90:GLU:H	1:B:90:GLU:CD	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:86:SER:C	1:C:88:MET:H	2.24	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:72:SER:O	1:B:85:LYS:NZ	2.38	0.45
1:B:158:LYS:O	1:B:159:ASN:HB3	2.17	0.45
1:B:108:THR:HA	1:B:124:GLU:O	2.16	0.45
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:A:88:MET:HE1	1:A:112:VAL:HG23	1.99	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:22:VAL:HG13	1:C:127:GLY:C	2.42	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:C:118:THR:CG2	1:C:119:LEU:N	2.79	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:B:160:GLY:C	1:B:161:ILE:HG23	2.42	0.44
1:C:118:THR:HG22	1:C:119:LEU:N	2.31	0.44
1:C:206:ALA:C	1:C:207:LEU:HD23	2.43	0.44
1:B:106:TYR:CD1	1:B:130:PHE:CZ	3.05	0.44
1:C:74:TYR:C	1:C:75:PRO:O	2.59	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: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:B:13:PRO:C	1:B:118:THR:HG23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:MET:HB2	1:C:198:ASN:CG	2.43	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:131:LYS:O	1:B:132:GLU:C	2.59	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:B:150:VAL:O	1:B:200:TYR:HA	2.18	0.43
1:B:109:ARG:HG2	1:B:110:ALA:N	2.34	0.43
1:B:198:ASN:ND2	1:B:198:ASN:H	2.15	0.43
1:A:220:LEU:HD21	1:A:222:GLU:HB2	2.01	0.43
1:C:78:MET:HE3	1:C:229:ILE:CD1	2.49	0.43
1:C:80:ARG:C	1:C:81:HIS:ND1	2.77	0.43
1:C:128:ILE:HD12	1:C:128:ILE:C	2.43	0.43
1:A:97:THR:CG2	1:A:99:PHE:CE1	3.00	0.43
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:C:224:VAL:C	1:C:225:THR:HG22	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:82:ASP:O	1:B:83:PHE:C	2.58	0.42
1:C:79:LYS:C	1:C:81:HIS:H	2.27	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:78:MET:HE3	1:A:78:MET:HB3	1.99	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:A:119:LEU:HD13	1:A:119:LEU:C	2.44	0.41
1:B:45:LYS:NZ	1:B:213:GLU:HB2	2.34	0.41
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:B:210:ASP:O	1:B:211:PRO:C	2.62	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:A:220:LEU:C	1:A:220:LEU:HD23	2.45	0.41
1:B:41:LYS:HE2	1:B:223:PHE:CE1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLY:C	1:A:128:ILE:HG23	2.44	0.41
1:B:106:TYR:CD1	1:B:130:PHE:HZ	2.38	0.41
1:C:199:HIS:HB2	1:C:229:ILE:HD12	2.01	0.41
1:A:104:GLY:C	1:A:130:PHE:CZ	2.98	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: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: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:B:14:ILE:HD12	1:B:34:GLU:C	2.46	0.40
1:C:11:VAL:HG11	1:C:34:GLU:OE1	2.21	0.40

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/236 (94%)	214 (96%)	7 (3%)	1 (0%)	24	16
1	B	221/236 (94%)	205 (93%)	15 (7%)	1 (0%)	24	16
1	C	221/236 (94%)	189 (86%)	24 (11%)	8 (4%)	2	0
All	All	664/708 (94%)	608 (92%)	46 (7%)	10 (2%)	8	2

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 ⓘ

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%)	164 (87%)	24 (13%)	4	1
1	B	184/206 (89%)	163 (89%)	21 (11%)	5	2
1	C	164/206 (80%)	133 (81%)	31 (19%)	1	0
All	All	536/618 (87%)	460 (86%)	76 (14%)	3	1

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	3	LYS
1	A	7	LEU
1	A	15	LEU
1	A	21	ASP
1	A	32	GLU
1	A	45	LYS
1	A	47	ILE
1	A	53	LEU
1	A	78	MET
1	A	97	THR
1	A	112	VAL
1	A	120	VAL
1	A	122	ARG
1	A	123	ILE
1	A	126	LYS
1	A	136	ILE
1	A	137	LEU
1	A	141	LEU
1	A	144	ASN
1	A	153	MET
1	A	171	ILE
1	A	177	GLN
1	A	229	ILE
1	B	3	LYS
1	B	25	HIS
1	B	47	ILE
1	B	76	ASP
1	B	79	LYS
1	B	90	GLU
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
1	B	170	ASN
1	B	175	SER
1	B	176	VAL
1	B	178	LEU
1	B	190	ASP
1	B	195	LEU

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Mol	Chain	Res	Type
1	B	215	ARG
1	B	220	LEU
1	C	7	LEU
1	C	18	LEU
1	C	38	THR
1	C	41	LYS
1	C	42	LEU
1	C	46	PHE
1	C	47	ILE
1	C	62	THR
1	C	77	HIS
1	C	83	PHE
1	C	95	GLU
1	C	98	ILE
1	C	99	PHE
1	C	105	ASN
1	C	117	ASP
1	C	123	ILE
1	C	125	LEU
1	C	128	ILE
1	C	133	ASP
1	C	141	LEU
1	C	152	ILE
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	224	VAL
1	C	225	THR
1	C	229	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	135	ASN
1	A	144	ASN
1	A	146	ASN
1	A	149	ASN

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Mol	Chain	Res	Type
1	A	170	ASN
1	A	177	GLN
1	A	184	GLN
1	B	121	ASN
1	B	144	ASN
1	B	159	ASN
1	B	170	ASN
1	C	69	GLN
1	C	81	HIS
1	C	146	ASN
1	C	149	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	22,23,24	2.60	9 (40%)	30,32,34	1.90	9 (30%)
1	CRO	B	66	1	22,23,24	2.54	9 (40%)	30,32,34	1.99	7 (23%)
1	CRO	C	66	1	22,23,24	2.58	8 (36%)	30,32,34	2.13	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	-	1/12/31/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRO	B	66	1	-	0/12/31/32	0/2/2/2
1	CRO	C	66	1	-	1/12/31/32	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CRO	CE1-CZ	6.80	1.51	1.39
1	B	66	CRO	CE1-CZ	6.63	1.51	1.39
1	A	66	CRO	CE1-CZ	5.24	1.48	1.39
1	A	66	CRO	CB2-CA2	5.24	1.40	1.35
1	A	66	CRO	CA3-N3	-4.54	1.38	1.47
1	B	66	CRO	CG2-CB2	-4.43	1.38	1.46
1	C	66	CRO	CE2-CZ	4.39	1.47	1.39
1	C	66	CRO	C1-N3	4.38	1.44	1.37
1	B	66	CRO	CE2-CZ	4.37	1.47	1.39
1	A	66	CRO	CE2-CZ	3.95	1.46	1.39
1	C	66	CRO	CG2-CB2	-3.83	1.39	1.46
1	C	66	CRO	CD1-CG2	3.72	1.47	1.39
1	A	66	CRO	CD1-CG2	3.56	1.46	1.39
1	B	66	CRO	OH-CZ	-3.29	1.29	1.37
1	B	66	CRO	CD1-CG2	3.11	1.45	1.39
1	A	66	CRO	C1-N3	3.05	1.42	1.37
1	B	66	CRO	C1-N2	3.02	1.36	1.32
1	B	66	CRO	C1-N3	2.87	1.42	1.37
1	C	66	CRO	OH-CZ	-2.69	1.30	1.37
1	B	66	CRO	CD2-CG2	2.62	1.44	1.39
1	A	66	CRO	CE1-CD1	-2.34	1.35	1.38
1	A	66	CRO	CD2-CG2	2.28	1.44	1.39
1	C	66	CRO	CB2-CA2	2.25	1.37	1.35
1	B	66	CRO	CA3-N3	-2.15	1.43	1.47
1	C	66	CRO	CE1-CD1	-2.13	1.35	1.38
1	A	66	CRO	CA2-N2	2.01	1.42	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CRO	C2-N3-C1	-5.23	105.64	108.07
1	B	66	CRO	CA1-C1-N3	-4.90	118.89	124.69
1	C	66	CRO	CA1-C1-N3	-4.51	119.35	124.69
1	B	66	CRO	CA1-C1-N2	4.25	129.65	123.88
1	A	66	CRO	CG2-CB2-CA2	4.23	134.89	129.87
1	C	66	CRO	N3-C1-N2	4.21	114.80	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CRO	CE2-CZ-CE1	-3.97	113.44	119.77
1	B	66	CRO	C3-CA3-N3	3.74	120.93	112.43
1	C	66	CRO	CE2-CZ-CE1	-3.63	113.98	119.77
1	A	66	CRO	O2-C2-CA2	3.55	133.29	131.02
1	B	66	CRO	O2-C2-CA2	3.51	133.26	131.02
1	A	66	CRO	CD2-CE2-CZ	3.43	123.50	119.88
1	B	66	CRO	CE2-CZ-CE1	-3.38	114.39	119.77
1	B	66	CRO	CD1-CE1-CZ	3.26	123.33	119.88
1	C	66	CRO	CG2-CB2-CA2	3.17	133.64	129.87
1	C	66	CRO	C1-CA1-N1	-2.98	104.45	109.78
1	C	66	CRO	CD2-CE2-CZ	2.81	122.86	119.88
1	A	66	CRO	C3-CA3-N3	2.75	118.69	112.43
1	A	66	CRO	CD1-CE1-CZ	2.54	122.57	119.88
1	A	66	CRO	CA2-N2-C1	2.34	107.63	105.80
1	C	66	CRO	C3-CA3-N3	2.27	117.59	112.43
1	A	66	CRO	CA1-C1-N3	-2.21	122.07	124.69
1	A	66	CRO	C1-CA1-N1	-2.05	106.12	109.78
1	B	66	CRO	CA2-N2-C1	2.04	107.40	105.80

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	A	66	CRO	N3-C1-CA1-CB1

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	B	66	CRO	2	0
1	C	66	CRO	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	226/236 (95%)	0.50	8 (3%)	47	50	22, 37, 60, 84	0
1	B	225/236 (95%)	0.65	9 (4%)	42	45	24, 41, 62, 81	0
1	C	225/236 (95%)	1.80	87 (38%)	1	0	31, 57, 88, 98	0
All	All	676/708 (95%)	0.98	104 (15%)	5	5	22, 44, 77, 98	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	PRO	5.8
1	C	91	GLY	5.1
1	C	116	GLY	4.9
1	C	90	GLU	4.9
1	C	50	THR	4.8
1	C	89	PRO	4.5
1	C	47	ILE	4.4
1	C	2	SER	4.2
1	C	121	ASN	4.0
1	C	97	THR	3.9
1	C	51	GLY	3.9
1	C	174	GLY	3.9
1	C	27	PHE	3.9
1	C	130	PHE	3.8
1	C	161	ILE	3.7
1	C	24	GLY	3.7
1	C	49	THR	3.5
1	C	48	SER	3.5
1	C	193	VAL	3.5
1	C	128	ILE	3.5
1	C	13	PRO	3.2
1	C	137	LEU	3.2
1	C	190	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	229	ILE	3.2
1	C	217	HIS	3.2
1	C	160	GLY	3.1
1	C	31	GLY	3.0
1	C	8	PHE	3.0
1	C	9	THR	3.0
1	C	191	GLY	3.0
1	C	30	SER	2.9
1	A	229	ILE	2.9
1	A	228	GLY	2.9
1	C	26	LYS	2.9
1	C	98	ILE	2.9
1	C	134	GLY	2.9
1	C	55	VAL	2.8
1	C	112	VAL	2.8
1	C	110	ALA	2.8
1	C	32	GLU	2.8
1	C	153	MET	2.8
1	C	194	LEU	2.8
1	A	80	ARG	2.8
1	B	173	ASP	2.8
1	A	1	MET	2.8
1	C	77	HIS	2.8
1	C	93	VAL	2.8
1	C	21	ASP	2.8
1	C	198	ASN	2.8
1	A	15	LEU	2.8
1	C	215	ARG	2.7
1	C	76	ASP	2.7
1	B	15	LEU	2.7
1	C	185	ASN	2.7
1	C	195	LEU	2.7
1	C	107	LYS	2.7
1	C	163	VAL	2.7
1	A	133	ASP	2.6
1	C	117	ASP	2.6
1	C	92	TYR	2.6
1	A	192	PRO	2.6
1	C	119	LEU	2.6
1	C	141	LEU	2.6
1	C	157	GLN	2.6
1	C	186	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	83	PHE	2.6
1	C	20	GLY	2.6
1	C	108	THR	2.5
1	C	53	LEU	2.5
1	C	154	ALA	2.5
1	B	133	ASP	2.5
1	C	118	THR	2.4
1	C	22	VAL	2.4
1	C	155	ASP	2.4
1	C	196	PRO	2.4
1	C	12	VAL	2.4
1	C	127	GLY	2.4
1	C	86	SER	2.4
1	C	175	SER	2.4
1	C	113	LYS	2.4
1	C	4	GLY	2.3
1	C	63	THR	2.3
1	B	25	HIS	2.3
1	B	214	LYS	2.3
1	C	120	VAL	2.3
1	C	28	SER	2.2
1	B	19	ASP	2.2
1	C	219	VAL	2.2
1	C	122	ARG	2.2
1	C	125	LEU	2.2
1	C	52	LYS	2.2
1	B	117	ASP	2.2
1	C	10	GLY	2.2
1	A	99	PHE	2.1
1	C	189	GLY	2.1
1	C	82	ASP	2.1
1	C	197	ASP	2.1
1	C	104	GLY	2.1
1	B	26	LYS	2.0
1	C	71	PHE	2.0
1	B	175	SER	2.0
1	C	184	GLN	2.0
1	C	15	LEU	2.0
1	C	23	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
1	CRO	C	66	22/23	0.92	0.11	22,41,56,60	0
1	CRO	A	66	22/23	0.96	0.08	14,28,38,70	0
1	CRO	B	66	22/23	0.97	0.06	19,25,33,52	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.