



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:09 AM UTC

PDB ID : 2WHU / pdb_00002whu
Title : Fluorescent Protein mKeima at pH 8.0
Authors : Violot, S.; Carpentier, P.; Blanchoin, L.; Bourgeois, D.
Deposited on : 2009-05-06
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

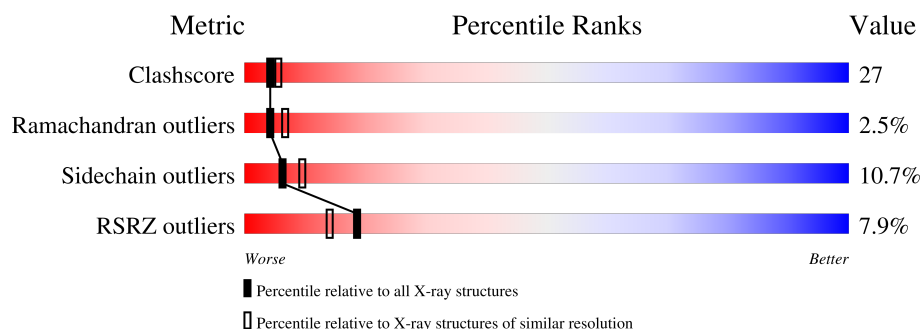
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	240	45% 33% 10% • 10%
1	B	240	4% 49% 35% 6% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7073 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 LARGE STOKES SHIFT FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1733	1102	290	330	11			
1	B	216	Total	C	N	O	S	0	0	0
			1727	1099	287	330	11			
1	C	216	Total	C	N	O	S	0	0	0
			1733	1102	290	330	11			
1	D	216	Total	C	N	O	S	0	0	0
			1733	1102	290	330	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	CRQ	GLN	chromophore	UNP Q1JV70
A	62	CRQ	TYR	chromophore	UNP Q1JV70
A	62	CRQ	GLY	chromophore	UNP Q1JV70
B	62	CRQ	GLN	chromophore	UNP Q1JV70
B	62	CRQ	TYR	chromophore	UNP Q1JV70
B	62	CRQ	GLY	chromophore	UNP Q1JV70
C	62	CRQ	GLN	chromophore	UNP Q1JV70
C	62	CRQ	TYR	chromophore	UNP Q1JV70
C	62	CRQ	GLY	chromophore	UNP Q1JV70
D	62	CRQ	GLN	chromophore	UNP Q1JV70
D	62	CRQ	TYR	chromophore	UNP Q1JV70
D	62	CRQ	GLY	chromophore	UNP Q1JV70

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		
2	B	24	Total	O	0	0
			24	24		

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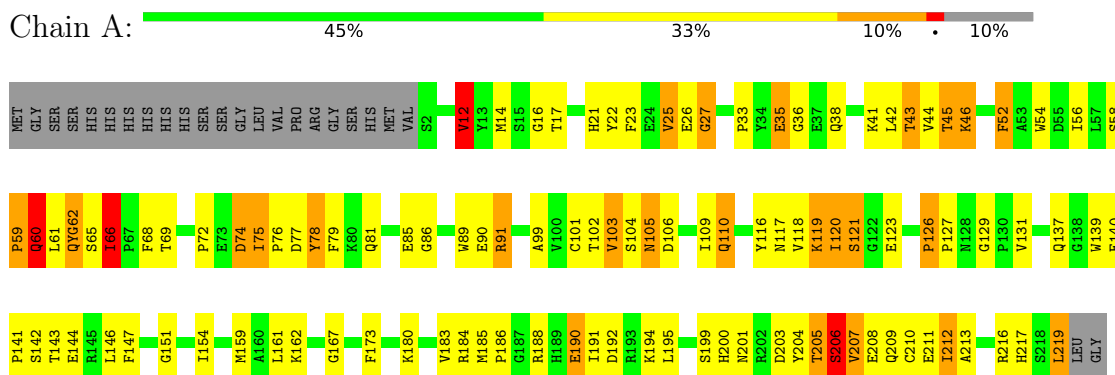
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	30	Total	O	0	0
			30	30		
2	D	29	Total	O	0	0
			29	29		

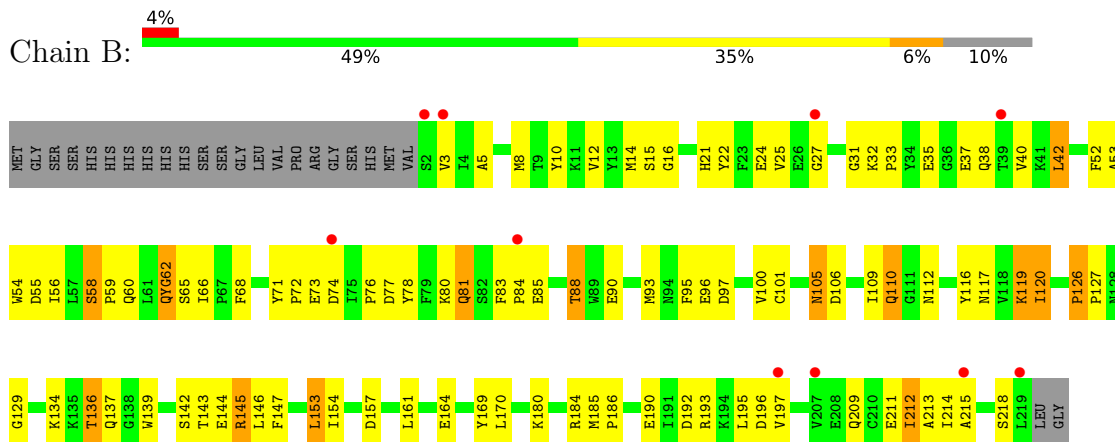
3 Residue-property plots

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.

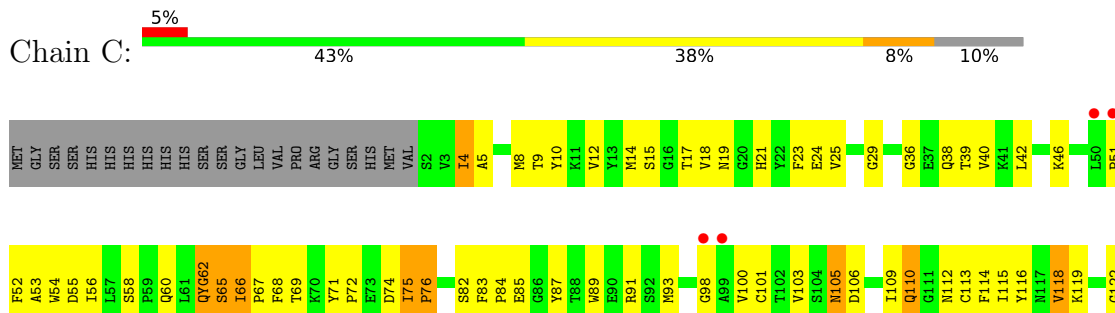
• Molecule 1: LARGE STOKES SHIFT FLUORESCENT PROTEIN

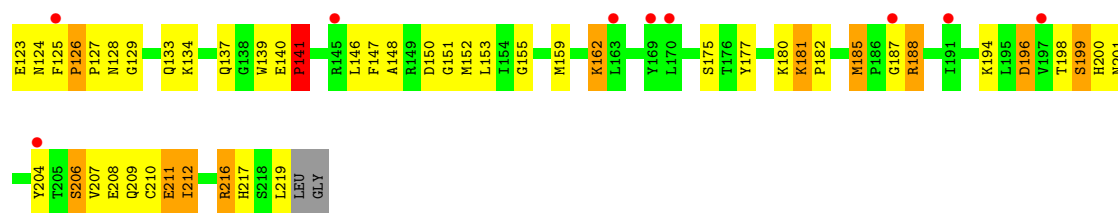


• Molecule 1: LARGE STOKES SHIFT FLUORESCENT PROTEIN

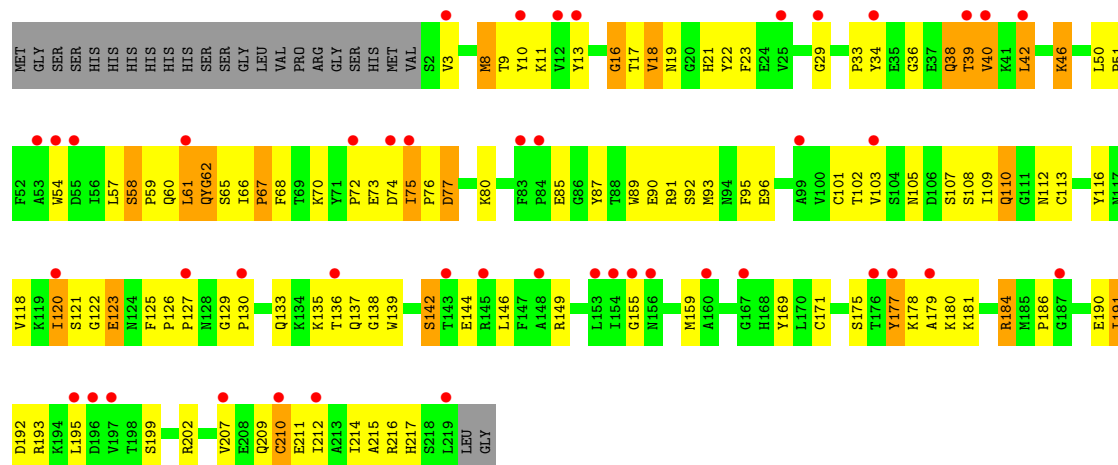
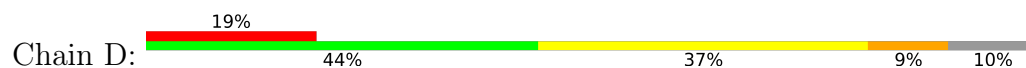


• Molecule 1: LARGE STOKES SHIFT FLUORESCENT PROTEIN





● Molecule 1: LARGE STOKES SHIFT FLUORESCENT PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.11Å 57.75Å 93.07Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	44.81 – 2.65 44.81 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.81-2.65) 99.7 (44.81-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.307 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7073	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CRQ

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	1.58	21/1754 (1.2%)	1.47	18/2369 (0.8%)
1	B	0.98	1/1748 (0.1%)	1.15	7/2362 (0.3%)
1	C	0.96	0/1754	1.21	8/2369 (0.3%)
1	D	1.00	2/1754 (0.1%)	1.24	7/2369 (0.3%)
All	All	1.16	24/7010 (0.3%)	1.27	40/9469 (0.4%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	VAL	CA-CB	17.92	1.74	1.55
1	A	103	VAL	CA-CB	10.45	1.69	1.54
1	A	22	TYR	CA-C	7.19	1.61	1.52
1	A	126	PRO	CA-C	-7.00	1.45	1.52
1	A	99	ALA	CA-CB	-6.93	1.41	1.53
1	A	16	GLY	N-CA	-6.74	1.38	1.45
1	A	44	VAL	N-CA	-6.01	1.38	1.46
1	A	102	THR	CA-CB	5.99	1.66	1.54
1	A	206	SER	N-CA	5.96	1.53	1.45
1	A	103	VAL	N-CA	-5.68	1.39	1.46
1	A	52	PHE	CA-C	5.56	1.59	1.52
1	B	100	VAL	CA-CB	5.52	1.61	1.54
1	A	101	CYS	CA-C	-5.50	1.45	1.52
1	A	22	TYR	N-CA	5.46	1.52	1.46
1	A	27	GLY	N-CA	-5.45	1.39	1.45
1	A	90	GLU	CA-C	-5.33	1.46	1.52
1	A	12	VAL	N-CA	-5.33	1.40	1.46
1	A	60	GLN	CA-CB	5.31	1.61	1.53
1	A	91	ARG	N-CA	-5.23	1.39	1.46
1	D	136	THR	CA-C	5.19	1.59	1.52
1	A	43	THR	CA-C	5.09	1.58	1.52
1	A	102	THR	N-CA	-5.05	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	75	ILE	CA-CB	5.02	1.58	1.54
1	A	121	SER	N-CA	-5.01	1.39	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	138	GLY	N-CA-C	8.89	120.40	111.95
1	B	126	PRO	CA-C-N	7.86	128.27	119.32
1	B	126	PRO	C-N-CA	7.86	128.27	119.32
1	D	142	SER	N-CA-C	7.68	118.13	108.45
1	A	59	PRO	CA-C-N	-7.49	110.68	122.73
1	A	59	PRO	C-N-CA	-7.49	110.68	122.73
1	A	109	ILE	CB-CA-C	-7.17	101.29	111.40
1	A	25	VAL	N-CA-C	-7.06	98.59	108.27
1	C	126	PRO	CA-C-N	6.65	126.78	119.87
1	C	126	PRO	C-N-CA	6.65	126.78	119.87
1	A	89	TRP	N-CA-C	6.63	118.28	108.60
1	D	120	ILE	N-CA-C	6.55	117.55	108.12
1	A	131	VAL	N-CA-CB	6.49	118.87	110.57
1	C	4	ILE	N-CA-C	6.41	116.86	107.37
1	A	207	VAL	N-CA-C	-6.31	99.17	107.88
1	D	16	GLY	N-CA-C	6.28	119.04	110.69
1	C	181	LYS	CA-C-N	6.26	127.66	119.84
1	C	181	LYS	C-N-CA	6.26	127.66	119.84
1	B	120	ILE	N-CA-C	6.25	116.86	108.11
1	A	142	SER	N-CA-C	6.14	116.38	108.34
1	A	206	SER	CA-C-O	-6.11	114.21	121.11
1	B	58	SER	CA-C-N	-6.08	113.70	120.45
1	B	58	SER	C-N-CA	-6.08	113.70	120.45
1	A	90	GLU	N-CA-C	-5.89	100.09	109.23
1	A	74	ASP	CA-C-N	-5.86	118.23	123.33
1	A	74	ASP	C-N-CA	-5.86	118.23	123.33
1	A	45	THR	N-CA-C	5.83	119.92	112.34
1	B	109	ILE	N-CA-C	5.79	116.20	108.27
1	A	66	ILE	N-CA-C	5.79	121.38	108.88
1	D	202	ARG	N-CA-C	5.73	118.30	111.71
1	D	136	THR	N-CA-C	5.70	119.34	110.17
1	C	100	VAL	N-CA-C	5.62	116.21	108.12
1	C	109	ILE	N-CA-C	5.51	116.97	108.44
1	A	205	THR	N-CA-C	5.38	119.70	113.18
1	A	129	GLY	CA-C-N	-5.28	114.31	119.64
1	A	129	GLY	C-N-CA	-5.28	114.31	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	PHE	N-CA-C	5.28	118.19	109.85
1	D	102	THR	CB-CA-C	5.15	118.13	109.48
1	C	185	MET	N-CA-C	5.12	116.28	109.93
1	B	196	ASP	N-CA-C	5.12	116.75	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1733	0	1662	86	0
1	B	1727	0	1650	86	0
1	C	1733	0	1662	95	0
1	D	1733	0	1662	105	0
2	A	64	0	0	7	0
2	B	24	0	0	3	0
2	C	30	0	0	3	0
2	D	29	0	0	3	0
All	All	7073	0	6636	368	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (368) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLY:HA2	1:A:185:MET:CE	1.72	1.18
1:D:77:ASP:OD2	1:D:80:LYS:HD2	1.49	1.13
1:D:58:SER:HA	1:D:209:GLN:HE22	0.98	1.07
1:A:58:SER:HA	1:A:209:GLN:HE22	1.19	1.06
1:D:58:SER:CA	1:D:209:GLN:HE22	1.68	1.06
1:D:184:ARG:HH11	1:D:184:ARG:HG3	1.26	1.00
1:A:151:GLY:HA2	1:A:185:MET:HE2	1.00	0.98
1:D:76:PRO:O	1:D:186:PRO:HG3	1.65	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TRP:HE1	1:A:209:GLN:HE21	1.10	0.97
1:C:58:SER:HB2	1:C:209:GLN:NE2	1.82	0.95
1:A:151:GLY:CA	1:A:185:MET:HE2	1.94	0.95
1:D:58:SER:HA	1:D:209:GLN:NE2	1.83	0.92
1:D:76:PRO:HD2	1:D:186:PRO:HB3	1.52	0.92
1:C:67:PRO:HD3	1:C:87:TYR:OH	1.70	0.92
1:D:184:ARG:HH11	1:D:184:ARG:CG	1.84	0.91
1:B:12:VAL:HG23	1:B:116:TYR:HB2	1.53	0.90
1:A:58:SER:HB2	1:A:59:PRO:HD3	1.54	0.89
1:D:77:ASP:OD2	1:D:80:LYS:CD	2.19	0.89
1:A:151:GLY:CA	1:A:185:MET:CE	2.51	0.86
1:D:175:SER:HB3	1:D:177:TYR:CE2	2.13	0.83
1:B:38:GLN:HE22	1:B:65:SER:HB3	1.45	0.81
1:D:23:PHE:HA	1:D:46:LYS:O	1.80	0.81
1:C:216:ARG:HG3	1:C:216:ARG:HH11	1.43	0.81
1:A:54:TRP:HE1	1:A:209:GLN:NE2	1.80	0.80
1:A:203:ASP:OD1	1:A:205:THR:HG23	1.80	0.80
1:D:89:TRP:HZ3	1:D:91:ARG:HB2	1.46	0.79
1:C:58:SER:HB2	1:C:209:GLN:HE22	1.45	0.78
1:D:58:SER:HB3	1:D:209:GLN:NE2	1.99	0.77
1:D:89:TRP:CZ3	1:D:91:ARG:HB2	2.20	0.77
1:B:54:TRP:HE1	1:B:209:GLN:HE21	1.32	0.76
1:D:107:SER:OG	1:D:116:TYR:CD1	2.38	0.76
1:A:65:SER:HB2	1:A:116:TYR:OH	1.85	0.76
1:D:62:CRQ:O2	1:D:91:ARG:NH2	2.13	0.76
1:D:33:PRO:HA	1:D:68:PHE:HA	1.67	0.75
1:A:151:GLY:C	1:A:185:MET:HE1	2.12	0.75
1:D:72:PRO:HG2	1:D:75:ILE:HD12	1.67	0.75
1:A:52:PHE:CD1	1:A:56:ILE:HD11	2.22	0.75
1:D:9:THR:OG1	1:D:113:CYS:HB2	1.88	0.74
1:C:10:TYR:CD1	1:C:116:TYR:HE2	2.05	0.74
1:A:151:GLY:O	1:A:185:MET:HE1	1.89	0.73
1:A:219:LEU:HD21	1:B:212:ILE:HG23	1.70	0.72
1:A:33:PRO:HA	1:A:68:PHE:HA	1.72	0.70
1:D:107:SER:OG	1:D:116:TYR:HD1	1.75	0.70
1:D:72:PRO:CG	1:D:75:ILE:HD12	2.21	0.70
1:D:96:GLU:OE2	1:D:169:TYR:HA	1.92	0.70
1:A:58:SER:HB2	1:A:59:PRO:CD	2.22	0.70
1:C:54:TRP:HB2	1:C:204:TYR:HD2	1.57	0.70
1:D:58:SER:CA	1:D:209:GLN:NE2	2.50	0.69
1:A:200:HIS:HD2	1:A:201:ASN:O	1.76	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:CRQ:HD2	1:B:62:CRQ:O2	1.93	0.69
1:C:147:PHE:HB3	1:C:188:ARG:HD3	1.75	0.69
1:B:144:GLU:HG2	1:B:146:LEU:HD11	1.75	0.69
1:A:54:TRP:CE2	1:A:207:VAL:HG11	2.27	0.69
1:A:58:SER:HA	1:A:209:GLN:NE2	2.03	0.68
1:B:5:ALA:HB3	1:B:8:MET:HG2	1.76	0.68
1:D:175:SER:CB	1:D:177:TYR:CE2	2.76	0.68
1:C:216:ARG:HH11	1:C:216:ARG:CG	2.07	0.67
1:C:10:TYR:CE2	1:C:29:GLY:HA3	2.30	0.67
1:C:198:THR:O	1:C:199:SER:HB3	1.95	0.67
1:C:62:CRQ:HD2	1:C:62:CRQ:O2	1.94	0.67
1:D:58:SER:CB	1:D:209:GLN:NE2	2.59	0.66
1:B:137:GLN:NE2	1:B:164:GLU:HG3	2.11	0.66
1:B:97:ASP:HB2	1:B:169:TYR:CE1	2.30	0.65
1:B:38:GLN:NE2	1:B:65:SER:HB3	2.11	0.65
1:C:10:TYR:CD1	1:C:116:TYR:CE2	2.85	0.65
1:D:184:ARG:HG3	1:D:184:ARG:NH1	2.06	0.64
1:D:133:GLN:HB2	1:D:135:LYS:HG2	1.79	0.64
1:C:18:VAL:HB	1:C:52:PHE:CE2	2.33	0.64
1:C:110:GLN:NE2	2:C:2014:HOH:O	2.31	0.64
1:C:128:ASN:O	1:C:133:GLN:HG2	1.98	0.64
1:C:211:GLU:HG3	1:C:212:ILE:N	2.14	0.63
1:A:26:GLU:HG3	1:A:45:THR:HG21	1.78	0.63
1:D:217:HIS:CD2	2:D:2009:HOH:O	2.51	0.63
1:C:17:THR:HA	1:C:21:HIS:O	1.99	0.63
1:A:81:GLN:OE1	1:A:183:VAL:HB	1.99	0.63
1:A:219:LEU:HD21	1:B:212:ILE:CG2	2.28	0.63
1:D:42:LEU:HD22	1:D:42:LEU:N	2.12	0.63
1:D:87:TYR:HB3	1:D:179:ALA:HA	1.80	0.63
1:A:66:ILE:HG21	1:A:79:PHE:CE2	2.34	0.62
1:B:5:ALA:H	1:B:8:MET:HE3	1.64	0.62
1:B:88:THR:HG22	1:B:105:ASN:O	1.99	0.62
1:A:23:PHE:HA	1:A:46:LYS:O	1.99	0.62
1:A:65:SER:HB2	1:A:116:TYR:CZ	2.35	0.62
1:C:58:SER:CB	1:C:209:GLN:HE22	2.11	0.62
1:D:199:SER:HB3	2:D:2021:HOH:O	1.99	0.62
1:A:144:GLU:O	1:A:190:GLU:HA	2.00	0.61
1:A:81:GLN:OE1	1:A:184:ARG:N	2.31	0.61
1:A:119:LYS:HE2	2:A:2032:HOH:O	1.99	0.61
1:C:14:MET:HA	1:C:118:VAL:O	2.00	0.61
1:B:12:VAL:HG23	1:B:116:TYR:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HD2	1:A:75:ILE:HG13	1.81	0.61
1:A:60:GLN:OE1	1:A:91:ARG:NH1	2.34	0.61
1:B:144:GLU:HG2	1:B:146:LEU:CD1	2.32	0.60
1:C:12:VAL:HG23	1:C:116:TYR:HB2	1.82	0.60
1:C:52:PHE:CE1	1:C:56:ILE:HD11	2.36	0.60
1:B:8:MET:HE2	1:B:112:ASN:HA	1.83	0.60
1:A:76:PRO:HD2	1:A:186:PRO:HB3	1.83	0.60
1:B:15:SER:HB3	1:B:24:GLU:HG2	1.83	0.60
1:D:62:CRQ:O2	1:D:62:CRQ:HD2	2.02	0.60
1:C:201:ASN:ND2	1:C:206:SER:HB2	2.17	0.60
1:B:32:LYS:HD2	1:B:35:GLU:HG2	1.84	0.59
1:B:83:PHE:HB3	1:B:84:PRO:HA	1.84	0.59
1:B:58:SER:CB	1:B:209:GLN:NE2	2.65	0.59
1:B:96:GLU:HG2	1:B:170:LEU:H	1.68	0.59
1:B:10:TYR:OH	1:B:40:VAL:HB	2.02	0.59
1:B:137:GLN:HE22	1:B:164:GLU:HG3	1.66	0.59
1:D:175:SER:CB	1:D:177:TYR:HE2	2.14	0.59
1:A:151:GLY:C	1:A:185:MET:CE	2.75	0.59
1:D:58:SER:CB	1:D:209:GLN:HE22	2.13	0.59
1:A:110:GLN:O	1:A:110:GLN:HG3	2.00	0.59
1:C:60:GLN:HG3	1:C:103:VAL:HG11	1.85	0.59
1:B:117:ASN:OD1	1:B:119:LYS:HE3	2.03	0.58
1:D:70:LYS:HB3	1:D:214:ILE:HG12	1.86	0.58
1:C:124:ASN:O	1:C:126:PRO:HD3	2.03	0.57
1:B:93:MET:HB2	1:B:101:CYS:HB2	1.86	0.57
1:A:12:VAL:HG21	1:A:61:LEU:CD2	2.34	0.57
1:D:10:TYR:CE2	1:D:29:GLY:HA3	2.39	0.57
1:C:211:GLU:CG	1:C:212:ILE:N	2.67	0.57
1:D:109:ILE:HG12	1:D:110:GLN:N	2.18	0.57
1:B:146:LEU:N	1:B:146:LEU:HD12	2.19	0.57
1:D:144:GLU:O	1:D:190:GLU:HA	2.05	0.57
1:B:53:ALA:HB2	1:B:134:LYS:HA	1.87	0.57
1:B:97:ASP:HB2	1:B:169:TYR:OH	2.05	0.57
1:D:76:PRO:O	1:D:186:PRO:CG	2.48	0.57
1:D:17:THR:HA	1:D:21:HIS:O	2.05	0.57
1:B:97:ASP:CB	1:B:169:TYR:OH	2.52	0.56
1:C:151:GLY:HA2	1:C:185:MET:HE2	1.87	0.56
1:C:151:GLY:CA	1:C:185:MET:HE2	2.35	0.56
1:C:134:LYS:NZ	2:C:2017:HOH:O	2.37	0.56
1:B:105:ASN:HA	1:B:117:ASN:O	2.05	0.56
1:D:76:PRO:HB2	1:D:186:PRO:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:MET:HB2	1:C:101:CYS:HB2	1.88	0.55
1:C:38:GLN:HE22	1:C:65:SER:HB3	1.70	0.55
1:B:16:GLY:O	1:B:22:TYR:HA	2.07	0.55
1:D:72:PRO:O	1:D:74:ASP:N	2.40	0.55
1:D:77:ASP:OD2	1:D:80:LYS:CE	2.55	0.55
1:C:54:TRP:HB2	1:C:204:TYR:CD2	2.40	0.55
1:C:155:GLY:N	1:C:175:SER:O	2.40	0.55
1:D:129:GLY:O	1:D:133:GLN:HG2	2.07	0.55
1:A:146:LEU:HA	1:A:154:ILE:O	2.06	0.55
1:D:216:ARG:NH1	1:D:216:ARG:HG3	2.21	0.54
1:B:5:ALA:H	1:B:8:MET:CE	2.20	0.54
1:A:65:SER:HB3	1:A:116:TYR:CE2	2.42	0.54
1:B:77:ASP:OD2	1:B:80:LYS:NZ	2.41	0.54
1:D:142:SER:O	1:D:192:ASP:HA	2.08	0.54
1:D:36:GLY:O	1:D:212:ILE:HA	2.06	0.54
1:D:177:TYR:N	1:D:177:TYR:CD2	2.76	0.54
1:B:97:ASP:OD2	1:B:126:PRO:CD	2.55	0.54
1:A:17:THR:HA	1:A:21:HIS:O	2.08	0.53
1:B:97:ASP:HB2	1:B:169:TYR:HE1	1.72	0.53
1:C:24:GLU:HB2	1:C:46:LYS:HB3	1.89	0.53
1:C:148:ALA:HB1	1:C:185:MET:HE3	1.91	0.53
1:D:11:LYS:HE3	1:D:13:TYR:CZ	2.43	0.53
1:D:54:TRP:CZ3	1:D:57:LEU:HD12	2.44	0.53
1:C:19:ASN:HD21	1:C:125:PHE:HB2	1.73	0.53
1:D:216:ARG:HG3	1:D:216:ARG:HH11	1.73	0.53
1:A:103:VAL:HG22	1:A:120:ILE:HD12	1.90	0.53
1:B:58:SER:HB2	1:B:209:GLN:NE2	2.23	0.53
1:C:139:TRP:CE3	1:C:159:MET:HE3	2.44	0.53
1:C:194:LYS:HE3	1:C:196:ASP:OD2	2.09	0.53
1:A:25:VAL:HA	1:A:43:THR:O	2.09	0.52
1:B:214:ILE:HG22	1:B:215:ALA:N	2.24	0.52
1:B:58:SER:CB	1:B:209:GLN:HE22	2.22	0.52
1:D:130:PRO:O	1:D:135:LYS:HB2	2.09	0.52
1:D:146:LEU:HD11	1:D:191:ILE:HG13	1.91	0.52
1:C:14:MET:HE1	1:C:60:GLN:HB2	1.90	0.52
1:D:217:HIS:HD2	2:D:2009:HOH:O	1.89	0.52
1:B:137:GLN:NE2	1:B:164:GLU:HA	2.25	0.52
1:A:110:GLN:NE2	1:C:15:SER:HB3	2.25	0.52
1:B:78:TYR:CE1	1:B:185:MET:HE1	2.44	0.52
1:A:194:LYS:HB3	1:A:212:ILE:HG22	1.93	0.51
1:B:27:GLY:HA3	1:B:42:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLU:OE2	1:D:155:GLY:HA3	2.10	0.51
1:A:26:GLU:HG3	1:A:45:THR:CG2	2.41	0.51
1:D:19:ASN:OD1	1:D:123:GLU:HA	2.10	0.51
1:D:34:TYR:HE1	1:D:80:LYS:HD3	1.75	0.51
1:C:58:SER:CA	1:C:209:GLN:HE22	2.23	0.51
1:D:184:ARG:CG	1:D:184:ARG:NH1	2.56	0.51
1:A:14:MET:HE3	1:A:61:LEU:HD21	1.90	0.51
1:B:139:TRP:CZ3	1:B:161:LEU:HG	2.46	0.51
1:C:66:ILE:O	1:C:67:PRO:C	2.53	0.51
1:C:198:THR:O	1:C:199:SER:CB	2.58	0.51
1:D:33:PRO:CA	1:D:68:PHE:HA	2.40	0.51
1:B:54:TRP:HE1	1:B:209:GLN:NE2	2.06	0.51
1:C:36:GLY:HA2	1:C:68:PHE:O	2.11	0.51
1:C:91:ARG:NH2	1:C:177:TYR:OH	2.42	0.51
1:C:216:ARG:CG	1:C:216:ARG:NH1	2.68	0.51
1:B:193:ARG:HG2	1:B:213:ALA:CB	2.41	0.51
1:B:62:CRQ:N1	1:B:62:CRQ:CA3	2.73	0.51
1:B:193:ARG:HG2	1:B:213:ALA:HB2	1.92	0.50
1:D:190:GLU:O	1:D:215:ALA:HA	2.10	0.50
1:A:14:MET:HE3	1:A:61:LEU:CD2	2.41	0.50
1:B:72:PRO:C	1:B:74:ASP:H	2.18	0.50
1:C:75:ILE:O	1:C:76:PRO:C	2.51	0.50
1:B:214:ILE:CG2	1:B:215:ALA:N	2.74	0.50
1:C:91:ARG:HB3	1:C:103:VAL:HB	1.94	0.50
1:D:175:SER:HB2	1:D:177:TYR:HE2	1.75	0.50
1:A:35:GLU:OE2	1:A:35:GLU:HA	2.12	0.50
1:D:77:ASP:CG	1:D:80:LYS:HD2	2.33	0.50
1:B:145:ARG:C	1:B:146:LEU:HD12	2.37	0.50
1:B:62:CRQ:N1	1:B:62:CRQ:C3	2.75	0.50
1:D:133:GLN:CB	1:D:135:LYS:HG2	2.41	0.49
1:B:147:PHE:CE2	1:B:154:ILE:HB	2.47	0.49
1:C:12:VAL:CG2	1:C:116:TYR:HB2	2.42	0.49
1:C:69:THR:O	1:C:71:TYR:HD1	1.96	0.49
1:C:74:ASP:OD2	1:C:217:HIS:CE1	2.65	0.49
1:C:53:ALA:O	1:C:54:TRP:C	2.55	0.49
1:C:54:TRP:HE1	1:C:209:GLN:HE21	1.59	0.49
1:B:76:PRO:O	1:B:186:PRO:HB3	2.12	0.49
1:C:105:ASN:C	1:C:105:ASN:ND2	2.71	0.49
1:B:218:SER:O	2:B:2023:HOH:O	2.20	0.48
1:A:12:VAL:HG21	1:A:61:LEU:HD23	1.95	0.48
1:C:85:GLU:OE1	1:C:85:GLU:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:PHE:CD1	1:B:56:ILE:HD11	2.48	0.48
1:B:60:GLN:NE2	1:B:93:MET:SD	2.86	0.48
1:B:72:PRO:C	1:B:74:ASP:N	2.72	0.48
1:B:97:ASP:OD2	1:B:126:PRO:HD2	2.13	0.48
1:D:34:TYR:CE1	1:D:80:LYS:HE3	2.48	0.48
1:D:85:GLU:OE1	1:D:85:GLU:N	2.32	0.48
1:B:120:ILE:O	1:B:120:ILE:HG23	2.13	0.48
1:B:144:GLU:CG	1:B:146:LEU:HD11	2.43	0.48
1:A:139:TRP:CE3	1:A:159:MET:HE3	2.49	0.48
1:A:147:PHE:CE2	1:A:154:ILE:HB	2.49	0.48
1:A:65:SER:CB	1:A:116:TYR:CE2	2.97	0.47
1:A:162:LYS:NZ	2:A:2042:HOH:O	2.46	0.47
1:D:72:PRO:C	1:D:74:ASP:N	2.71	0.47
1:D:85:GLU:O	1:D:180:LYS:HD3	2.14	0.47
1:D:135:LYS:HA	1:D:135:LYS:HD3	1.68	0.47
1:B:112:ASN:HB2	2:B:2012:HOH:O	2.13	0.47
1:D:87:TYR:HB2	1:D:178:LYS:O	2.14	0.47
1:C:150:ASP:C	1:C:152:MET:H	2.23	0.47
1:A:195:LEU:HD13	1:A:211:GLU:HB2	1.95	0.47
1:B:81:GLN:OE1	1:B:184:ARG:HB2	2.15	0.47
1:D:16:GLY:O	1:D:22:TYR:HA	2.15	0.47
1:D:103:VAL:HG22	1:D:120:ILE:HD12	1.96	0.47
1:C:38:GLN:O	1:C:210:CYS:HA	2.14	0.47
1:B:31:GLY:O	1:B:68:PHE:HE2	1.97	0.47
1:B:110:GLN:HE21	1:B:110:GLN:HA	1.80	0.47
1:D:109:ILE:CG1	1:D:110:GLN:N	2.77	0.47
1:C:137:GLN:N	1:C:162:LYS:O	2.48	0.47
1:D:18:VAL:HA	1:D:122:GLY:O	2.15	0.47
1:D:130:PRO:HA	1:D:135:LYS:HB2	1.97	0.47
1:C:19:ASN:ND2	1:C:125:PHE:HB2	2.30	0.46
1:A:69:THR:HG21	1:A:191:ILE:HD13	1.97	0.46
1:A:105:ASN:C	1:A:105:ASN:ND2	2.73	0.46
1:A:117:ASN:HD22	1:C:115:ILE:HD12	1.80	0.46
1:A:86:GLY:O	1:A:180:LYS:HB2	2.15	0.46
1:B:16:GLY:HA3	1:B:120:ILE:O	2.15	0.46
1:B:40:VAL:HG13	1:B:42:LEU:HD21	1.98	0.46
1:C:15:SER:O	1:C:119:LYS:HA	2.15	0.46
1:A:66:ILE:HG21	1:A:79:PHE:CZ	2.51	0.46
1:D:8:MET:CE	1:D:112:ASN:HA	2.45	0.46
1:B:195:LEU:HD12	1:B:211:GLU:HB2	1.97	0.46
1:D:34:TYR:CD1	1:D:80:LYS:HE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HG3	2:A:2054:HOH:O	2.14	0.46
1:B:77:ASP:O	1:B:81:GLN:HB2	2.16	0.46
1:D:67:PRO:HD3	1:D:87:TYR:OH	2.16	0.46
1:B:97:ASP:HB2	1:B:169:TYR:CZ	2.51	0.45
1:B:110:GLN:O	1:B:110:GLN:HG3	2.15	0.45
1:B:144:GLU:O	1:B:190:GLU:HA	2.16	0.45
1:C:89:TRP:CZ3	1:C:91:ARG:HB2	2.51	0.45
1:C:152:MET:HE3	1:C:152:MET:HB2	1.87	0.45
1:C:58:SER:HA	1:C:209:GLN:HE22	1.82	0.45
1:B:21:HIS:ND1	2:B:2001:HOH:O	2.36	0.45
1:D:66:ILE:N	1:D:67:PRO:HD2	2.32	0.45
1:A:212:ILE:HD13	1:A:213:ALA:N	2.32	0.45
1:B:95:PHE:CD1	1:B:169:TYR:CE2	3.04	0.45
1:D:54:TRP:HE1	1:D:209:GLN:HE21	1.65	0.45
1:D:107:SER:OG	1:D:116:TYR:CE1	2.63	0.45
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.47	0.45
1:B:33:PRO:HA	1:B:68:PHE:HA	1.99	0.45
1:D:11:LYS:HE3	1:D:13:TYR:OH	2.17	0.45
1:D:58:SER:HA	1:D:61:LEU:HD12	1.99	0.45
1:A:143:THR:HG23	1:A:192:ASP:OD1	2.17	0.45
1:C:10:TYR:HD1	1:C:116:TYR:CE2	2.34	0.45
1:C:23:PHE:HA	1:C:46:LYS:O	2.17	0.45
1:D:59:PRO:O	1:D:62:CRQ:C2	2.65	0.45
1:D:8:MET:HE2	1:D:112:ASN:HA	1.99	0.44
1:C:106:ASP:OD2	1:C:180:LYS:NZ	2.38	0.44
1:D:72:PRO:C	1:D:74:ASP:H	2.25	0.44
1:B:126:PRO:HA	1:B:127:PRO:HD3	1.82	0.44
1:C:83:PHE:HB3	1:C:84:PRO:HA	1.99	0.44
1:A:159:MET:HE2	1:A:173:PHE:CZ	2.53	0.44
1:C:14:MET:HB3	1:C:25:VAL:HB	1.98	0.44
1:D:126:PRO:HA	1:D:127:PRO:HD2	1.84	0.44
1:D:195:LEU:HD12	1:D:210:CYS:O	2.18	0.44
1:C:126:PRO:HA	1:C:127:PRO:HD3	1.68	0.44
1:D:39:THR:O	1:D:40:VAL:HB	2.18	0.44
1:A:120:ILE:HG13	1:A:121:SER:N	2.32	0.43
1:B:77:ASP:OD2	1:B:80:LYS:CE	2.66	0.43
1:C:62:CRQ:HD2	1:C:62:CRQ:C2	2.48	0.43
1:C:128:ASN:HA	1:C:133:GLN:HE21	1.82	0.43
1:C:66:ILE:H	1:C:66:ILE:HG12	1.49	0.43
1:D:54:TRP:CE2	1:D:207:VAL:HG11	2.54	0.43
1:A:27:GLY:HA2	1:A:41:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:OE1	1:A:65:SER:OG	2.36	0.43
1:A:140:GLU:O	1:A:141:PRO:C	2.61	0.43
1:C:12:VAL:HB	1:C:116:TYR:HD2	1.82	0.43
1:A:74:ASP:OD2	1:A:217:HIS:NE2	2.49	0.43
1:B:106:ASP:OD2	1:B:180:LYS:NZ	2.21	0.43
1:D:89:TRP:CE2	1:D:105:ASN:HB3	2.54	0.43
1:D:95:PHE:CD1	1:D:171:CYS:HB2	2.54	0.43
1:D:50:LEU:HA	1:D:51:PRO:HD2	1.88	0.43
1:A:36:GLY:O	1:A:212:ILE:HA	2.19	0.43
1:A:62:CRQ:HD2	1:A:62:CRQ:O2	2.19	0.43
1:D:109:ILE:CG1	1:D:110:GLN:H	2.32	0.43
1:D:10:TYR:CD2	1:D:29:GLY:HA3	2.54	0.43
1:B:14:MET:HE1	1:B:60:GLN:HB2	2.01	0.43
1:A:203:ASP:O	1:A:204:TYR:C	2.62	0.42
1:B:143:THR:OG1	1:B:192:ASP:OD1	2.31	0.42
1:C:55:ASP:CG	2:C:2008:HOH:O	2.63	0.42
1:A:137:GLN:O	1:A:162:LYS:HE2	2.20	0.42
1:A:208:GLU:HB3	2:A:2062:HOH:O	2.19	0.42
1:C:8:MET:HE3	1:C:112:ASN:HA	2.02	0.42
1:B:142:SER:HB2	1:B:157:ASP:OD1	2.19	0.42
1:C:10:TYR:OH	1:C:40:VAL:HB	2.20	0.42
1:A:52:PHE:N	1:A:52:PHE:CD2	2.86	0.42
1:B:58:SER:N	1:B:59:PRO:CD	2.82	0.42
1:A:146:LEU:CD1	1:A:191:ILE:HG13	2.49	0.42
1:B:58:SER:HB3	1:B:209:GLN:NE2	2.35	0.42
1:C:9:THR:O	1:C:113:CYS:HA	2.19	0.42
1:C:200:HIS:CD2	1:C:204:TYR:CE1	3.07	0.42
1:A:103:VAL:CG2	1:A:120:ILE:HD12	2.49	0.42
1:A:126:PRO:HA	1:A:127:PRO:HD3	1.94	0.42
1:A:139:TRP:O	2:A:2042:HOH:O	2.21	0.42
1:D:10:TYR:CD1	1:D:116:TYR:HE2	2.38	0.42
1:A:58:SER:CB	1:A:59:PRO:CD	2.95	0.41
1:D:193:ARG:HA	1:D:212:ILE:O	2.19	0.41
1:D:93:MET:HB2	1:D:101:CYS:HB2	2.02	0.41
1:C:5:ALA:HB3	1:C:8:MET:HG3	2.01	0.41
1:C:54:TRP:CE2	1:C:207:VAL:HG11	2.55	0.41
1:A:200:HIS:CD2	1:A:201:ASN:O	2.66	0.41
1:C:19:ASN:OD1	1:C:124:ASN:N	2.51	0.41
1:B:153:LEU:HD11	1:B:186:PRO:HG2	2.02	0.41
1:D:38:GLN:HE22	1:D:65:SER:CB	2.33	0.41
1:B:78:TYR:HE1	1:B:185:MET:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:GLU:HG3	1:C:212:ILE:H	1.82	0.41
1:D:62:CRQ:HD2	1:D:62:CRQ:C2	2.51	0.41
1:D:139:TRP:CE3	1:D:159:MET:HE3	2.55	0.41
1:C:54:TRP:CE3	1:C:207:VAL:HG21	2.55	0.41
1:C:89:TRP:HZ3	1:C:91:ARG:HB2	1.86	0.41
1:D:75:ILE:HA	1:D:76:PRO:HD3	1.98	0.41
1:C:75:ILE:HA	1:C:76:PRO:HD2	1.95	0.41
1:D:125:PHE:O	1:D:126:PRO:C	2.63	0.41
1:A:203:ASP:OD1	1:A:203:ASP:C	2.64	0.41
1:C:39:THR:HA	1:C:209:GLN:O	2.21	0.41
1:C:140:GLU:O	1:C:141:PRO:C	2.62	0.41
1:A:104:SER:HB3	2:A:2028:HOH:O	2.20	0.41
1:A:106:ASP:OD2	1:A:180:LYS:NZ	2.51	0.41
1:B:95:PHE:O	1:B:96:GLU:C	2.64	0.41
1:D:42:LEU:N	1:D:42:LEU:CD2	2.82	0.41
1:A:201:ASN:CG	1:A:206:SER:H	2.27	0.40
1:D:76:PRO:HG2	1:D:186:PRO:HA	2.03	0.40
1:C:8:MET:CE	1:C:114:PHE:CE2	3.04	0.40
1:A:77:ASP:O	1:A:78:TYR:C	2.64	0.40
1:C:14:MET:CE	1:C:60:GLN:HB3	2.51	0.40
1:C:38:GLN:NE2	1:C:65:SER:HB3	2.36	0.40
1:C:82:SER:O	1:C:181:LYS:HE2	2.22	0.40
1:D:87:TYR:CB	1:D:179:ALA:HA	2.49	0.40
1:A:85:GLU:O	1:A:180:LYS:HD2	2.21	0.40
1:A:91:ARG:HH11	1:A:91:ARG:HD2	1.59	0.40
1:A:208:GLU:HG3	2:A:2058:HOH:O	2.22	0.40
1:B:55:ASP:OD2	1:B:136:THR:OG1	2.39	0.40
1:C:18:VAL:HA	1:C:122:GLY:O	2.21	0.40
1:C:84:PRO:HD2	1:C:85:GLU:OE1	2.22	0.40
1:B:77:ASP:CG	1:B:80:LYS:HZ3	2.29	0.40
1:C:187:GLY:O	1:C:188:ARG:C	2.65	0.40
1:C:207:VAL:HG12	1:C:208:GLU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/240 (88%)	186 (88%)	22 (10%)	3 (1%)	9	14
1	B	211/240 (88%)	186 (88%)	20 (10%)	5 (2%)	4	7
1	C	211/240 (88%)	179 (85%)	23 (11%)	9 (4%)	2	2
1	D	211/240 (88%)	188 (89%)	19 (9%)	4 (2%)	6	10
All	All	844/960 (88%)	739 (88%)	84 (10%)	21 (2%)	4	7

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	199	SER
1	D	40	VAL
1	D	73	GLU
1	A	78	TYR
1	A	188	ARG
1	B	81	GLN
1	C	98	GLY
1	C	129	GLY
1	B	73	GLU
1	B	129	GLY
1	C	162	LYS
1	C	188	ARG
1	A	167	GLY
1	C	76	PRO
1	B	85	GLU
1	D	77	ASP
1	B	197	VAL
1	C	72	PRO
1	C	141	PRO
1	C	182	PRO
1	D	67	PRO

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	187/207 (90%)	166 (89%)	21 (11%)	6	8
1	B	186/207 (90%)	171 (92%)	15 (8%)	11	18
1	C	187/207 (90%)	168 (90%)	19 (10%)	7	10
1	D	187/207 (90%)	162 (87%)	25 (13%)	4	5
All	All	747/828 (90%)	667 (89%)	80 (11%)	6	9

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	35	GLU
1	A	42	LEU
1	A	46	LYS
1	A	60	GLN
1	A	66	ILE
1	A	75	ILE
1	A	105	ASN
1	A	110	GLN
1	A	118	VAL
1	A	119	LYS
1	A	120	ILE
1	A	123	GLU
1	A	161	LEU
1	A	190	GLU
1	A	199	SER
1	A	206	SER
1	A	210	CYS
1	A	212	ILE
1	A	216	ARG
1	A	219	LEU
1	B	3	VAL
1	B	25	VAL
1	B	37	GLU
1	B	42	LEU
1	B	66	ILE
1	B	71	TYR
1	B	88	THR
1	B	90	GLU
1	B	105	ASN
1	B	110	GLN

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Mol	Chain	Res	Type
1	B	119	LYS
1	B	136	THR
1	B	145	ARG
1	B	153	LEU
1	B	212	ILE
1	C	4	ILE
1	C	42	LEU
1	C	51	PRO
1	C	65	SER
1	C	66	ILE
1	C	75	ILE
1	C	105	ASN
1	C	110	GLN
1	C	118	VAL
1	C	123	GLU
1	C	141	PRO
1	C	146	LEU
1	C	153	LEU
1	C	196	ASP
1	C	206	SER
1	C	211	GLU
1	C	212	ILE
1	C	216	ARG
1	C	219	LEU
1	D	3	VAL
1	D	8	MET
1	D	18	VAL
1	D	38	GLN
1	D	39	THR
1	D	42	LEU
1	D	46	LYS
1	D	58	SER
1	D	60	GLN
1	D	61	LEU
1	D	90	GLU
1	D	92	SER
1	D	108	SER
1	D	110	GLN
1	D	118	VAL
1	D	121	SER
1	D	123	GLU
1	D	137	GLN

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Mol	Chain	Res	Type
1	D	149	ARG
1	D	177	TYR
1	D	181	LYS
1	D	184	ARG
1	D	191	ILE
1	D	210	CYS
1	D	211	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	117	ASN
1	A	128	ASN
1	A	200	HIS
1	A	209	GLN
1	B	21	HIS
1	B	110	GLN
1	B	112	ASN
1	B	137	GLN
1	B	156	ASN
1	B	200	HIS
1	B	209	GLN
1	B	217	HIS
1	C	94	ASN
1	C	105	ASN
1	C	110	GLN
1	C	124	ASN
1	C	133	GLN
1	C	200	HIS
1	C	209	GLN
1	C	217	HIS
1	D	38	GLN
1	D	124	ASN
1	D	133	GLN
1	D	200	HIS
1	D	209	GLN
1	D	217	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	CRQ	C	62	1	25,25,26	3.25	3 (12%)	28,34,36	3.50	9 (32%)
1	CRQ	A	62	1	25,25,26	3.21	6 (24%)	28,34,36	3.79	10 (35%)
1	CRQ	B	62	1	25,25,26	3.30	4 (16%)	28,34,36	2.96	8 (28%)
1	CRQ	D	62	1	25,25,26	3.47	4 (16%)	28,34,36	3.39	8 (28%)

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	CRQ	C	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	A	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	B	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	D	62	1	-	3/10/32/33	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	CRQ	CB2-CA2	16.26	1.50	1.35
1	B	62	CRQ	CB2-CA2	15.45	1.50	1.35
1	C	62	CRQ	CB2-CA2	14.99	1.49	1.35
1	A	62	CRQ	CB2-CA2	14.11	1.48	1.35
1	A	62	CRQ	C2-N3	-3.89	1.31	1.40
1	C	62	CRQ	C2-N3	-3.50	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	CRQ	C2-N3	-3.46	1.32	1.40
1	B	62	CRQ	C2-N3	-3.40	1.32	1.40
1	B	62	CRQ	O2-C2	2.70	1.28	1.23
1	A	62	CRQ	C1-CA1	2.67	1.51	1.48
1	A	62	CRQ	O2-C2	2.51	1.28	1.23
1	C	62	CRQ	O2-C2	2.46	1.28	1.23
1	A	62	CRQ	CA2-N2	-2.44	1.33	1.38
1	D	62	CRQ	O2-C2	2.29	1.27	1.23
1	A	62	CRQ	CE1-CZ	2.28	1.43	1.39
1	B	62	CRQ	C1-N3	-2.24	1.34	1.38
1	D	62	CRQ	C1-N2	2.22	1.38	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	CRQ	CB2-CA2-C2	13.19	138.34	122.36
1	C	62	CRQ	CB2-CA2-C2	12.81	137.88	122.36
1	D	62	CRQ	CB2-CA2-C2	12.05	136.96	122.36
1	B	62	CRQ	CB2-CA2-C2	10.91	135.58	122.36
1	C	62	CRQ	CB2-CA2-N2	-9.71	115.58	128.76
1	A	62	CRQ	CB2-CA2-N2	-9.59	115.74	128.76
1	D	62	CRQ	CB2-CA2-N2	-8.26	117.55	128.76
1	B	62	CRQ	CB2-CA2-N2	-7.72	118.28	128.76
1	A	62	CRQ	N3-C1-N2	-5.64	105.93	112.62
1	C	62	CRQ	CG2-CB2-CA2	-5.54	123.28	129.87
1	A	62	CRQ	CG2-CB2-CA2	-4.94	123.99	129.87
1	D	62	CRQ	C2-CA2-N2	-4.83	105.49	108.95
1	D	62	CRQ	CG2-CB2-CA2	-4.71	124.26	129.87
1	D	62	CRQ	N3-C1-N2	-4.28	107.54	112.62
1	A	62	CRQ	C2-CA2-N2	-4.23	105.92	108.95
1	B	62	CRQ	C2-CA2-N2	-3.94	106.13	108.95
1	A	62	CRQ	CA2-N2-C1	3.49	110.51	104.09
1	A	62	CRQ	CD2-CG2-CD1	3.45	122.77	117.65
1	C	62	CRQ	C2-CA2-N2	-3.37	106.54	108.95
1	B	62	CRQ	CG2-CB2-CA2	-3.36	125.88	129.87
1	B	62	CRQ	N3-C1-N2	-3.35	108.64	112.62
1	D	62	CRQ	C3-CA3-N3	-3.31	104.89	112.43
1	D	62	CRQ	CA2-C2-N3	2.99	106.01	103.50
1	D	62	CRQ	CA2-N2-C1	2.93	109.47	104.09
1	C	62	CRQ	CG1-CB1-CA1	-2.90	104.72	113.51
1	A	62	CRQ	CE1-CD1-CG2	-2.54	117.95	121.22
1	C	62	CRQ	N3-C1-N2	-2.51	109.64	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	CRQ	O3-C3-CA3	-2.46	114.40	125.47
1	B	62	CRQ	CA2-N2-C1	2.43	108.56	104.09
1	A	62	CRQ	CA2-C2-N3	2.40	105.52	103.50
1	B	62	CRQ	CA3-N3-C1	-2.40	123.67	128.39
1	C	62	CRQ	CA2-N2-C1	2.23	108.20	104.09
1	B	62	CRQ	O3-C3-CA3	-2.19	115.59	125.47
1	C	62	CRQ	CE1-CD1-CG2	-2.17	118.42	121.22
1	C	62	CRQ	C3-CA3-N3	-2.04	107.79	112.43

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	62	CRQ	N2-CA2-CB2-CG2
1	A	62	CRQ	C2-CA2-CB2-CG2
1	B	62	CRQ	C2-CA2-CB2-CG2
1	C	62	CRQ	N2-CA2-CB2-CG2
1	C	62	CRQ	C2-CA2-CB2-CG2
1	D	62	CRQ	C1-CA1-CB1-CG1
1	D	62	CRQ	C2-CA2-CB2-CG2
1	B	62	CRQ	N2-CA2-CB2-CG2
1	D	62	CRQ	N2-CA2-CB2-CG2
1	B	62	CRQ	CA1-CB1-CG1-CD3
1	A	62	CRQ	C3-CA3-N3-C1

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	62	CRQ	2	0
1	A	62	CRQ	1	0
1	B	62	CRQ	3	0
1	D	62	CRQ	4	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	215/240 (89%)	0.06	0 100 100	11, 36, 58, 68	0
1	B	215/240 (89%)	0.94	10 (4%) 36 28	45, 68, 80, 86	0
1	C	215/240 (89%)	0.90	13 (6%) 27 21	41, 68, 81, 91	0
1	D	215/240 (89%)	1.43	45 (20%) 2 1	52, 69, 83, 90	0
All	All	860/960 (89%)	0.83	68 (7%) 18 14	11, 65, 81, 91	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	PHE	3.6
1	D	160	ALA	3.2
1	D	219	LEU	3.2
1	C	170	LEU	3.2
1	D	207	VAL	3.0
1	D	74	ASP	3.0
1	D	148	ALA	2.8
1	D	195	LEU	2.8
1	D	25	VAL	2.8
1	D	75	ILE	2.8
1	B	219	LEU	2.8
1	D	179	ALA	2.8
1	D	72	PRO	2.7
1	D	212	ILE	2.7
1	D	12	VAL	2.7
1	C	145	ARG	2.7
1	D	130	PRO	2.7
1	D	197	VAL	2.7
1	D	187	GLY	2.7
1	D	3	VAL	2.7
1	D	196	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	74	ASP	2.6
1	D	153	LEU	2.6
1	C	163	LEU	2.6
1	D	177	TYR	2.6
1	B	3	VAL	2.6
1	D	155	GLY	2.5
1	D	61	LEU	2.5
1	D	84	PRO	2.5
1	D	103	VAL	2.5
1	B	197	VAL	2.4
1	B	207	VAL	2.4
1	D	42	LEU	2.4
1	D	127	PRO	2.4
1	C	125	PHE	2.4
1	C	204	TYR	2.4
1	D	53	ALA	2.4
1	D	154	ILE	2.3
1	D	136	THR	2.3
1	C	187	GLY	2.3
1	B	39	THR	2.3
1	B	2	SER	2.3
1	C	98	GLY	2.3
1	D	40	VAL	2.3
1	B	27	GLY	2.3
1	D	55	ASP	2.3
1	C	99	ALA	2.2
1	D	54	TRP	2.2
1	D	120	ILE	2.2
1	C	50	LEU	2.2
1	C	191	ILE	2.2
1	D	143	THR	2.2
1	C	197	VAL	2.2
1	D	145	ARG	2.1
1	D	13	TYR	2.1
1	D	34	TYR	2.1
1	D	39	THR	2.1
1	D	176	THR	2.1
1	C	51	PRO	2.1
1	C	169	TYR	2.1
1	D	10	TYR	2.1
1	B	215	ALA	2.1
1	D	167	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	99	ALA	2.0
1	B	84	PRO	2.0
1	D	156	ASN	2.0
1	D	29	GLY	2.0
1	D	210	CYS	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	CRQ	D	62	24/25	0.84	0.18	63,68,74,75	0
1	CRQ	B	62	24/25	0.86	0.17	67,72,82,83	0
1	CRQ	C	62	24/25	0.91	0.13	56,61,70,71	0
1	CRQ	A	62	24/25	0.91	0.12	35,43,44,45	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.