Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 AM GMT

PDB ID	:	2H8Q
Title	:	Crystal Structure of a Redshifted Mutant (K83M) of the Red Fluorescent Protein dRFP583/dsRed
Authors	:	Yarbrough, C.A.; Remington, S.J.
Deposited on	:	2006-06-07
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

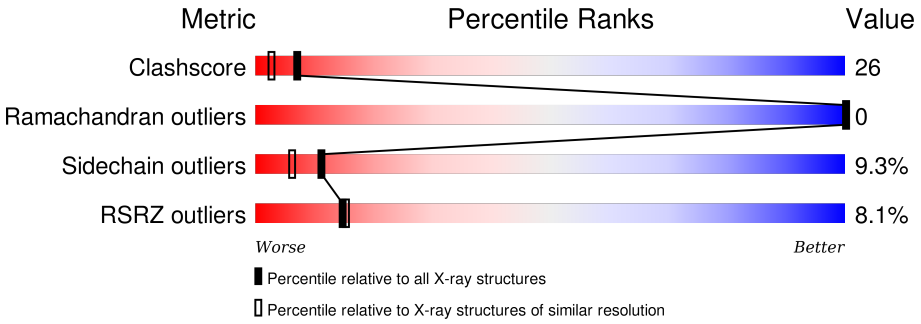
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	217	6% 47% 36% 16%
1	B	217	10% 46% 37% 16%
1	C	217	7% 47% 35% 17%
1	D	217	10% 46% 36% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7624 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 Red fluorescent protein drFP583.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1761	1144	289	320	8			
1	B	217	Total	C	N	O	S	0	0	0
			1761	1144	289	320	8			
1	C	217	Total	C	N	O	S	0	0	0
			1761	1144	289	320	8			
1	D	217	Total	C	N	O	S	0	0	0
			1761	1144	289	320	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
A	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
A	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
A	83	MET	LYS	ENGINEERED	UNP Q9U6Y8
B	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
B	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
B	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
B	83	MET	LYS	ENGINEERED	UNP Q9U6Y8
C	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
C	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
C	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
C	83	MET	LYS	ENGINEERED	UNP Q9U6Y8
D	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
D	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
D	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
D	83	MET	LYS	ENGINEERED	UNP Q9U6Y8

- Molecule 2 is water.

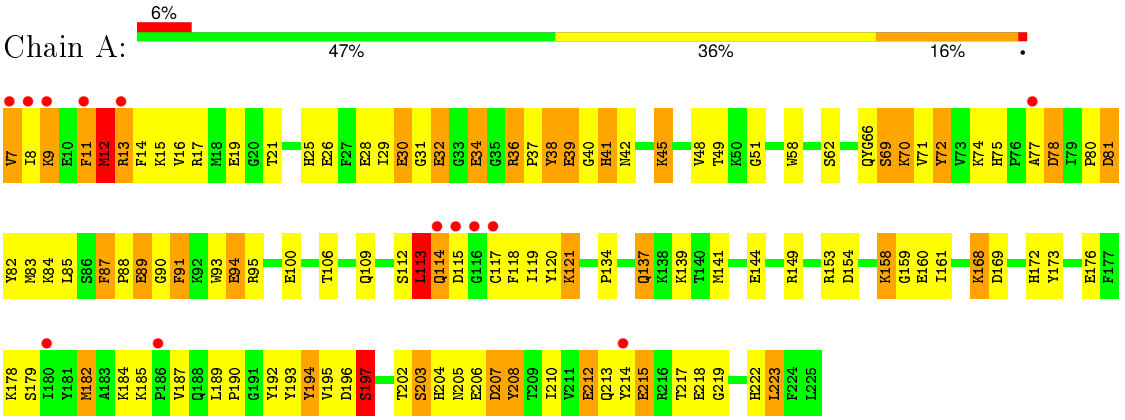
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	146	Total O 146 146	0	0
2	B	146	Total O 146 146	0	0
2	C	144	Total O 144 144	0	0
2	D	144	Total O 144 144	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

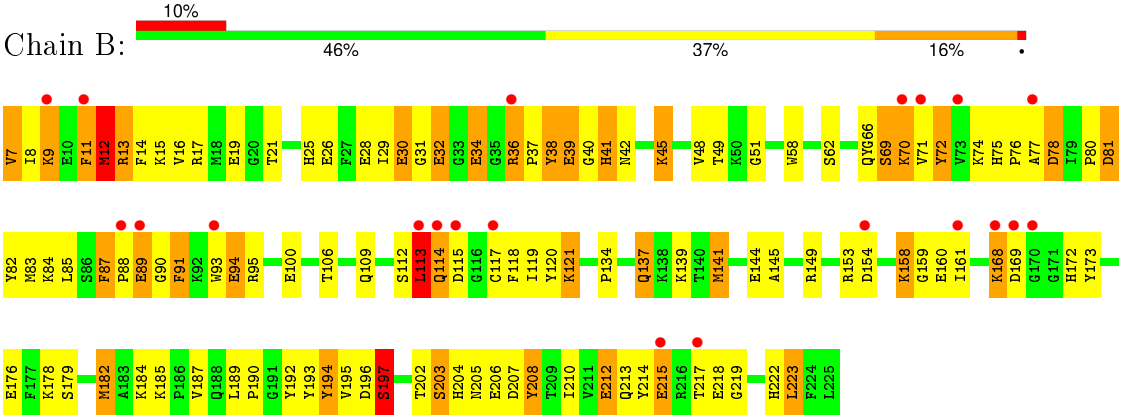
- Molecule 1: Red fluorescent protein drFP583

Chain A:



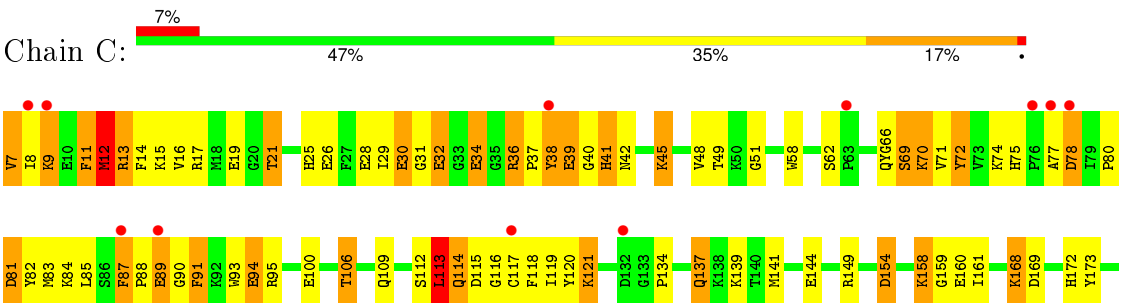
- Molecule 1: Red fluorescent protein drFP583

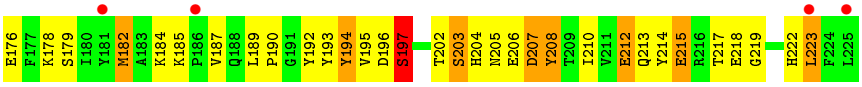
Chain B:



- Molecule 1: Red fluorescent protein drFP583

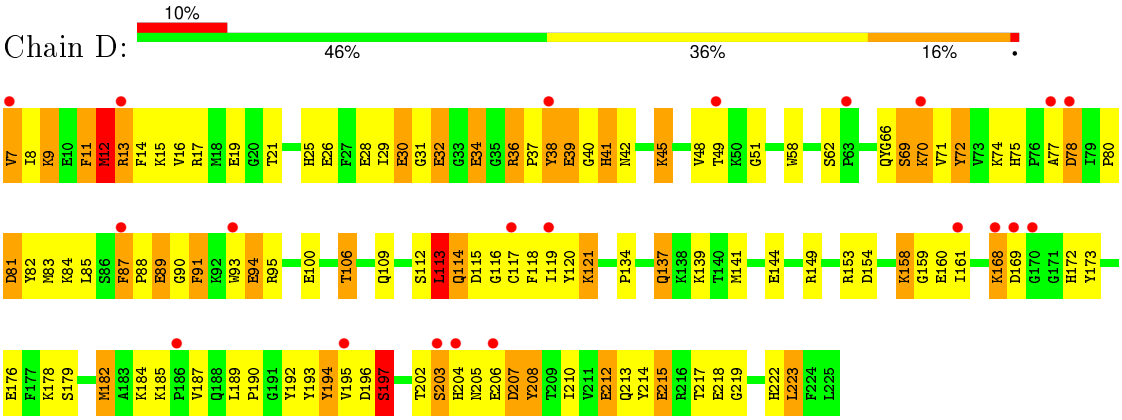
Chain C:





- Molecule 1: Red fluorescent protein drFP583

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	92.93Å 92.93Å 431.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.00 29.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	80.0 (5.00-2.00) 81.7 (29.98-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.00Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.230 , 0.268 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 76.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	3 of 61886 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7624	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 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	1.37	15/1786 (0.8%)	1.79	49/2409 (2.0%)
1	B	1.37	15/1786 (0.8%)	1.79	49/2409 (2.0%)
1	C	1.37	14/1786 (0.8%)	1.79	49/2409 (2.0%)
1	D	1.37	15/1786 (0.8%)	1.79	49/2409 (2.0%)
All	All	1.37	59/7144 (0.8%)	1.79	196/9636 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	1	0
1	C	1	0
1	D	1	0
All	All	4	0

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	218	GLU	CD-OE2	10.02	1.36	1.25
1	B	218	GLU	CD-OE2	10.02	1.36	1.25
1	C	218	GLU	CD-OE2	10.01	1.36	1.25
1	C	32	GLU	CD-OE2	9.99	1.36	1.25
1	A	32	GLU	CD-OE2	9.98	1.36	1.25
1	D	32	GLU	CD-OE2	9.97	1.36	1.25
1	A	218	GLU	CD-OE2	9.96	1.36	1.25
1	B	32	GLU	CD-OE2	9.93	1.36	1.25
1	A	94	GLU	CD-OE2	9.89	1.36	1.25
1	B	94	GLU	CD-OE2	9.89	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	GLU	CD-OE2	9.86	1.36	1.25
1	C	94	GLU	CD-OE2	9.84	1.36	1.25
1	A	176	GLU	CD-OE2	9.21	1.35	1.25
1	B	176	GLU	CD-OE2	9.21	1.35	1.25
1	C	176	GLU	CD-OE2	9.19	1.35	1.25
1	D	176	GLU	CD-OE2	9.14	1.35	1.25
1	B	100	GLU	CD-OE2	9.06	1.35	1.25
1	C	100	GLU	CD-OE2	9.04	1.35	1.25
1	D	100	GLU	CD-OE2	9.02	1.35	1.25
1	A	100	GLU	CD-OE2	9.01	1.35	1.25
1	D	215	GLU	CD-OE2	8.68	1.35	1.25
1	A	215	GLU	CD-OE2	8.62	1.35	1.25
1	C	215	GLU	CD-OE2	8.61	1.35	1.25
1	B	215	GLU	CD-OE2	8.59	1.35	1.25
1	B	212	GLU	CD-OE2	8.29	1.34	1.25
1	C	212	GLU	CD-OE2	8.26	1.34	1.25
1	A	212	GLU	CD-OE2	8.21	1.34	1.25
1	D	212	GLU	CD-OE2	8.15	1.34	1.25
1	A	34	GLU	CD-OE2	8.14	1.34	1.25
1	D	34	GLU	CD-OE2	8.13	1.34	1.25
1	C	34	GLU	CD-OE2	8.08	1.34	1.25
1	B	34	GLU	CD-OE2	8.05	1.34	1.25
1	D	30	GLU	CD-OE2	7.94	1.34	1.25
1	C	30	GLU	CD-OE2	7.91	1.34	1.25
1	A	30	GLU	CD-OE2	7.91	1.34	1.25
1	B	30	GLU	CD-OE2	7.87	1.34	1.25
1	D	19	GLU	CD-OE2	7.16	1.33	1.25
1	C	39	GLU	CD-OE2	7.14	1.33	1.25
1	B	39	GLU	CD-OE2	7.13	1.33	1.25
1	B	19	GLU	CD-OE2	7.13	1.33	1.25
1	C	19	GLU	CD-OE2	7.13	1.33	1.25
1	A	19	GLU	CD-OE2	7.13	1.33	1.25
1	D	39	GLU	CD-OE2	7.13	1.33	1.25
1	A	39	GLU	CD-OE2	7.09	1.33	1.25
1	A	26	GLU	CD-OE2	6.68	1.32	1.25
1	C	26	GLU	CD-OE2	6.67	1.32	1.25
1	B	26	GLU	CD-OE2	6.61	1.32	1.25
1	D	26	GLU	CD-OE2	6.59	1.32	1.25
1	C	160	GLU	CD-OE2	6.17	1.32	1.25
1	B	160	GLU	CD-OE2	6.11	1.32	1.25
1	D	160	GLU	CD-OE2	6.07	1.32	1.25
1	A	160	GLU	CD-OE2	6.05	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	206	GLU	CD-OE2	5.13	1.31	1.25
1	A	206	GLU	CD-OE2	5.13	1.31	1.25
1	B	206	GLU	CD-OE2	5.09	1.31	1.25
1	B	153	ARG	CZ-NH2	5.06	1.39	1.33
1	D	153	ARG	CZ-NH2	5.05	1.39	1.33
1	C	206	GLU	CD-OE2	5.03	1.31	1.25
1	A	153	ARG	CZ-NH2	5.01	1.39	1.33

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	95	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	C	95	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	B	95	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	D	95	ARG	NE-CZ-NH1	10.57	125.58	120.30
1	B	78	ASP	CB-CG-OD2	-10.49	108.86	118.30
1	A	78	ASP	CB-CG-OD2	-10.48	108.87	118.30
1	D	78	ASP	CB-CG-OD2	-10.46	108.89	118.30
1	A	81	ASP	CB-CG-OD2	-10.43	108.91	118.30
1	C	78	ASP	CB-CG-OD2	-10.42	108.92	118.30
1	B	81	ASP	CB-CG-OD2	-10.42	108.92	118.30
1	C	81	ASP	CB-CG-OD2	-10.41	108.93	118.30
1	D	81	ASP	CB-CG-OD2	-10.40	108.94	118.30
1	B	114	GLN	N-CA-CB	10.19	128.95	110.60
1	A	114	GLN	N-CA-CB	10.18	128.92	110.60
1	C	114	GLN	N-CA-CB	10.17	128.91	110.60
1	D	114	GLN	N-CA-CB	10.14	128.86	110.60
1	A	197	SER	N-CA-CB	9.88	125.33	110.50
1	D	197	SER	N-CA-CB	9.88	125.31	110.50
1	B	197	SER	N-CA-CB	9.87	125.30	110.50
1	C	197	SER	N-CA-CB	9.85	125.28	110.50
1	A	36	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	C	36	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	B	36	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	D	36	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	B	81	ASP	CB-CG-OD1	8.79	126.22	118.30
1	A	81	ASP	CB-CG-OD1	8.78	126.20	118.30
1	D	81	ASP	CB-CG-OD1	8.79	126.21	118.30
1	C	81	ASP	CB-CG-OD1	8.77	126.19	118.30
1	B	192	TYR	CB-CG-CD1	-8.43	115.94	121.00
1	C	192	TYR	CB-CG-CD1	-8.38	115.97	121.00
1	A	207	ASP	CB-CG-OD2	-8.37	110.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	192	TYR	CB-CG-CD1	-8.36	115.98	121.00
1	A	154	ASP	CB-CG-OD1	8.35	125.81	118.30
1	C	207	ASP	CB-CG-OD2	-8.34	110.79	118.30
1	D	154	ASP	CB-CG-OD1	8.33	125.80	118.30
1	B	207	ASP	CB-CG-OD2	-8.33	110.81	118.30
1	D	207	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	C	154	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	192	TYR	CB-CG-CD1	-8.31	116.02	121.00
1	B	154	ASP	CB-CG-OD1	8.22	125.70	118.30
1	B	196	ASP	CB-CG-OD1	8.19	125.67	118.30
1	A	196	ASP	CB-CG-OD1	8.13	125.61	118.30
1	C	196	ASP	CB-CG-OD1	8.12	125.61	118.30
1	D	196	ASP	CB-CG-OD1	8.10	125.59	118.30
1	C	95	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	95	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	A	95	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	B	81	ASP	CB-CA-C	7.67	125.73	110.40
1	A	81	ASP	CB-CA-C	7.66	125.72	110.40
1	D	81	ASP	CB-CA-C	7.65	125.70	110.40
1	C	81	ASP	CB-CA-C	7.64	125.69	110.40
1	D	95	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	196	ASP	CB-CG-OD2	-7.62	111.45	118.30
1	A	196	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	C	196	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	D	196	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	B	208	TYR	CZ-CE2-CD2	-7.51	113.04	119.80
1	D	208	TYR	CZ-CE2-CD2	-7.50	113.05	119.80
1	A	208	TYR	CZ-CE2-CD2	-7.48	113.07	119.80
1	C	208	TYR	CZ-CE2-CD2	-7.47	113.08	119.80
1	D	113	LEU	N-CA-CB	6.91	124.22	110.40
1	B	113	LEU	N-CA-CB	6.90	124.20	110.40
1	A	113	LEU	N-CA-CB	6.90	124.20	110.40
1	C	113	LEU	N-CA-CB	6.87	124.13	110.40
1	B	72	TYR	CB-CG-CD1	-6.83	116.91	121.00
1	A	72	TYR	CB-CG-CD1	-6.82	116.91	121.00
1	D	72	TYR	CB-CG-CD1	-6.78	116.93	121.00
1	C	72	TYR	CB-CG-CD1	-6.78	116.94	121.00
1	D	11	PHE	N-CA-CB	6.67	122.60	110.60
1	B	11	PHE	N-CA-CB	6.66	122.59	110.60
1	A	11	PHE	N-CA-CB	6.66	122.59	110.60
1	C	11	PHE	N-CA-CB	6.64	122.55	110.60
1	D	70	LYS	CB-CA-C	6.42	123.24	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	70	LYS	CB-CA-C	6.42	123.23	110.40
1	A	70	LYS	CB-CA-C	6.42	123.23	110.40
1	B	70	LYS	CB-CA-C	6.41	123.23	110.40
1	A	93	TRP	N-CA-CB	6.40	122.12	110.60
1	B	93	TRP	N-CA-CB	6.40	122.11	110.60
1	D	93	TRP	N-CA-CB	6.39	122.10	110.60
1	C	93	TRP	N-CA-CB	6.37	122.06	110.60
1	B	194	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	C	194	TYR	CB-CG-CD2	-6.16	117.30	121.00
1	D	194	TYR	CB-CG-CD2	-6.16	117.30	121.00
1	A	194	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	A	12	MET	CG-SD-CE	6.05	109.88	100.20
1	D	193	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	C	13	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	193	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	D	13	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	12	MET	CG-SD-CE	6.04	109.86	100.20
1	C	12	MET	CG-SD-CE	6.04	109.86	100.20
1	D	12	MET	CG-SD-CE	6.03	109.85	100.20
1	B	193	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	C	193	TYR	CB-CG-CD1	-6.01	117.40	121.00
1	C	34	GLU	CA-CB-CG	-6.00	100.19	113.40
1	D	34	GLU	CA-CB-CG	-6.00	100.20	113.40
1	B	34	GLU	CA-CB-CG	-5.99	100.21	113.40
1	A	34	GLU	CA-CB-CG	-5.99	100.23	113.40
1	A	13	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	13	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	21	THR	CA-CB-CG2	-5.82	104.25	112.40
1	C	21	THR	CA-CB-CG2	-5.82	104.25	112.40
1	D	173	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	B	21	THR	CA-CB-CG2	-5.81	104.27	112.40
1	D	21	THR	CA-CB-CG2	-5.80	104.27	112.40
1	B	182	MET	CG-SD-CE	-5.79	90.94	100.20
1	D	182	MET	CG-SD-CE	-5.78	90.96	100.20
1	C	182	MET	CG-SD-CE	-5.76	90.98	100.20
1	C	173	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	87	PHE	CB-CA-C	5.75	121.90	110.40
1	C	87	PHE	CB-CA-C	5.75	121.90	110.40
1	A	182	MET	CG-SD-CE	-5.75	91.01	100.20
1	B	87	PHE	CB-CA-C	5.75	121.89	110.40
1	D	87	PHE	CB-CA-C	5.74	121.87	110.40
1	A	173	TYR	CB-CG-CD2	-5.73	117.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	173	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	D	154	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	B	154	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	69	SER	CB-CA-C	5.66	120.86	110.10
1	D	69	SER	CB-CA-C	5.66	120.85	110.10
1	B	69	SER	CB-CA-C	5.66	120.85	110.10
1	C	69	SER	CB-CA-C	5.65	120.84	110.10
1	D	106	THR	N-CA-CB	5.62	120.99	110.30
1	C	154	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	C	106	THR	N-CA-CB	5.61	120.96	110.30
1	A	208	TYR	CG-CD1-CE1	-5.61	116.81	121.30
1	A	106	THR	N-CA-CB	5.60	120.95	110.30
1	B	106	THR	N-CA-CB	5.59	120.93	110.30
1	C	208	TYR	CG-CD1-CE1	-5.59	116.83	121.30
1	A	154	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	208	TYR	CG-CD1-CE1	-5.57	116.84	121.30
1	D	208	TYR	CG-CD1-CE1	-5.57	116.84	121.30
1	C	77	ALA	N-CA-CB	-5.55	102.33	110.10
1	A	77	ALA	N-CA-CB	-5.54	102.35	110.10
1	B	77	ALA	N-CA-CB	-5.53	102.36	110.10
1	D	77	ALA	N-CA-CB	-5.52	102.38	110.10
1	D	206	GLU	CG-CD-OE2	-5.34	107.62	118.30
1	C	62	SER	CB-CA-C	5.34	120.24	110.10
1	C	206	GLU	CG-CD-OE2	-5.34	107.63	118.30
1	D	62	SER	CB-CA-C	5.33	120.23	110.10
1	A	41	HIS	CB-CA-C	-5.33	99.75	110.40
1	B	41	HIS	CB-CA-C	-5.33	99.75	110.40
1	B	62	SER	CB-CA-C	5.32	120.22	110.10
1	D	41	HIS	CB-CA-C	-5.32	99.75	110.40
1	A	206	GLU	CG-CD-OE2	-5.32	107.66	118.30
1	D	91	PHE	CB-CA-C	-5.32	99.76	110.40
1	B	206	GLU	CG-CD-OE2	-5.32	107.67	118.30
1	C	41	HIS	CB-CA-C	-5.31	99.77	110.40
1	A	62	SER	CB-CA-C	5.31	120.18	110.10
1	A	91	PHE	CB-CA-C	-5.31	99.79	110.40
1	B	48	VAL	CG1-CB-CG2	5.30	119.38	110.90
1	C	91	PHE	CB-CA-C	-5.30	99.80	110.40
1	A	48	VAL	CG1-CB-CG2	5.29	119.37	110.90
1	D	48	VAL	CG1-CB-CG2	5.29	119.37	110.90
1	B	91	PHE	CB-CA-C	-5.29	99.83	110.40
1	C	48	VAL	CG1-CB-CG2	5.27	119.34	110.90
1	C	94	GLU	N-CA-CB	5.23	120.01	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	42	ASN	CB-CA-C	5.23	120.86	110.40
1	D	94	GLU	N-CA-CB	5.22	120.00	110.60
1	B	42	ASN	CB-CA-C	5.22	120.83	110.40
1	A	42	ASN	CB-CA-C	5.22	120.83	110.40
1	A	94	GLU	N-CA-CB	5.21	119.98	110.60
1	A	178	LYS	N-CA-CB	5.21	119.97	110.60
1	B	178	LYS	N-CA-CB	5.21	119.97	110.60
1	B	94	GLU	N-CA-CB	5.20	119.96	110.60
1	D	178	LYS	N-CA-CB	5.20	119.95	110.60
1	C	42	ASN	CB-CA-C	5.20	120.79	110.40
1	C	178	LYS	N-CA-CB	5.20	119.95	110.60
1	C	121	LYS	N-CA-CB	5.19	119.95	110.60
1	D	121	LYS	N-CA-CB	5.17	119.91	110.60
1	B	121	LYS	N-CA-CB	5.16	119.89	110.60
1	A	121	LYS	N-CA-CB	5.15	119.88	110.60
1	B	45	LYS	CB-CA-C	5.12	120.65	110.40
1	A	45	LYS	CB-CA-C	5.12	120.64	110.40
1	D	45	LYS	CB-CA-C	5.11	120.63	110.40
1	C	45	LYS	CB-CA-C	5.11	120.61	110.40
1	D	17	ARG	N-CA-CB	5.07	119.72	110.60
1	C	203	SER	N-CA-CB	-5.07	102.90	110.50
1	A	141	MET	CG-SD-CE	5.06	108.30	100.20
1	B	17	ARG	N-CA-CB	5.06	119.71	110.60
1	D	203	SER	N-CA-CB	-5.06	102.91	110.50
1	C	137	GLN	CA-CB-CG	-5.06	102.27	113.40
1	C	17	ARG	N-CA-CB	5.06	119.70	110.60
1	B	137	GLN	CA-CB-CG	-5.06	102.28	113.40
1	B	203	SER	N-CA-CB	-5.06	102.92	110.50
1	A	203	SER	N-CA-CB	-5.05	102.92	110.50
1	B	141	MET	CG-SD-CE	5.05	108.29	100.20
1	D	137	GLN	CA-CB-CG	-5.05	102.28	113.40
1	A	137	GLN	CA-CB-CG	-5.05	102.30	113.40
1	C	141	MET	CG-SD-CE	5.04	108.27	100.20
1	C	169	ASP	CB-CA-C	5.04	120.47	110.40
1	D	141	MET	CG-SD-CE	5.03	108.25	100.20
1	A	17	ARG	N-CA-CB	5.03	119.64	110.60
1	A	169	ASP	CB-CA-C	5.02	120.44	110.40
1	D	169	ASP	CB-CA-C	5.02	120.43	110.40
1	B	169	ASP	CB-CA-C	5.00	120.41	110.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	81	ASP	CA
1	B	81	ASP	CA
1	C	81	ASP	CA
1	D	81	ASP	CA

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	1761	0	1697	91	0
1	B	1761	0	1697	91	1
1	C	1761	0	1697	93	0
1	D	1761	0	1697	91	0
2	A	146	0	0	13	0
2	B	146	0	0	13	3
2	C	144	0	0	12	1
2	D	144	0	0	13	1
All	All	7624	0	6788	364	4

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 26.

All (364) 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:D:118:PHE:O	1:D:119:ILE:HD13	1.76	0.86
1:C:118:PHE:O	1:C:119:ILE:HD13	1.76	0.85
1:B:118:PHE:O	1:B:119:ILE:HD13	1.76	0.84
1:A:118:PHE:O	1:A:119:ILE:HD13	1.76	0.84
1:D:13:ARG:HG2	1:D:34:GLU:HB2	1.61	0.83
1:D:9:LYS:HG2	1:D:12:MET:SD	2.20	0.81
1:C:9:LYS:HG2	1:C:12:MET:SD	2.20	0.81
1:C:13:ARG:HG2	1:C:34:GLU:HB2	1.61	0.81
1:B:9:LYS:HG2	1:B:12:MET:SD	2.20	0.81
1:A:9:LYS:HG2	1:A:12:MET:SD	2.20	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:HG2	1:A:34:GLU:HB2	1.61	0.81
1:B:13:ARG:HG2	1:B:34:GLU:HB2	1.61	0.81
1:B:45:LYS:HB2	1:B:212:GLU:HG2	1.63	0.80
1:D:45:LYS:HB2	1:D:212:GLU:HG2	1.63	0.80
1:A:45:LYS:HB2	1:A:212:GLU:HG2	1.63	0.79
1:C:45:LYS:HB2	1:C:212:GLU:HG2	1.63	0.79
1:D:11:PHE:HB2	1:D:36:ARG:NH1	2.03	0.74
1:A:11:PHE:HB2	1:A:36:ARG:NH1	2.03	0.73
1:B:11:PHE:HB2	1:B:36:ARG:NH1	2.03	0.73
1:C:11:PHE:HB2	1:C:36:ARG:NH1	2.03	0.73
1:C:40:GLY:HA2	1:C:72:TYR:O	1.88	0.73
1:D:40:GLY:HA2	1:D:72:TYR:O	1.88	0.73
1:B:14:PHE:HB3	1:B:118:PHE:HB2	1.71	0.72
1:A:40:GLY:HA2	1:A:72:TYR:O	1.88	0.72
1:B:40:GLY:HA2	1:B:72:TYR:O	1.88	0.72
1:D:14:PHE:HB3	1:D:118:PHE:HB2	1.71	0.72
1:A:14:PHE:HB3	1:A:118:PHE:HB2	1.71	0.71
1:C:70:LYS:HB2	2:C:419:HOH:O	1.91	0.71
1:C:14:PHE:HB3	1:C:118:PHE:HB2	1.71	0.71
1:D:13:ARG:HA	1:D:34:GLU:HA	1.74	0.70
1:A:70:LYS:HB2	2:A:332:HOH:O	1.91	0.70
1:B:13:ARG:HA	1:B:34:GLU:HA	1.74	0.70
1:B:70:LYS:HB2	2:B:336:HOH:O	1.91	0.70
1:A:13:ARG:HA	1:A:34:GLU:HA	1.74	0.69
1:A:113:LEU:HD23	1:A:114:GLN:H	1.56	0.69
1:C:113:LEU:HD23	1:C:114:GLN:H	1.56	0.69
1:C:13:ARG:HA	1:C:34:GLU:HA	1.74	0.69
1:C:114:GLN:O	1:C:117:CYS:N	2.19	0.69
1:B:114:GLN:O	1:B:117:CYS:N	2.19	0.69
1:D:70:LYS:HB2	2:D:336:HOH:O	1.91	0.69
1:A:66:CRQ:HG12	1:A:215:GLU:OE2	1.93	0.69
1:C:66:CRQ:HG12	1:C:215:GLU:OE2	1.93	0.69
1:A:114:GLN:O	1:A:117:CYS:N	2.19	0.68
1:B:66:CRQ:HG12	1:B:215:GLU:OE2	1.93	0.68
1:D:114:GLN:O	1:D:117:CYS:N	2.19	0.68
1:B:113:LEU:HD23	1:B:114:GLN:H	1.56	0.68
1:D:66:CRQ:HG12	1:D:215:GLU:OE2	1.93	0.68
1:B:13:ARG:NH1	1:B:34:GLU:OE1	2.27	0.68
1:D:113:LEU:HD23	1:D:114:GLN:H	1.56	0.68
1:D:13:ARG:NH1	1:D:34:GLU:OE1	2.27	0.68
1:C:13:ARG:NH1	1:C:34:GLU:OE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:NH1	1:A:34:GLU:OE1	2.27	0.68
1:B:11:PHE:HB2	1:B:36:ARG:HH12	1.60	0.67
1:D:11:PHE:HB2	1:D:36:ARG:HH12	1.60	0.66
1:C:144:GLU:OE2	1:C:172:HIS:HE1	1.79	0.66
1:A:9:LYS:HD3	1:A:9:LYS:H	1.61	0.65
1:A:144:GLU:OE2	1:A:172:HIS:HE1	1.79	0.65
1:C:9:LYS:HD3	1:C:9:LYS:H	1.61	0.65
1:B:9:LYS:HD3	1:B:9:LYS:H	1.61	0.65
1:C:11:PHE:HB2	1:C:36:ARG:HH12	1.60	0.64
1:D:9:LYS:HD3	1:D:9:LYS:H	1.61	0.64
1:B:144:GLU:OE2	1:B:172:HIS:HE1	1.79	0.64
1:A:11:PHE:HB2	1:A:36:ARG:HH12	1.60	0.64
1:D:144:GLU:OE2	1:D:172:HIS:HE1	1.79	0.64
1:A:8:ILE:HG22	1:A:38:TYR:OH	1.98	0.64
1:C:8:ILE:HG22	1:C:38:TYR:OH	1.98	0.63
1:B:8:ILE:HG22	1:B:38:TYR:OH	1.98	0.63
1:C:7:VAL:O	1:C:9:LYS:NZ	2.29	0.63
1:C:217:THR:HG22	2:C:317:HOH:O	1.98	0.63
1:D:8:ILE:HG22	1:D:38:TYR:OH	1.98	0.63
1:A:217:THR:HG22	2:A:234:HOH:O	1.99	0.63
1:A:83:MET:HG3	1:A:91:PHE:CZ	2.34	0.62
1:D:83:MET:HG3	1:D:91:PHE:CZ	2.34	0.62
1:B:83:MET:HG3	1:B:91:PHE:CZ	2.34	0.62
1:A:158:LYS:HE2	2:A:274:HOH:O	2.00	0.62
1:B:217:THR:HG22	2:B:237:HOH:O	1.99	0.62
1:C:83:MET:HG3	1:C:91:PHE:CZ	2.34	0.62
1:D:217:THR:HG22	2:D:238:HOH:O	1.99	0.62
1:B:7:VAL:O	1:B:9:LYS:NZ	2.29	0.61
1:C:8:ILE:HG22	1:C:38:TYR:CZ	2.36	0.61
1:B:8:ILE:HG22	1:B:38:TYR:CZ	2.36	0.61
1:A:90:GLY:O	1:A:184:LYS:HB2	2.01	0.61
1:A:8:ILE:HG22	1:A:38:TYR:CZ	2.36	0.61
1:D:90:GLY:O	1:D:184:LYS:HB2	2.01	0.61
1:A:9:LYS:HD3	1:A:9:LYS:N	2.16	0.61
1:B:158:LYS:HE2	2:B:277:HOH:O	2.00	0.61
1:D:8:ILE:HG22	1:D:38:TYR:CZ	2.36	0.61
1:C:9:LYS:HD3	1:C:9:LYS:N	2.16	0.61
1:C:158:LYS:HE2	2:C:358:HOH:O	2.00	0.61
1:C:90:GLY:O	1:C:184:LYS:HB2	2.01	0.60
1:D:158:LYS:HE2	2:D:278:HOH:O	2.00	0.60
1:B:90:GLY:O	1:B:184:LYS:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:VAL:O	1:C:9:LYS:HD3	2.02	0.60
1:B:9:LYS:N	1:B:9:LYS:HD3	2.16	0.60
1:D:9:LYS:HD3	1:D:9:LYS:N	2.16	0.60
1:B:13:ARG:HG2	1:B:34:GLU:CB	2.31	0.60
1:A:7:VAL:O	1:A:9:LYS:HD3	2.02	0.60
1:A:49:THR:HA	2:A:326:HOH:O	2.02	0.59
1:C:13:ARG:HG2	1:C:34:GLU:CB	2.31	0.59
1:A:8:ILE:HD13	1:A:84:LYS:HG2	1.85	0.59
1:D:8:ILE:HD13	1:D:84:LYS:HG2	1.85	0.59
1:C:8:ILE:HD13	1:C:84:LYS:HG2	1.85	0.59
1:A:13:ARG:HG2	1:A:34:GLU:CB	2.31	0.59
1:B:114:GLN:O	1:B:115:ASP:C	2.41	0.59
1:B:7:VAL:O	1:B:9:LYS:HD3	2.02	0.59
1:D:81:ASP:OD2	1:D:84:LYS:HD2	2.03	0.59
1:C:49:THR:HA	2:C:413:HOH:O	2.02	0.59
1:D:13:ARG:HG2	1:D:34:GLU:CB	2.31	0.58
1:B:81:ASP:OD2	1:B:84:LYS:HD2	2.03	0.58
1:B:8:ILE:HD13	1:B:84:LYS:HG2	1.85	0.58
1:D:7:VAL:O	1:D:9:LYS:HD3	2.02	0.58
1:D:7:VAL:O	1:D:9:LYS:NZ	2.29	0.58
1:A:7:VAL:O	1:A:9:LYS:NZ	2.29	0.58
1:B:78:ASP:OD1	1:B:78:ASP:N	2.36	0.58
1:A:81:ASP:OD2	1:A:84:LYS:HD2	2.03	0.58
1:A:8:ILE:HD11	1:A:87:PHE:HB2	1.85	0.58
1:C:81:ASP:OD2	1:C:84:LYS:HD2	2.03	0.58
1:D:49:THR:HA	2:D:330:HOH:O	2.02	0.58
1:C:8:ILE:HD11	1:C:87:PHE:HB2	1.85	0.58
1:C:185:LYS:O	1:C:187:VAL:HG13	2.04	0.57
1:B:89:GLU:CD	1:B:185:LYS:HD3	2.24	0.57
1:B:49:THR:HA	2:B:330:HOH:O	2.02	0.57
1:A:89:GLU:CD	1:A:185:LYS:HD3	2.24	0.57
1:C:114:GLN:O	1:C:115:ASP:C	2.41	0.57
1:B:8:ILE:HD11	1:B:87:PHE:HB2	1.85	0.57
1:D:8:ILE:HD11	1:D:87:PHE:HB2	1.85	0.57
1:A:185:LYS:O	1:A:187:VAL:HG13	2.04	0.57
1:C:89:GLU:CD	1:C:185:LYS:HD3	2.24	0.56
1:A:149:ARG:HD2	1:A:149:ARG:C	2.26	0.56
1:B:185:LYS:O	1:B:187:VAL:HG13	2.04	0.56
1:B:149:ARG:HD2	1:B:149:ARG:C	2.26	0.56
1:D:149:ARG:C	1:D:149:ARG:HD2	2.26	0.56
1:D:89:GLU:CD	1:D:185:LYS:HD3	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ARG:HD2	1:C:149:ARG:C	2.26	0.56
1:D:185:LYS:O	1:D:187:VAL:HG13	2.04	0.56
1:C:71:VAL:HG11	1:C:118:PHE:CE1	2.41	0.56
1:A:71:VAL:HG11	1:A:118:PHE:CE1	2.41	0.56
1:B:58:TRP:HE1	1:B:213:GLN:HE21	1.54	0.56
1:D:58:TRP:HE1	1:D:213:GLN:HE21	1.54	0.56
1:A:58:TRP:HE1	1:A:213:GLN:HE21	1.54	0.56
1:C:58:TRP:HE1	1:C:213:GLN:HE21	1.54	0.56
1:D:91:PHE:HA	1:D:184:LYS:HD2	1.89	0.55
1:C:91:PHE:HA	1:C:184:LYS:HD2	1.89	0.55
1:D:71:VAL:HG11	1:D:118:PHE:CE1	2.41	0.55
1:D:114:GLN:O	1:D:115:ASP:C	2.41	0.55
1:B:91:PHE:HA	1:B:184:LYS:HD2	1.89	0.55
1:B:71:VAL:HG11	1:B:118:PHE:CE1	2.41	0.55
1:A:91:PHE:HA	1:A:184:LYS:HD2	1.89	0.55
1:B:89:GLU:H	1:B:89:GLU:CD	2.10	0.55
1:A:114:GLN:O	1:A:115:ASP:C	2.41	0.55
1:D:94:GLU:OE2	2:D:255:HOH:O	2.18	0.55
1:B:94:GLU:OE2	2:B:254:HOH:O	2.18	0.55
1:C:94:GLU:OE2	2:C:334:HOH:O	2.18	0.54
1:C:89:GLU:H	1:C:89:GLU:CD	2.10	0.54
1:D:25:HIS:HE1	1:D:51:GLY:O	1.91	0.54
1:C:89:GLU:CG	1:C:185:LYS:HD3	2.38	0.54
1:A:89:GLU:CG	1:A:185:LYS:HD3	2.38	0.54
1:D:78:ASP:OD1	1:D:78:ASP:N	2.36	0.54
1:C:25:HIS:HE1	1:C:51:GLY:O	1.91	0.54
1:B:89:GLU:CG	1:B:185:LYS:HD3	2.38	0.54
1:B:25:HIS:HE1	1:B:51:GLY:O	1.91	0.54
1:D:89:GLU:H	1:D:89:GLU:CD	2.10	0.53
1:D:204:HIS:ND1	1:D:205:ASN:O	2.41	0.53
1:A:25:HIS:HE1	1:A:51:GLY:O	1.91	0.53
1:D:89:GLU:CG	1:D:185:LYS:HD3	2.38	0.53
1:C:58:TRP:HE1	1:C:213:GLN:NE2	2.07	0.53
1:B:41:HIS:CE1	1:B:214:TYR:HH	2.26	0.53
1:A:58:TRP:HE1	1:A:213:GLN:NE2	2.07	0.53
1:B:113:LEU:CD2	1:B:114:GLN:H	2.22	0.53
1:D:113:LEU:HD23	1:D:114:GLN:N	2.24	0.53
1:A:113:LEU:CD2	1:A:114:GLN:H	2.22	0.52
1:A:89:GLU:CD	1:A:89:GLU:H	2.10	0.52
1:C:41:HIS:CE1	1:C:214:TYR:HH	2.28	0.52
1:B:113:LEU:HD23	1:B:114:GLN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:HIS:CE1	1:A:214:TYR:HH	2.28	0.52
1:C:113:LEU:CD2	1:C:114:GLN:H	2.22	0.52
1:B:58:TRP:HE1	1:B:213:GLN:NE2	2.07	0.52
1:C:113:LEU:HD23	1:C:114:GLN:N	2.24	0.52
1:A:113:LEU:HD23	1:A:114:GLN:N	2.24	0.51
1:D:113:LEU:CD2	1:D:114:GLN:H	2.22	0.51
1:D:58:TRP:HE1	1:D:213:GLN:NE2	2.06	0.51
1:A:94:GLU:OE2	2:A:251:HOH:O	2.18	0.51
1:B:31:GLY:O	1:B:32:GLU:HG2	2.10	0.51
1:C:78:ASP:N	1:C:78:ASP:OD1	2.36	0.51
1:B:7:VAL:N	2:B:314:HOH:O	2.44	0.51
1:A:78:ASP:N	1:A:78:ASP:OD1	2.36	0.51
1:C:31:GLY:O	1:C:32:GLU:HG2	2.11	0.51
1:D:31:GLY:O	1:D:32:GLU:HG2	2.11	0.51
1:D:91:PHE:CA	1:D:184:LYS:HD2	2.41	0.51
1:A:91:PHE:CA	1:A:184:LYS:HD2	2.41	0.51
1:D:7:VAL:N	2:D:314:HOH:O	2.44	0.51
1:B:91:PHE:CA	1:B:184:LYS:HD2	2.41	0.50
1:A:83:MET:HG3	1:A:91:PHE:CE2	2.47	0.50
1:D:41:HIS:CE1	1:D:214:TYR:HH	2.29	0.50
1:D:83:MET:HG3	1:D:91:PHE:CE2	2.47	0.50
1:A:31:GLY:O	1:A:32:GLU:HG2	2.10	0.50
1:A:7:VAL:N	2:A:310:HOH:O	2.44	0.50
1:D:36:ARG:NH1	1:D:36:ARG:HG2	2.26	0.50
1:C:7:VAL:N	2:C:396:HOH:O	2.44	0.50
1:C:91:PHE:CA	1:C:184:LYS:HD2	2.41	0.50
1:B:36:ARG:HG2	1:B:36:ARG:NH1	2.26	0.50
1:B:83:MET:HG3	1:B:91:PHE:CE2	2.47	0.50
1:C:36:ARG:NH1	1:C:36:ARG:HG2	2.26	0.49
1:A:9:LYS:N	1:A:12:MET:SD	2.85	0.49
1:B:194:TYR:HE1	2:B:370:HOH:O	1.95	0.49
1:C:83:MET:HG3	1:C:91:PHE:CE2	2.47	0.49
1:A:194:TYR:HE1	2:A:366:HOH:O	1.95	0.49
1:C:9:LYS:N	1:C:12:MET:SD	2.85	0.49
1:D:9:LYS:N	1:D:12:MET:SD	2.85	0.49
1:C:194:TYR:HE1	2:C:453:HOH:O	1.95	0.49
1:A:36:ARG:HG2	1:A:36:ARG:NH1	2.26	0.49
1:A:113:LEU:CD2	1:A:114:GLN:N	2.76	0.49
1:B:9:LYS:N	1:B:12:MET:SD	2.85	0.49
1:C:113:LEU:CD2	1:C:114:GLN:N	2.76	0.49
1:C:204:HIS:ND1	1:C:205:ASN:O	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ASP:O	1:D:85:LEU:HG	2.13	0.49
1:B:12:MET:HG3	1:B:37:PRO:HG2	1.95	0.48
1:A:12:MET:HG3	1:A:37:PRO:HG2	1.95	0.48
1:C:12:MET:HG3	1:C:37:PRO:HG2	1.95	0.48
1:C:81:ASP:O	1:C:85:LEU:HG	2.13	0.48
1:D:113:LEU:CD2	1:D:114:GLN:N	2.76	0.48
1:D:194:TYR:HE1	2:D:369:HOH:O	1.95	0.48
1:D:12:MET:HG3	1:D:37:PRO:HG2	1.95	0.48
1:B:81:ASP:O	1:B:85:LEU:HG	2.13	0.48
1:A:83:MET:CG	1:A:91:PHE:CZ	2.97	0.48
1:B:113:LEU:CD2	1:B:114:GLN:N	2.76	0.47
1:C:45:LYS:HB2	1:C:212:GLU:CG	2.40	0.47
1:A:81:ASP:O	1:A:85:LEU:HG	2.13	0.47
1:A:45:LYS:HB2	1:A:212:GLU:CG	2.40	0.47
1:C:195:VAL:HG22	1:C:219:GLY:HA2	1.97	0.47
1:B:45:LYS:HB2	1:B:212:GLU:CG	2.40	0.47
1:C:75:HIS:CG	1:C:81:ASP:HB2	2.50	0.47
1:B:83:MET:CG	1:B:91:PHE:CZ	2.97	0.47
1:C:83:MET:CG	1:C:91:PHE:CZ	2.97	0.47
1:D:195:VAL:HG22	1:D:219:GLY:HA2	1.97	0.47
1:A:195:VAL:HG22	1:A:219:GLY:HA2	1.97	0.47
1:D:75:HIS:CG	1:D:81:ASP:HB2	2.50	0.47
1:B:204:HIS:ND1	1:B:205:ASN:O	2.41	0.47
1:D:45:LYS:HB2	1:D:212:GLU:CG	2.40	0.47
1:B:75:HIS:CG	1:B:81:ASP:HB2	2.50	0.46
1:C:222:HIS:HB2	2:C:453:HOH:O	2.15	0.46
1:A:75:HIS:CG	1:A:81:ASP:HB2	2.50	0.46
1:B:222:HIS:HB2	2:B:370:HOH:O	2.15	0.46
1:A:137:GLN:HB3	2:A:371:HOH:O	2.15	0.46
1:D:83:MET:CG	1:D:91:PHE:CZ	2.97	0.46
1:D:222:HIS:HB2	2:D:369:HOH:O	2.15	0.46
1:A:222:HIS:HB2	2:A:366:HOH:O	2.15	0.45
1:B:195:VAL:HG22	1:B:219:GLY:HA2	1.97	0.45
1:A:7:VAL:HG11	1:A:88:PRO:HB3	1.99	0.45
1:A:204:HIS:ND1	1:A:205:ASN:O	2.41	0.45
1:B:7:VAL:HG11	1:B:88:PRO:HB3	1.99	0.45
1:C:210:ILE:HD13	1:C:210:ILE:HG21	1.64	0.45
1:D:210:ILE:HG21	1:D:210:ILE:HD13	1.64	0.45
1:C:7:VAL:HG11	1:C:88:PRO:HB3	1.99	0.45
1:B:69:SER:HB2	1:B:120:TYR:OH	2.17	0.45
1:D:69:SER:HB2	1:D:120:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:HIS:HE1	2:C:363:HOH:O	1.99	0.45
1:A:69:SER:HB2	1:A:120:TYR:OH	2.17	0.45
1:D:137:GLN:HB2	1:D:139:LYS:HE3	1.98	0.45
1:A:75:HIS:HE1	2:A:279:HOH:O	1.99	0.45
1:B:134:PRO:HA	1:B:139:LYS:HD2	1.99	0.45
1:B:137:GLN:HB2	1:B:139:LYS:HE3	1.99	0.45
1:D:36:ARG:O	1:D:39:GLU:N	2.46	0.44
1:B:36:ARG:O	1:B:39:GLU:N	2.46	0.44
1:D:134:PRO:HA	1:D:139:LYS:HD2	1.99	0.44
1:C:69:SER:HB2	1:C:120:TYR:OH	2.17	0.44
1:D:223:LEU:HD12	1:D:223:LEU:HA	1.75	0.44
1:C:36:ARG:O	1:C:39:GLU:N	2.46	0.44
1:A:36:ARG:O	1:A:39:GLU:N	2.46	0.44
1:A:168:LYS:NZ	1:C:154:ASP:OD1	2.26	0.44
1:D:168:LYS:HD3	2:D:306:HOH:O	2.18	0.44
1:D:7:VAL:HG11	1:D:88:PRO:HB3	1.99	0.44
1:C:204:HIS:CE1	1:C:208:TYR:CZ	3.06	0.44
1:C:137:GLN:HB2	1:C:139:LYS:HE3	1.98	0.44
1:B:75:HIS:HE1	2:B:282:HOH:O	1.99	0.44
1:A:204:HIS:CE1	1:A:208:TYR:CZ	3.06	0.44
1:B:168:LYS:HD3	2:B:306:HOH:O	2.18	0.44
1:D:11:PHE:CE2	1:D:13:ARG:HG3	2.53	0.44
1:C:11:PHE:CE2	1:C:13:ARG:HG3	2.53	0.44
1:D:75:HIS:HE1	2:D:283:HOH:O	1.99	0.44
1:C:168:LYS:HD3	2:C:388:HOH:O	2.18	0.44
1:A:28:GLU:C	1:A:29:ILE:HG13	2.38	0.44
1:B:11:PHE:CE2	1:B:13:ARG:HG3	2.53	0.43
1:D:204:HIS:CE1	1:D:208:TYR:CZ	3.06	0.43
1:A:137:GLN:HB2	1:A:139:LYS:HE3	1.99	0.43
1:A:134:PRO:HA	1:A:139:LYS:HD2	1.99	0.43
1:C:134:PRO:HA	1:C:139:LYS:HD2	1.99	0.43
1:A:168:LYS:HD3	2:A:302:HOH:O	2.18	0.43
1:A:80:PRO:HG2	1:A:190:PRO:HA	2.01	0.43
1:D:202:THR:O	1:D:203:SER:HB3	2.18	0.43
1:A:11:PHE:CE2	1:A:13:ARG:HG3	2.53	0.43
1:A:149:ARG:O	1:A:159:GLY:HA2	2.19	0.43
1:B:204:HIS:CE1	1:B:208:TYR:CZ	3.06	0.43
1:B:210:ILE:HG21	1:B:210:ILE:HD13	1.64	0.43
1:D:149:ARG:O	1:D:159:GLY:HA2	2.19	0.43
1:B:202:THR:O	1:B:203:SER:HB3	2.18	0.43
1:C:80:PRO:HG2	1:C:190:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:THR:O	1:C:203:SER:HB3	2.18	0.43
1:C:207:ASP:OD2	1:C:207:ASP:N	2.52	0.43
1:C:109:GLN:HG2	1:C:121:LYS:O	2.19	0.43
1:C:149:ARG:O	1:C:159:GLY:HA2	2.19	0.43
1:C:28:GLU:C	1:C:29:ILE:HG13	2.39	0.43
1:A:210:ILE:HD13	1:A:210:ILE:HG21	1.64	0.43
1:A:109:GLN:HG2	1:A:121:LYS:O	2.19	0.43
1:A:207:ASP:OD2	1:A:207:ASP:N	2.52	0.42
1:C:8:ILE:CD1	1:C:87:PHE:HB2	2.48	0.42
1:D:8:ILE:CD1	1:D:87:PHE:HB2	2.48	0.42
1:C:21:THR:HG22	2:D:255:HOH:O	2.18	0.42
1:A:202:THR:O	1:A:203:SER:HB3	2.18	0.42
1:B:109:GLN:HG2	1:B:121:LYS:O	2.19	0.42
1:B:28:GLU:C	1:B:29:ILE:HG13	2.38	0.42
1:A:8:ILE:CD1	1:A:87:PHE:HB2	2.48	0.42
1:D:109:GLN:HG2	1:D:121:LYS:O	2.19	0.42
1:C:9:LYS:H	1:C:9:LYS:CD	2.25	0.42
1:A:222:HIS:CD2	2:A:366:HOH:O	2.72	0.42
1:B:168:LYS:HE3	1:B:168:LYS:HB3	1.60	0.42
1:C:222:HIS:CD2	2:C:453:HOH:O	2.72	0.42
1:D:80:PRO:HG2	1:D:190:PRO:HA	2.01	0.42
1:C:223:LEU:HA	1:C:223:LEU:HD12	1.75	0.42
1:D:28:GLU:C	1:D:29:ILE:HG13	2.39	0.42
1:B:149:ARG:O	1:B:159:GLY:HA2	2.19	0.42
1:D:16:VAL:HG23	1:D:120:TYR:HB2	2.01	0.42
1:A:16:VAL:HG23	1:A:120:TYR:HB2	2.02	0.42
1:C:16:VAL:HG23	1:C:120:TYR:HB2	2.01	0.42
1:B:80:PRO:HG2	1:B:190:PRO:HA	2.01	0.42
1:B:8:ILE:HD11	1:B:87:PHE:CB	2.50	0.41
1:D:8:ILE:HD11	1:D:87:PHE:CB	2.50	0.41
1:B:222:HIS:CD2	2:B:370:HOH:O	2.72	0.41
1:D:207:ASP:N	1:D:207:ASP:OD2	2.52	0.41
1:B:8:ILE:CD1	1:B:87:PHE:HB2	2.48	0.41
1:D:222:HIS:CD2	2:D:369:HOH:O	2.72	0.41
1:A:66:CRQ:CZ	1:A:197:SER:HB2	2.51	0.41
1:D:66:CRQ:CZ	1:D:197:SER:HB2	2.51	0.41
1:B:41:HIS:CE1	2:B:321:HOH:O	2.73	0.41
1:C:41:HIS:CE1	2:C:404:HOH:O	2.73	0.41
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.75	0.41
1:C:106:THR:HG23	1:D:106:THR:HG23	2.02	0.41
1:A:82:TYR:CD1	1:A:189:LEU:HD23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:LEU:HD23	1:C:117:CYS:O	2.21	0.41
1:C:66:CRQ:CZ	1:C:197:SER:HB2	2.51	0.41
1:B:66:CRQ:CZ	1:B:197:SER:HB2	2.51	0.41
1:B:16:VAL:HG23	1:B:120:TYR:HB2	2.01	0.41
1:A:9:LYS:H	1:A:9:LYS:CD	2.25	0.41
1:B:82:TYR:CD1	1:B:189:LEU:HD23	2.56	0.41
1:C:25:HIS:CE1	1:C:51:GLY:O	2.72	0.41
1:A:41:HIS:CE1	2:A:317:HOH:O	2.74	0.41
1:D:41:HIS:CE1	2:D:321:HOH:O	2.73	0.41
1:B:223:LEU:HA	1:B:223:LEU:HD12	1.75	0.41
1:C:82:TYR:CD1	1:C:189:LEU:HD23	2.56	0.41
1:B:113:LEU:HD23	1:B:117:CYS:O	2.21	0.41
1:C:114:GLN:O	1:C:116:GLY:N	2.54	0.40
1:C:8:ILE:HD11	1:C:87:PHE:CB	2.50	0.40
1:D:82:TYR:CD1	1:D:189:LEU:HD23	2.56	0.40
1:A:113:LEU:HD23	1:A:117:CYS:O	2.21	0.40
1:B:141:MET:HG3	1:B:168:LYS:HA	2.03	0.40
1:B:37:PRO:HA	1:B:72:TYR:HA	2.03	0.40
1:D:113:LEU:HD23	1:D:117:CYS:C	2.42	0.40
1:D:113:LEU:HD23	1:D:117:CYS:O	2.21	0.40
1:D:37:PRO:HA	1:D:72:TYR:HA	2.03	0.40
1:A:89:GLU:CD	1:A:89:GLU:N	2.74	0.40
1:B:25:HIS:CE1	1:B:51:GLY:O	2.72	0.40
1:A:25:HIS:CE1	1:A:51:GLY:O	2.72	0.40
1:B:76:PRO:HG3	2:B:343:HOH:O	2.21	0.40
1:D:114:GLN:O	1:D:116:GLY:N	2.54	0.40

All (4) 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:B:330:HOH:O	2:D:309:HOH:O[11_556]	2.09	0.11
2:B:362:HOH:O	2:B:370:HOH:O[11_656]	2.13	0.07
2:C:445:HOH:O	2:C:453:HOH:O[7_556]	2.14	0.06
1:B:145:ALA:O	2:B:370:HOH:O[11_656]	2.15	0.05

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	214/217 (99%)	205 (96%)	9 (4%)	0	100	100
1	B	214/217 (99%)	205 (96%)	9 (4%)	0	100	100
1	C	214/217 (99%)	205 (96%)	9 (4%)	0	100	100
1	D	214/217 (99%)	205 (96%)	9 (4%)	0	100	100
All	All	856/868 (99%)	820 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/190 (96%)	166 (91%)	17 (9%)	11	6
1	B	183/190 (96%)	166 (91%)	17 (9%)	11	6
1	C	183/190 (96%)	166 (91%)	17 (9%)	11	6
1	D	183/190 (96%)	166 (91%)	17 (9%)	11	6
All	All	732/760 (96%)	664 (91%)	68 (9%)	11	6

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	9	LYS

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Mol	Chain	Res	Type
1	A	12	MET
1	A	15	LYS
1	A	30	GLU
1	A	38	TYR
1	A	74	LYS
1	A	89	GLU
1	A	112	SER
1	A	113	LEU
1	A	158	LYS
1	A	161	ILE
1	A	168	LYS
1	A	179	SER
1	A	182	MET
1	A	197	SER
1	A	223	LEU
1	B	7	VAL
1	B	9	LYS
1	B	12	MET
1	B	15	LYS
1	B	30	GLU
1	B	38	TYR
1	B	74	LYS
1	B	89	GLU
1	B	112	SER
1	B	113	LEU
1	B	158	LYS
1	B	161	ILE
1	B	168	LYS
1	B	179	SER
1	B	182	MET
1	B	197	SER
1	B	223	LEU
1	C	7	VAL
1	C	9	LYS
1	C	12	MET
1	C	15	LYS
1	C	30	GLU
1	C	38	TYR
1	C	74	LYS
1	C	89	GLU
1	C	112	SER
1	C	113	LEU

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Mol	Chain	Res	Type
1	C	158	LYS
1	C	161	ILE
1	C	168	LYS
1	C	179	SER
1	C	182	MET
1	C	197	SER
1	C	223	LEU
1	D	7	VAL
1	D	9	LYS
1	D	12	MET
1	D	15	LYS
1	D	30	GLU
1	D	38	TYR
1	D	74	LYS
1	D	89	GLU
1	D	112	SER
1	D	113	LEU
1	D	158	LYS
1	D	161	ILE
1	D	168	LYS
1	D	179	SER
1	D	182	MET
1	D	197	SER
1	D	223	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	42	ASN
1	A	172	HIS
1	B	25	HIS
1	B	42	ASN
1	B	172	HIS
1	C	25	HIS
1	C	42	ASN
1	C	172	HIS
1	D	25	HIS
1	D	42	ASN
1	D	172	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	A	66	1	24,25,26	2.06	8 (33%)	25,34,36	3.80	7 (28%)
1	CRQ	B	66	1	24,25,26	2.07	8 (33%)	25,34,36	3.79	7 (28%)
1	CRQ	C	66	1	24,25,26	2.06	8 (33%)	25,34,36	3.80	7 (28%)
1	CRQ	D	66	1	24,25,26	2.07	8 (33%)	25,34,36	3.79	7 (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	A	66	1	-	0/10/32/33	0/2/2/2
1	CRQ	B	66	1	-	0/10/32/33	0/2/2/2
1	CRQ	C	66	1	-	0/10/32/33	0/2/2/2
1	CRQ	D	66	1	-	0/10/32/33	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CRQ	OH-CZ	-5.42	1.24	1.37
1	B	66	CRQ	OH-CZ	-5.42	1.24	1.37
1	D	66	CRQ	OH-CZ	-5.41	1.24	1.37
1	A	66	CRQ	OH-CZ	-5.41	1.24	1.37
1	D	66	CRQ	CG2-CB2	-3.33	1.40	1.46
1	A	66	CRQ	CG2-CB2	-3.30	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRQ	CG2-CB2	-3.30	1.40	1.46
1	C	66	CRQ	CG2-CB2	-3.30	1.40	1.46
1	B	66	CRQ	CA3-N3	-3.11	1.42	1.47
1	C	66	CRQ	CA3-N3	-3.09	1.42	1.47
1	D	66	CRQ	CA3-N3	-3.09	1.42	1.47
1	A	66	CRQ	CA3-N3	-3.08	1.42	1.47
1	B	66	CRQ	CD1-CG2	2.19	1.43	1.39
1	A	66	CRQ	CD1-CG2	2.21	1.43	1.39
1	C	66	CRQ	CD1-CG2	2.22	1.43	1.39
1	D	66	CRQ	CD1-CG2	2.24	1.43	1.39
1	C	66	CRQ	CB2-CA2	2.40	1.37	1.35
1	A	66	CRQ	CB2-CA2	2.40	1.37	1.35
1	B	66	CRQ	CB2-CA2	2.43	1.37	1.35
1	D	66	CRQ	CB2-CA2	2.50	1.37	1.35
1	C	66	CRQ	CE2-CZ	3.05	1.45	1.38
1	B	66	CRQ	CE2-CZ	3.05	1.45	1.38
1	A	66	CRQ	CE2-CZ	3.07	1.45	1.38
1	D	66	CRQ	CE2-CZ	3.07	1.45	1.38
1	A	66	CRQ	CE1-CZ	3.20	1.45	1.38
1	C	66	CRQ	CE1-CZ	3.21	1.45	1.38
1	D	66	CRQ	CE1-CZ	3.23	1.45	1.38
1	B	66	CRQ	CE1-CZ	3.26	1.45	1.38
1	D	66	CRQ	CA1-N	3.80	1.39	1.28
1	A	66	CRQ	CA1-N	3.81	1.39	1.28
1	B	66	CRQ	CA1-N	3.82	1.40	1.28
1	C	66	CRQ	CA1-N	3.83	1.40	1.28

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	CRQ	CB1-CA1-N	-15.43	96.58	124.94
1	C	66	CRQ	CB1-CA1-N	-15.42	96.59	124.94
1	B	66	CRQ	CB1-CA1-N	-15.42	96.60	124.94
1	D	66	CRQ	CB1-CA1-N	-15.41	96.62	124.94
1	B	66	CRQ	CE2-CZ-CE1	-3.27	115.13	119.79
1	A	66	CRQ	CE2-CZ-CE1	-3.26	115.14	119.79
1	D	66	CRQ	CE2-CZ-CE1	-3.25	115.16	119.79
1	C	66	CRQ	CE2-CZ-CE1	-3.24	115.17	119.79
1	B	66	CRQ	CE2-CD2-CG2	2.40	124.29	121.29
1	A	66	CRQ	CE2-CD2-CG2	2.42	124.32	121.29
1	D	66	CRQ	CE2-CD2-CG2	2.45	124.35	121.29
1	C	66	CRQ	CE2-CD2-CG2	2.47	124.37	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	CRQ	C-CA3-N3	3.80	121.32	113.00
1	B	66	CRQ	C-CA3-N3	3.80	121.32	113.00
1	C	66	CRQ	C-CA3-N3	3.80	121.32	113.00
1	D	66	CRQ	C-CA3-N3	3.82	121.36	113.00
1	A	66	CRQ	CG2-CB2-CA2	4.50	136.05	130.22
1	B	66	CRQ	CG2-CB2-CA2	4.50	136.06	130.22
1	B	66	CRQ	CA2-C2-N3	4.54	105.67	103.40
1	D	66	CRQ	CA2-C2-N3	4.54	105.68	103.40
1	C	66	CRQ	CG2-CB2-CA2	4.54	136.12	130.22
1	D	66	CRQ	CG2-CB2-CA2	4.55	136.12	130.22
1	A	66	CRQ	CA2-C2-N3	4.57	105.69	103.40
1	C	66	CRQ	CA2-C2-N3	4.61	105.71	103.40
1	D	66	CRQ	O2-C2-CA2	5.51	133.92	130.95
1	B	66	CRQ	O2-C2-CA2	5.57	133.95	130.95
1	C	66	CRQ	O2-C2-CA2	5.57	133.95	130.95
1	A	66	CRQ	O2-C2-CA2	5.62	133.98	130.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRQ	2	0
1	B	66	CRQ	2	0
1	C	66	CRQ	2	0
1	D	66	CRQ	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	216/217 (99%)	0.32	13 (6%)	25	27	28, 44, 65, 82	0
1	B	216/217 (99%)	0.42	21 (9%)	10	10	28, 44, 65, 82	0
1	C	216/217 (99%)	0.43	15 (6%)	20	21	30, 45, 66, 82	0
1	D	216/217 (99%)	0.60	21 (9%)	10	10	29, 45, 65, 82	0
All	All	864/868 (99%)	0.44	70 (8%)	15	15	28, 44, 66, 82	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	169	ASP	5.7
1	D	168	LYS	5.1
1	D	13	ARG	4.9
1	C	77	ALA	3.9
1	D	70	LYS	3.9
1	B	9	LYS	3.9
1	A	7	VAL	3.9
1	D	93	TRP	3.7
1	D	161	ILE	3.6
1	D	7	VAL	3.6
1	B	117	CYS	3.5
1	A	114	GLN	3.5
1	D	195	VAL	3.4
1	A	116	GLY	3.4
1	C	9	LYS	3.4
1	D	186	PRO	3.3
1	D	119	ILE	3.2
1	B	114	GLN	3.1
1	C	63	PRO	3.0
1	C	78	ASP	2.9
1	B	161	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	168	LYS	2.9
1	B	11	PHE	2.8
1	B	77	ALA	2.8
1	D	206	GLU	2.8
1	B	215	GLU	2.8
1	A	77	ALA	2.7
1	B	93	TRP	2.7
1	C	223	LEU	2.7
1	B	154	ASP	2.7
1	A	13	ARG	2.7
1	A	9	LYS	2.7
1	B	36	ARG	2.7
1	C	132	ASP	2.6
1	A	115	ASP	2.6
1	C	225	LEU	2.6
1	B	70	LYS	2.5
1	B	71	VAL	2.5
1	D	117	CYS	2.5
1	D	49	THR	2.5
1	C	117	CYS	2.4
1	A	8	ILE	2.4
1	B	169	ASP	2.4
1	C	76	PRO	2.4
1	A	117	CYS	2.4
1	B	217	THR	2.4
1	D	38	TYR	2.4
1	D	203	SER	2.4
1	A	180	ILE	2.3
1	B	88	PRO	2.3
1	D	78	ASP	2.3
1	C	87	PHE	2.3
1	B	89	GLU	2.3
1	A	186	PRO	2.3
1	D	204	HIS	2.3
1	D	87	PHE	2.2
1	D	63	PRO	2.2
1	D	77	ALA	2.2
1	A	11	PHE	2.2
1	C	186	PRO	2.2
1	B	113	LEU	2.1
1	C	8	ILE	2.1
1	C	38	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	181	TYR	2.1
1	D	170	GLY	2.1
1	C	89	GLU	2.0
1	B	73	VAL	2.0
1	B	115	ASP	2.0
1	A	214	TYR	2.0
1	B	170	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	CRQ	A	66	24/25	0.91	0.20	-	34,43,54,64	0
1	CRQ	D	66	24/25	0.91	0.22	-	35,44,54,65	0
1	CRQ	B	66	24/25	0.94	0.21	-	34,43,54,64	0
1	CRQ	C	66	24/25	0.93	0.17	-	36,44,55,65	0

6.3 Carbohydrates (i)

There are no carbohydrates 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.