



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 11:52 AM UTC

PDB ID : 2G6X / pdb_00002g6x
Title : Crystal structure of a novel green fluorescent protein from marine copepod
Pontellina plumata
Authors : Evdokimov, A.G.; Pokross, M.E.; Chudakov, D.M.
Deposited on : 2006-02-26
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

<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

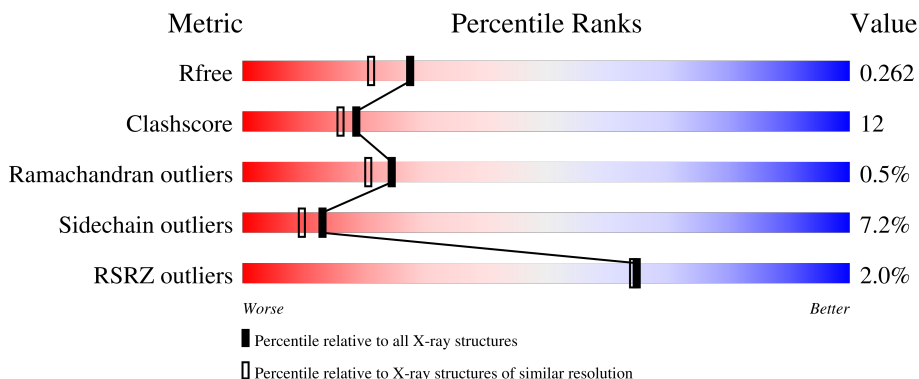
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	217	2% 68% 24% 6%
1	B	217	2% 70% 24% 6%
1	C	217	2% 73% 23%
1	D	217	% 63% 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7109 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	1	0
			1700	1077	289	324	10			
1	B	216	Total	C	N	O	S	0	2	0
			1718	1090	291	327	10			
1	C	216	Total	C	N	O	S	0	1	0
			1718	1087	294	328	9			
1	D	215	Total	C	N	O	S	0	0	0
			1703	1077	290	327	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	-	cloning artifact	GB 33243028
A	5	GLU	LYS	engineered mutation	GB 33243028
A	58	CR2	GLY	chromophore	GB 33243028
A	58	CR2	TYR	chromophore	GB 33243028
A	58	CR2	GLY	chromophore	GB 33243028
A	117	MET	VAL	engineered mutation	GB 33243028
A	149	ASP	VAL	engineered mutation	GB 33243028
A	151	ASP	VAL	engineered mutation	GB 33243028
A	155	THR	ALA	engineered mutation	GB 33243028
A	168	SER	PHE	engineered mutation	GB 33243028
A	200	ASP	LEU	engineered mutation	GB 33243028
A	219	ASP	ILE	engineered mutation	GB 33243028
B	1	LEU	-	cloning artifact	GB 33243028
B	5	GLU	LYS	engineered mutation	GB 33243028
B	58	CR2	GLY	chromophore	GB 33243028
B	58	CR2	TYR	chromophore	GB 33243028
B	58	CR2	GLY	chromophore	GB 33243028
B	117	MET	VAL	engineered mutation	GB 33243028
B	149	ASP	VAL	engineered mutation	GB 33243028
B	151	ASP	VAL	engineered mutation	GB 33243028
B	155	THR	ALA	engineered mutation	GB 33243028

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Chain	Residue	Modelled	Actual	Comment	Reference
B	168	SER	PHE	engineered mutation	GB 33243028
B	200	ASP	LEU	engineered mutation	GB 33243028
B	219	ASP	ILE	engineered mutation	GB 33243028
C	1	LEU	-	cloning artifact	GB 33243028
C	5	GLU	LYS	engineered mutation	GB 33243028
C	58	CR2	GLY	chromophore	GB 33243028
C	58	CR2	TYR	chromophore	GB 33243028
C	58	CR2	GLY	chromophore	GB 33243028
C	117	MET	VAL	engineered mutation	GB 33243028
C	149	ASP	VAL	engineered mutation	GB 33243028
C	151	ASP	VAL	engineered mutation	GB 33243028
C	155	THR	ALA	engineered mutation	GB 33243028
C	168	SER	PHE	engineered mutation	GB 33243028
C	200	ASP	LEU	engineered mutation	GB 33243028
C	219	ASP	ILE	engineered mutation	GB 33243028
D	1	LEU	-	cloning artifact	GB 33243028
D	5	GLU	LYS	engineered mutation	GB 33243028
D	58	CR2	GLY	chromophore	GB 33243028
D	58	CR2	TYR	chromophore	GB 33243028
D	58	CR2	GLY	chromophore	GB 33243028
D	117	MET	VAL	engineered mutation	GB 33243028
D	149	ASP	VAL	engineered mutation	GB 33243028
D	151	ASP	VAL	engineered mutation	GB 33243028
D	155	THR	ALA	engineered mutation	GB 33243028
D	168	SER	PHE	engineered mutation	GB 33243028
D	200	ASP	LEU	engineered mutation	GB 33243028
D	219	ASP	ILE	engineered mutation	GB 33243028

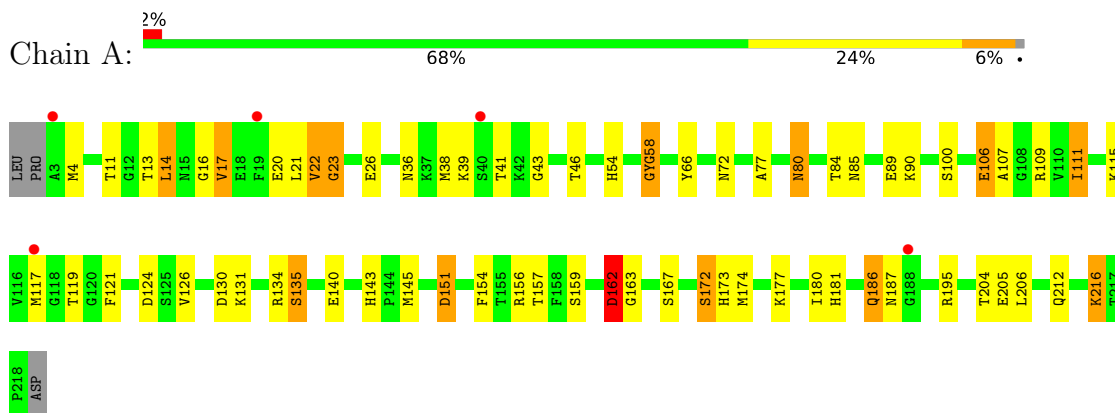
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	66	Total O 66 66	0	0
2	B	78	Total O 78 78	0	0
2	C	58	Total O 58 58	0	0
2	D	68	Total O 68 68	0	0

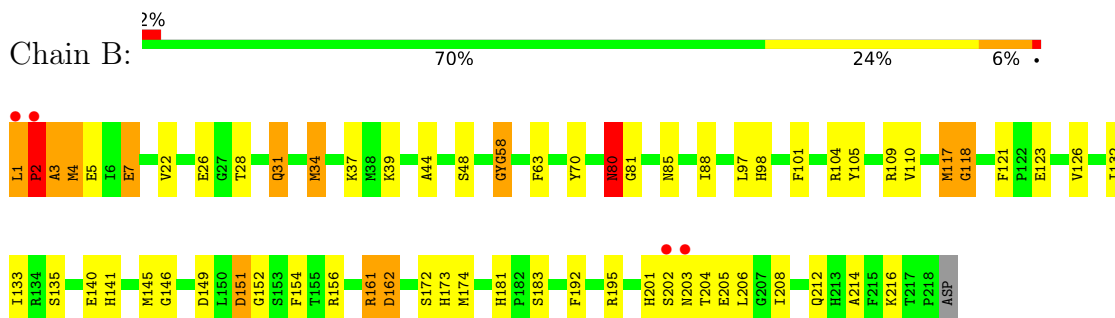
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

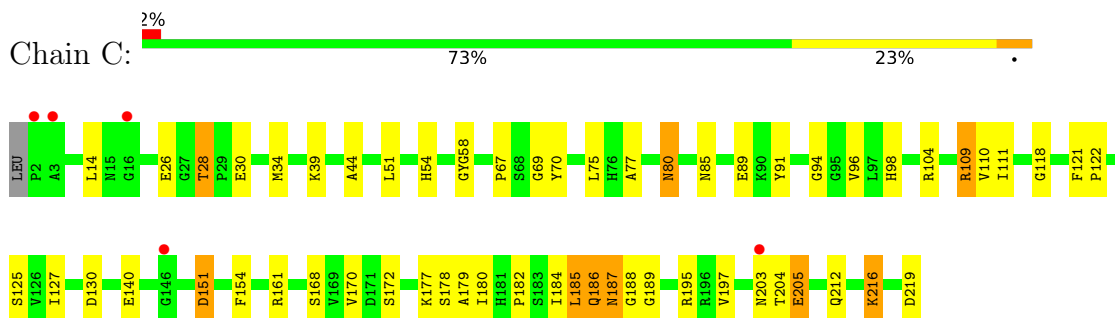
- Molecule 1: green fluorescent protein 2



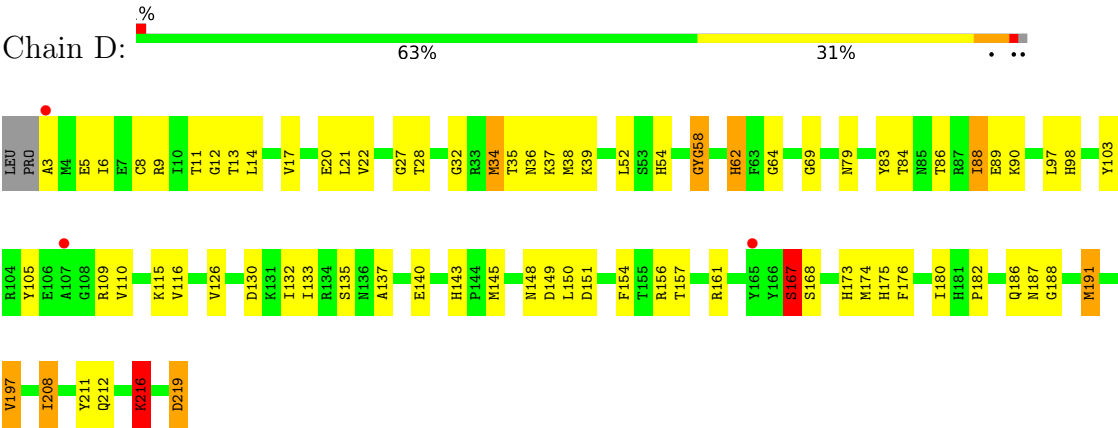
- Molecule 1: green fluorescent protein 2



- Molecule 1: green fluorescent protein 2



- Molecule 1: green fluorescent protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.75Å 97.91Å 172.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.00 86.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (100.00-2.00) 98.1 (86.16-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.246 0.214 , 0.262	Depositor DCC
R_{free} test set	2807 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7109	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: CR2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	0/1728	1.64	23/2331 (1.0%)
1	B	0.73	0/1750	1.65	28/2362 (1.2%)
1	C	0.63	0/1747	1.58	14/2357 (0.6%)
1	D	0.69	0/1728	1.62	27/2332 (1.2%)
All	All	0.69	0/6953	1.62	92/9382 (1.0%)

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	0	1
1	B	0	3
1	D	0	2
All	All	0	6

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	THR	CA-C-N	9.92	129.55	119.24
1	B	28	THR	C-N-CA	9.92	129.55	119.24
1	A	135	SER	CB-CA-C	-9.44	94.46	109.84
1	B	80	ASN	N-CA-C	9.19	121.26	110.41
1	C	189	GLY	CA-C-N	-8.47	112.08	120.21
1	C	189	GLY	C-N-CA	-8.47	112.08	120.21
1	C	69	GLY	N-CA-C	-7.97	105.21	114.69
1	D	34	MET	CG-SD-CE	7.70	117.83	100.90
1	A	121	PHE	CA-C-N	-7.67	112.85	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	PHE	C-N-CA	-7.67	112.85	120.21
1	C	28	THR	CB-CA-C	7.57	120.73	110.13
1	C	51	LEU	N-CA-C	-7.51	103.10	111.82
1	C	121	PHE	CA-C-N	7.19	127.19	119.78
1	C	121	PHE	C-N-CA	7.19	127.19	119.78
1	A	162	ASP	N-CA-C	7.19	126.11	110.80
1	D	35	THR	N-CA-C	-7.11	98.51	109.24
1	B	48	SER	CA-C-N	-6.98	112.51	119.56
1	B	48	SER	C-N-CA	-6.98	112.51	119.56
1	D	132	ILE	CA-C-N	-6.93	113.42	122.16
1	D	132	ILE	C-N-CA	-6.93	113.42	122.16
1	A	163	GLY	N-CA-C	-6.92	96.78	113.18
1	C	203	ASN	N-CA-C	-6.89	104.91	113.38
1	A	151	ASP	OD1-CG-OD2	6.75	139.09	122.90
1	A	111	ILE	CA-C-N	-6.59	116.40	122.80
1	A	111	ILE	C-N-CA	-6.59	116.40	122.80
1	B	162	ASP	CB-CG-OD1	-6.50	103.44	118.40
1	B	156	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	B	63	PHE	CA-C-N	-6.44	117.63	122.33
1	B	63	PHE	C-N-CA	-6.44	117.63	122.33
1	C	151	ASP	N-CA-CB	-6.43	100.48	110.57
1	D	6	ILE	N-CA-C	-6.40	98.25	107.78
1	D	143	HIS	CA-C-N	-6.38	113.38	120.14
1	D	143	HIS	C-N-CA	-6.38	113.38	120.14
1	D	21	LEU	CD1-CG-CD2	-6.24	97.07	110.80
1	A	23	GLY	N-CA-C	6.17	118.89	110.69
1	A	16	GLY	N-CA-C	6.15	123.23	115.42
1	B	146	GLY	N-CA-C	-6.13	98.66	113.18
1	B	161	ARG	CB-CG-CD	6.12	125.39	111.30
1	A	151	ASP	N-CA-CB	-6.10	100.43	110.68
1	B	132	ILE	N-CA-CB	6.06	117.13	110.53
1	D	28	THR	CB-CA-C	6.01	118.15	110.34
1	B	3	ALA	N-CA-C	5.99	118.51	107.73
1	A	151	ASP	CB-CG-OD2	-5.98	104.64	118.40
1	D	216	LYS	N-CA-C	-5.95	105.69	113.12
1	A	143	HIS	O-C-N	5.92	126.08	121.88
1	B	133	ILE	N-CA-C	5.91	119.44	113.47
1	A	131	LYS	N-CA-C	5.87	118.46	111.71
1	A	130	ASP	N-CA-C	-5.80	106.11	112.72
1	C	94	GLY	CA-C-N	5.80	125.49	119.92
1	C	94	GLY	C-N-CA	5.80	125.49	119.92
1	B	161	ARG	CA-CB-CG	-5.78	102.54	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	208	ILE	CA-C-N	-5.75	115.68	123.10
1	D	208	ILE	C-N-CA	-5.75	115.68	123.10
1	B	181	HIS	CA-C-N	5.75	125.60	119.28
1	B	181	HIS	C-N-CA	5.75	125.60	119.28
1	A	186	GLN	CB-CA-C	5.70	120.27	110.01
1	A	14	LEU	CA-CB-CG	-5.64	96.57	116.30
1	B	22	VAL	CA-C-N	-5.62	111.66	120.55
1	B	22	VAL	C-N-CA	-5.62	111.66	120.55
1	B	31	GLN	CB-CG-CD	-5.61	103.06	112.60
1	B	4	MET	N-CA-C	5.52	118.24	110.23
1	B	121	PHE	CA-C-N	5.47	125.38	119.85
1	B	121	PHE	C-N-CA	5.47	125.38	119.85
1	C	75	LEU	CB-CG-CD2	-5.42	94.45	110.70
1	B	101	PHE	N-CA-CB	-5.41	102.07	110.57
1	D	69	GLY	N-CA-C	-5.41	107.64	115.27
1	B	2	PRO	N-CA-C	5.33	123.45	112.47
1	D	135	SER	CB-CA-C	-5.30	100.57	109.53
1	D	52	LEU	N-CA-C	5.30	119.75	113.28
1	D	173	HIS	CA-C-O	5.30	125.86	120.24
1	A	26	GLU	CA-C-N	-5.28	113.76	121.26
1	A	26	GLU	C-N-CA	-5.28	113.76	121.26
1	B	161	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	17	VAL	N-CA-C	5.23	116.28	108.54
1	D	173	HIS	CA-C-N	-5.22	115.74	123.05
1	D	173	HIS	C-N-CA	-5.22	115.74	123.05
1	B	135	SER	CB-CA-C	-5.21	100.93	109.53
1	A	43	GLY	N-CA-C	5.20	119.45	112.17
1	D	133	ILE	N-CA-C	5.20	119.10	113.43
1	D	197	VAL	N-CA-CB	-5.18	102.95	111.45
1	C	184	ILE	N-CA-C	-5.18	106.09	111.58
1	D	27	GLY	N-CA-C	5.15	118.09	110.42
1	D	88	ILE	CA-C-N	-5.14	115.75	123.00
1	D	88	ILE	C-N-CA	-5.14	115.75	123.00
1	D	167	SER	N-CA-CB	5.13	118.75	111.05
1	D	167	SER	N-CA-C	5.08	117.59	109.81
1	C	205	GLU	N-CA-C	5.06	116.87	108.02
1	D	103	TYR	N-CA-C	5.05	116.87	109.24
1	D	137	ALA	N-CA-C	5.05	117.21	110.35
1	A	66	TYR	CB-CA-C	5.03	116.44	108.84
1	A	36	ASN	N-CA-C	-5.03	100.08	108.32
1	B	118	GLY	O-C-N	-5.01	119.75	123.61

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	ASP	Peptide
1	B	2	PRO	Peptide
1	B	201	HIS	Peptide
1	B	208	ILE	Peptide
1	D	208	ILE	Peptide
1	D	3	ALA	Peptide

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	1700	0	1600	41	0
1	B	1718	0	1625	42	0
1	C	1718	0	1615	40	0
1	D	1703	0	1595	43	0
2	A	66	0	0	5	0
2	B	78	0	0	7	0
2	C	58	0	0	0	0
2	D	68	0	0	1	1
All	All	7109	0	6435	158	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 12.

All (158) 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:187:ASN:HD21	1:C:216:LYS:HE3	1.19	1.05
1:C:182:PRO:O	1:C:186:GLN:HG2	1.55	1.04
1:C:187:ASN:ND2	1:C:216:LYS:HE3	1.74	1.01
1:B:34:MET:HE1	1:B:58:CR2:HA12	1.48	0.95
1:B:1:LEU:HB2	1:B:2:PRO:HD3	1.53	0.91
1:B:34:MET:HE1	1:B:58:CR2:CA1	2.03	0.89
1:B:1:LEU:HB2	1:B:2:PRO:CD	2.03	0.87
1:A:54:HIS:HE1	1:A:89:GLU:OE1	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ASN:HD21	1:C:216:LYS:CE	1.90	0.83
1:A:145[A]:MET:SD	2:A:273:HOH:O	2.37	0.81
1:C:54:HIS:HE1	1:C:89:GLU:OE1	1.67	0.78
1:A:156:ARG:NH1	2:A:266:HOH:O	2.17	0.76
1:C:109:ARG:CB	1:C:109:ARG:HH11	2.00	0.74
1:C:187:ASN:CG	1:C:216:LYS:HE3	2.12	0.74
1:A:23:GLY:HA3	1:A:38:MET:HG2	1.70	0.72
1:B:88:ILE:HD11	1:B:98:HIS:HD2	1.55	0.72
1:D:88:ILE:HD11	1:D:98:HIS:HD2	1.55	0.72
1:B:80:ASN:HD22	1:B:80:ASN:C	1.99	0.71
1:A:54:HIS:CE1	1:A:89:GLU:OE1	2.42	0.70
1:B:202[B]:SER:OG	1:B:205:GLU:HB2	1.92	0.70
1:B:1:LEU:CB	1:B:2:PRO:HD3	2.20	0.70
1:D:54:HIS:HE1	1:D:89:GLU:OE1	1.73	0.70
1:B:34:MET:HE2	2:B:230:HOH:O	1.92	0.69
1:D:187:ASN:HD21	1:D:216:LYS:HE3	1.55	0.69
1:B:81:GLY:CA	2:B:272:HOH:O	2.40	0.69
1:A:173:HIS:HB3	2:A:236:HOH:O	1.92	0.69
1:B:81:GLY:N	2:B:272:HOH:O	2.17	0.69
1:C:130:ASP:CG	1:C:161[A]:ARG:HH12	2.00	0.68
1:D:157:THR:HG22	1:D:167:SER:HB3	1.75	0.68
1:B:104:ARG:HD3	2:B:280:HOH:O	1.95	0.66
1:A:54:HIS:CD2	2:A:266:HOH:O	2.48	0.66
1:A:80:ASN:C	1:A:80:ASN:HD22	2.04	0.66
1:B:34:MET:CE	2:B:230:HOH:O	2.45	0.63
1:B:7:GLU:OE2	1:B:109:ARG:HD3	1.98	0.63
1:C:109:ARG:HB2	1:C:109:ARG:NH1	2.13	0.63
1:D:62:HIS:CD2	1:D:62:HIS:H	2.15	0.63
1:D:88:ILE:HD11	1:D:98:HIS:CD2	2.34	0.63
1:B:204:THR:HG21	2:B:239:HOH:O	1.98	0.63
1:D:187:ASN:ND2	1:D:216:LYS:HE3	2.14	0.62
1:D:11:THR:HG22	1:D:20:GLU:HG3	1.82	0.62
1:B:88:ILE:CD1	1:B:98:HIS:HD2	2.14	0.61
1:B:195:ARG:HG2	1:B:212:GLN:HG2	1.81	0.61
1:C:39:LYS:HE2	1:C:205:GLU:OE1	2.03	0.59
1:D:13:THR:HA	1:D:17:VAL:O	2.02	0.59
1:C:216:LYS:HZ3	1:C:216:LYS:HB3	1.68	0.58
1:B:204:THR:CG2	2:B:239:HOH:O	2.49	0.58
1:C:54:HIS:CE1	1:C:89:GLU:OE1	2.55	0.58
1:C:109:ARG:CB	1:C:109:ARG:NH1	2.68	0.57
1:A:39:LYS:HG2	1:A:205:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ARG:HH11	1:C:109:ARG:HB3	1.68	0.57
1:A:22:VAL:HG22	1:A:41:THR:CG2	2.36	0.55
1:C:130:ASP:OD2	1:C:161[A]:ARG:NH1	2.39	0.55
1:D:58:CR2:N2	1:D:58:CR2:HD1	2.22	0.55
1:D:9:ARG:HG3	1:D:22:VAL:HG12	1.88	0.55
1:A:11:THR:HG22	1:A:20:GLU:HG3	1.87	0.55
1:D:5:GLU:HG3	1:D:109:ARG:HG3	1.88	0.55
1:B:145[A]:MET:HE3	1:C:122:PRO:HA	1.88	0.55
1:C:187:ASN:OD1	1:C:216:LYS:HE3	2.07	0.55
1:A:140:GLU:HA	1:A:154:PHE:HB3	1.89	0.54
1:C:85:ASN:HD21	1:C:172:SER:HB3	1.72	0.54
1:D:54:HIS:H	1:D:54:HIS:CD2	2.26	0.53
1:A:124:ASP:OD1	1:A:124:ASP:C	2.52	0.53
1:A:187:ASN:HD21	1:A:216:LYS:HD2	1.73	0.53
1:D:54:HIS:CE1	1:D:89:GLU:OE1	2.58	0.52
1:C:195:ARG:HG2	1:C:212:GLN:HG2	1.91	0.52
1:B:97:LEU:HD23	1:B:118:GLY:CA	2.39	0.52
1:B:85:ASN:ND2	1:B:174:MET:HG3	2.25	0.51
1:A:90:LYS:HE2	1:D:90:LYS:HE3	1.91	0.51
1:D:191:MET:HA	1:D:191:MET:HE2	1.93	0.51
1:A:85:ASN:HD21	1:A:172:SER:HB3	1.76	0.51
1:A:195:ARG:HG2	1:A:212:GLN:HG2	1.92	0.51
1:C:109:ARG:HH11	1:C:109:ARG:HB2	1.68	0.51
1:A:117:MET:HE3	1:D:98:HIS:CE1	2.46	0.50
1:A:117:MET:HE3	1:D:98:HIS:HE1	1.74	0.50
1:C:67:PRO:HG2	1:C:70:TYR:CD1	2.47	0.50
1:B:44:ALA:HB1	1:B:203:ASN:ND2	2.26	0.50
1:D:148:ASN:HB3	1:D:176:PHE:O	2.11	0.49
1:A:77:ALA:HA	1:A:80:ASN:ND2	2.27	0.49
1:A:135:SER:OG	1:A:156:ARG:NH1	2.45	0.49
1:B:97:LEU:HD23	1:B:118:GLY:HA2	1.94	0.49
1:A:21:LEU:CD2	1:A:206:LEU:HD13	2.43	0.49
1:B:34:MET:HE1	1:B:58:CR2:HA11	1.91	0.49
1:B:80:ASN:C	1:B:80:ASN:ND2	2.64	0.48
1:D:145:MET:HB2	1:D:149:ASP:HB2	1.96	0.48
1:D:34:MET:HE2	1:D:36:ASN:HB2	1.96	0.48
1:C:44:ALA:HA	1:C:204:THR:HG22	1.95	0.48
1:D:150:LEU:HG	1:D:180:ILE:HD13	1.95	0.48
1:C:219:ASP:OD2	1:D:219:ASP:C	2.57	0.47
1:D:130:ASP:O	1:D:161:ARG:NH1	2.45	0.47
1:D:188:GLY:N	2:D:286:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLU:HG2	1:C:170:VAL:HG13	1.97	0.47
1:A:109:ARG:HD3	1:A:111:ILE:HD11	1.97	0.47
1:B:140:GLU:HA	1:B:154:PHE:HB3	1.96	0.46
1:C:39:LYS:HE3	1:C:39:LYS:HB2	1.74	0.46
1:D:88:ILE:HD13	1:D:88:ILE:HA	1.81	0.46
1:A:80:ASN:C	1:A:80:ASN:ND2	2.68	0.46
1:A:84:THR:O	1:A:174:MET:HA	2.16	0.46
1:A:23:GLY:HA3	1:A:38:MET:CG	2.44	0.45
1:C:54:HIS:CD2	1:C:54:HIS:H	2.34	0.45
1:A:77:ALA:HA	1:A:80:ASN:HD21	1.81	0.45
1:C:77:ALA:HA	1:C:80:ASN:ND2	2.31	0.45
1:C:104:ARG:HB3	1:C:111:ILE:HB	1.98	0.45
1:C:187:ASN:OD1	1:C:216:LYS:CE	2.65	0.45
1:C:96:VAL:O	1:C:118:GLY:HA2	2.17	0.45
1:D:34:MET:CE	1:D:36:ASN:HB2	2.46	0.45
1:B:70:TYR:HA	1:B:183:SER:HB2	1.98	0.45
1:B:149:ASP:HB3	1:B:173:HIS:CE1	2.52	0.45
1:B:141:HIS:O	1:B:152:GLY:HA2	2.17	0.45
1:C:180:ILE:O	1:C:185:LEU:HD22	2.17	0.45
1:C:216:LYS:HZ2	1:C:216:LYS:HG3	1.62	0.44
1:D:8:CYS:SG	1:D:38:MET:HE1	2.57	0.44
1:D:154:PHE:HE1	1:D:156:ARG:HD2	1.82	0.44
1:B:2:PRO:HB2	1:B:3:ALA:H	1.54	0.44
1:C:80:ASN:C	1:C:80:ASN:HD22	2.25	0.44
1:A:106:GLU:O	1:A:107:ALA:C	2.60	0.44
1:D:62:HIS:HE1	1:D:105:TYR:OH	2.00	0.44
1:D:54:HIS:H	1:D:54:HIS:HD2	1.63	0.44
1:D:64:GLY:HA2	1:D:212:GLN:HB2	2.00	0.44
1:B:192:PHE:O	1:B:214:ALA:HA	2.17	0.44
1:A:134:ARG:HD2	2:A:271:HOH:O	2.19	0.43
1:B:5:GLU:HG3	1:B:109:ARG:NH2	2.33	0.43
1:B:39:LYS:HA	1:B:204:THR:O	2.18	0.43
1:D:97:LEU:HA	1:D:97:LEU:HD12	1.80	0.43
1:A:22:VAL:CG2	1:A:41:THR:CG2	2.96	0.43
1:A:90:LYS:HE3	1:D:90:LYS:NZ	2.33	0.43
1:A:157:THR:HG22	1:A:167:SER:HB3	1.99	0.43
1:D:90:LYS:O	1:D:168:SER:HA	2.19	0.43
1:D:140:GLU:HA	1:D:154:PHE:HB3	2.00	0.43
1:C:140:GLU:HG3	1:C:154:PHE:HD2	1.83	0.43
1:B:4:MET:HB2	1:B:4:MET:HE3	1.49	0.43
1:C:30:GLU:H	1:C:30:GLU:CD	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:HA	1:A:17:VAL:O	2.18	0.43
1:C:186:GLN:HE21	1:C:186:GLN:HA	1.84	0.43
1:C:178:SER:O	1:C:179:ALA:C	2.61	0.43
1:B:145[B]:MET:HE2	1:B:151:ASP:OD2	2.18	0.42
1:D:11:THR:O	1:D:115:LYS:HA	2.20	0.42
1:D:32:GLY:O	1:D:211:TYR:HA	2.19	0.42
1:B:58:CR2:N2	1:B:58:CR2:HD1	2.34	0.42
1:A:115:LYS:HE2	1:A:115:LYS:HB2	1.87	0.42
1:B:80:ASN:ND2	1:B:80:ASN:O	2.52	0.42
1:A:39:LYS:HG2	1:A:205:GLU:CG	2.49	0.42
1:A:58:CR2:N2	1:A:58:CR2:HD1	2.34	0.42
1:B:37:LYS:HA	1:B:206:LEU:O	2.19	0.42
1:B:85:ASN:HD21	1:B:172:SER:HB3	1.85	0.42
1:A:134:ARG:HG2	1:A:159:SER:HB2	2.01	0.42
1:C:125:SER:OG	1:C:127:ILE:HG12	2.20	0.41
1:A:4:MET:HE3	1:A:4:MET:HB2	1.97	0.41
1:B:88:ILE:CD1	1:B:98:HIS:CD2	3.01	0.41
1:C:91:TYR:CD2	1:C:168:SER:HB3	2.56	0.41
1:A:72:ASN:OD1	1:A:72:ASN:C	2.64	0.41
1:A:119:THR:HG21	1:D:86:THR:OG1	2.20	0.41
1:B:105:TYR:CE2	1:B:110:VAL:HG23	2.56	0.40
1:D:12:GLY:HA3	1:D:116:VAL:O	2.22	0.40
1:D:182:PRO:O	1:D:186:GLN:HB2	2.21	0.40
1:A:180:ILE:O	1:A:181:HIS:C	2.61	0.40
1:B:117:MET:HG2	1:C:98:HIS:CE1	2.57	0.40
1:D:84:THR:O	1:D:174:MET:HA	2.22	0.40
1:D:83:TYR:HA	1:D:175:HIS:O	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:D:224:HOH:O	2:D:224:HOH:O[4_565]	2.18	0.02

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	210/217 (97%)	197 (94%)	12 (6%)	1 (0%)	24	21
1	B	213/217 (98%)	205 (96%)	7 (3%)	1 (0%)	24	21
1	C	212/217 (98%)	206 (97%)	4 (2%)	2 (1%)	14	9
1	D	210/217 (97%)	207 (99%)	3 (1%)	0	100	100
All	All	845/868 (97%)	815 (96%)	26 (3%)	4 (0%)	24	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	B	2	PRO
1	C	187	ASN
1	C	188	GLY

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	181/183 (99%)	168 (93%)	13 (7%)	13	10
1	B	184/183 (100%)	171 (93%)	13 (7%)	13	10
1	C	183/183 (100%)	170 (93%)	13 (7%)	13	10
1	D	181/183 (99%)	168 (93%)	13 (7%)	13	10
All	All	729/732 (100%)	677 (93%)	52 (7%)	13	10

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	22	VAL

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Mol	Chain	Res	Type
1	A	46	THR
1	A	80	ASN
1	A	100	SER
1	A	106	GLU
1	A	126	VAL
1	A	151	ASP
1	A	172	SER
1	A	177	LYS
1	A	186	GLN
1	A	204	THR
1	A	216	LYS
1	B	1	LEU
1	B	7	GLU
1	B	26	GLU
1	B	31	GLN
1	B	34	MET
1	B	80	ASN
1	B	117	MET
1	B	123	GLU
1	B	126	VAL
1	B	151	ASP
1	B	161	ARG
1	B	162	ASP
1	B	216	LYS
1	C	14	LEU
1	C	26	GLU
1	C	28	THR
1	C	34	MET
1	C	80	ASN
1	C	109	ARG
1	C	110	VAL
1	C	151	ASP
1	C	177	LYS
1	C	185	LEU
1	C	186	GLN
1	C	197	VAL
1	C	216	LYS
1	D	14	LEU
1	D	37	LYS
1	D	39	LYS
1	D	62	HIS
1	D	79	ASN

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Mol	Chain	Res	Type
1	D	110	VAL
1	D	126	VAL
1	D	151	ASP
1	D	167	SER
1	D	191	MET
1	D	197	VAL
1	D	216	LYS
1	D	219	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	54	HIS
1	A	80	ASN
1	A	85	ASN
1	A	187	ASN
1	B	80	ASN
1	B	85	ASN
1	B	98	HIS
1	B	143	HIS
1	B	148	ASN
1	C	54	HIS
1	C	76	HIS
1	C	80	ASN
1	C	85	ASN
1	C	173	HIS
1	C	186	GLN
1	C	187	ASN
1	D	54	HIS
1	D	62	HIS
1	D	98	HIS
1	D	187	ASN

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	CR2	B	58	1	20,20,21	3.47	6 (30%)	25,27,29	3.90	10 (40%)
1	CR2	C	58	1	20,20,21	3.53	5 (25%)	25,27,29	2.33	7 (28%)
1	CR2	A	58	1	20,20,21	3.30	5 (25%)	25,27,29	3.54	14 (56%)
1	CR2	D	58	1	20,20,21	3.33	7 (35%)	25,27,29	3.26	8 (32%)

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	CR2	B	58	1	-	0/6/25/26	0/2/2/2
1	CR2	C	58	1	-	0/6/25/26	0/2/2/2
1	CR2	A	58	1	-	0/6/25/26	0/2/2/2
1	CR2	D	58	1	-	1/6/25/26	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	58	CR2	CB2-CA2	11.03	1.45	1.35
1	C	58	CR2	CB2-CA2	10.54	1.45	1.35
1	D	58	CR2	CB2-CA2	9.83	1.44	1.35
1	A	58	CR2	CB2-CA2	8.74	1.43	1.35
1	A	58	CR2	CA2-C2	-8.70	1.39	1.48
1	C	58	CR2	CA2-C2	-8.54	1.39	1.48
1	B	58	CR2	CA2-C2	-8.19	1.39	1.48
1	D	58	CR2	CA2-C2	-8.08	1.39	1.48
1	C	58	CR2	CA3-N3	-5.99	1.36	1.47
1	A	58	CR2	CA3-N3	-4.85	1.38	1.47
1	B	58	CR2	CA3-N3	-4.28	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	58	CR2	CA3-N3	-4.18	1.39	1.47
1	A	58	CR2	CG2-CB2	-3.64	1.40	1.46
1	D	58	CR2	O2-C2	3.26	1.29	1.23
1	B	58	CR2	O2-C2	3.22	1.29	1.23
1	A	58	CR2	O2-C2	3.10	1.29	1.23
1	C	58	CR2	O2-C2	2.95	1.29	1.23
1	B	58	CR2	CG2-CB2	-2.70	1.41	1.46
1	D	58	CR2	C1-N2	2.30	1.36	1.32
1	D	58	CR2	CG2-CB2	-2.27	1.42	1.46
1	D	58	CR2	CA1-C1	2.17	1.52	1.49
1	B	58	CR2	C1-N2	2.02	1.36	1.32
1	C	58	CR2	C1-N2	2.01	1.36	1.32

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	CR2	C2-N3-C1	-9.65	103.74	108.08
1	D	58	CR2	O2-C2-CA2	-9.16	125.17	131.02
1	B	58	CR2	CA2-C2-N3	8.02	110.23	103.50
1	A	58	CR2	O2-C2-CA2	7.82	136.01	131.02
1	D	58	CR2	C2-N3-C1	-6.92	104.97	108.08
1	A	58	CR2	CE2-CD2-CG2	-6.54	112.78	121.22
1	B	58	CR2	O2-C2-CA2	-6.36	126.96	131.02
1	B	58	CR2	C1-CA1-N1	-6.33	98.86	112.85
1	D	58	CR2	CA2-C2-N3	6.07	108.60	103.50
1	A	58	CR2	C2-CA2-N2	5.94	113.21	108.95
1	B	58	CR2	C3-CA3-N3	5.93	125.93	112.43
1	A	58	CR2	C3-CA3-N3	5.76	125.54	112.43
1	A	58	CR2	CD1-CE1-CZ	-5.68	113.87	119.88
1	C	58	CR2	CA2-C2-N3	5.63	108.23	103.50
1	B	58	CR2	CD1-CE1-CZ	-5.52	114.03	119.88
1	D	58	CR2	CG2-CB2-CA2	-5.46	123.37	129.87
1	A	58	CR2	C1-CA1-N1	-5.12	101.52	112.85
1	A	58	CR2	CD2-CG2-CD1	5.08	125.19	117.65
1	C	58	CR2	C1-CA1-N1	-4.94	101.92	112.85
1	B	58	CR2	CE2-CZ-CE1	4.36	126.70	119.77
1	C	58	CR2	C2-N3-C1	-4.08	106.24	108.08
1	B	58	CR2	CD2-CG2-CD1	4.05	123.66	117.65
1	C	58	CR2	O3-C3-CA3	-4.03	107.31	125.47
1	D	58	CR2	C3-CA3-N3	4.01	121.56	112.43
1	C	58	CR2	O2-C2-CA2	-3.97	128.49	131.02
1	D	58	CR2	C1-CA1-N1	-3.61	104.86	112.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	CR2	C3-CA3-N3	3.43	120.24	112.43
1	B	58	CR2	CE2-CD2-CG2	-3.37	116.86	121.22
1	A	58	CR2	CD2-CG2-CB2	-2.82	111.53	121.22
1	A	58	CR2	O3-C3-CA3	-2.75	113.08	125.47
1	A	58	CR2	CB2-CA2-N2	-2.74	125.05	128.76
1	A	58	CR2	CE2-CZ-CE1	2.67	124.01	119.77
1	B	58	CR2	C2-CA2-N2	-2.56	107.12	108.95
1	A	58	CR2	CD2-CE2-CZ	2.51	122.53	119.88
1	D	58	CR2	CD1-CE1-CZ	2.50	122.52	119.88
1	C	58	CR2	CG2-CB2-CA2	-2.31	127.12	129.87
1	A	58	CR2	O2-C2-N3	-2.26	119.60	124.31
1	D	58	CR2	CE1-CD1-CG2	-2.23	118.34	121.22
1	A	58	CR2	OH-CZ-CE2	-2.16	113.97	120.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	58	CR2	C3-CA3-N3-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	58	CR2	4	0
1	A	58	CR2	1	0
1	D	58	CR2	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	213/217 (98%)	0.47	5 (2%) 61 60	21, 34, 46, 53	1 (0%)
1	B	215/217 (99%)	0.19	4 (1%) 66 66	21, 31, 48, 62	2 (0%)
1	C	215/217 (99%)	0.28	5 (2%) 61 60	21, 34, 48, 62	1 (0%)
1	D	214/217 (98%)	0.25	3 (1%) 73 73	23, 33, 47, 60	0
All	All	857/868 (98%)	0.30	17 (1%) 65 64	21, 33, 48, 62	4 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	LEU	4.1
1	B	202[A]	SER	4.0
1	C	2	PRO	3.9
1	D	3	ALA	3.5
1	B	2	PRO	3.2
1	A	188	GLY	3.0
1	B	203	ASN	3.0
1	C	146	GLY	2.7
1	A	19	PHE	2.6
1	D	107	ALA	2.4
1	A	40	SER	2.2
1	A	117	MET	2.2
1	C	16	GLY	2.1
1	D	165	TYR	2.1
1	C	203	ASN	2.1
1	A	3	ALA	2.0
1	C	3	ALA	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($\text{\AA}^2$)	Q<0.9
1	CR2	D	58	19/20	0.92	0.07	26,29,31,31	0
1	CR2	A	58	19/20	0.93	0.08	25,28,29,29	0
1	CR2	C	58	19/20	0.94	0.07	25,28,31,31	0
1	CR2	B	58	19/20	0.96	0.06	21,24,26,27	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.