



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:33 PM UTC

PDB ID : 1EMC / pdb_00001emc
Title : GREEN FLUORESCENT PROTEIN FROM AEQUOREA VICTORIA, MUTANT
Authors : Palm, G.; Zdanov, A.; Wlodawer, A.
Deposited on : 1997-03-31
Resolution : 2.30 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

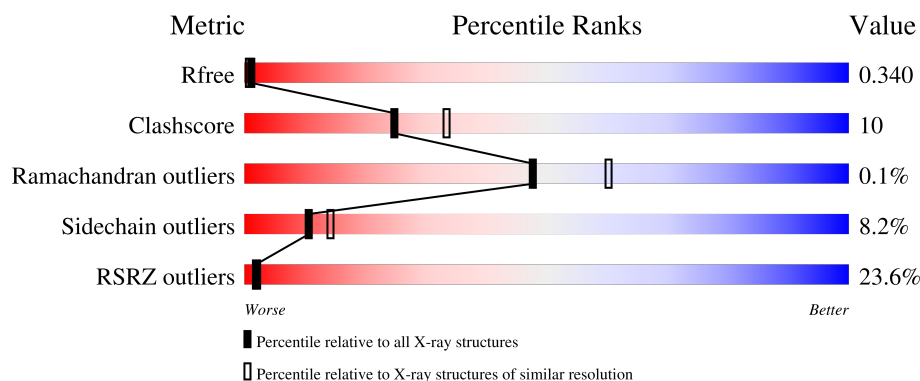
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	237	11% 68% 24% 5%
1	B	237	5% 67% 25% 5%
1	C	237	41% 59% 32% 5%
1	D	237	33% 66% 26% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7354 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GREEN FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	1	0
			1795	1142	302	345	6			
1	B	225	Total	C	N	O	S	0	1	0
			1795	1142	302	345	6			
1	C	226	Total	C	N	O	S	0	1	0
			1811	1151	308	346	6			
1	D	225	Total	C	N	O	S	0	1	0
			1795	1142	302	345	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	GYS	SER	chromophore	UNP P42212
A	66	GYS	TYR	chromophore	UNP P42212
A	66	GYS	GLY	chromophore	UNP P42212
A	80	ARG	GLN	conflict	UNP P42212
A	167	THR	ILE	engineered mutation	UNP P42212
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	GYS	SER	chromophore	UNP P42212
B	66	GYS	TYR	chromophore	UNP P42212
B	66	GYS	GLY	chromophore	UNP P42212
B	80	ARG	GLN	conflict	UNP P42212
B	167	THR	ILE	engineered mutation	UNP P42212
C	64	LEU	PHE	engineered mutation	UNP P42212
C	66	GYS	SER	chromophore	UNP P42212
C	66	GYS	TYR	chromophore	UNP P42212
C	66	GYS	GLY	chromophore	UNP P42212
C	80	ARG	GLN	conflict	UNP P42212
C	167	THR	ILE	engineered mutation	UNP P42212
D	64	LEU	PHE	engineered mutation	UNP P42212
D	66	GYS	SER	chromophore	UNP P42212
D	66	GYS	TYR	chromophore	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	66	GYS	GLY	chromophore	UNP P42212
D	80	ARG	GLN	conflict	UNP P42212
D	167	THR	ILE	engineered mutation	UNP P42212

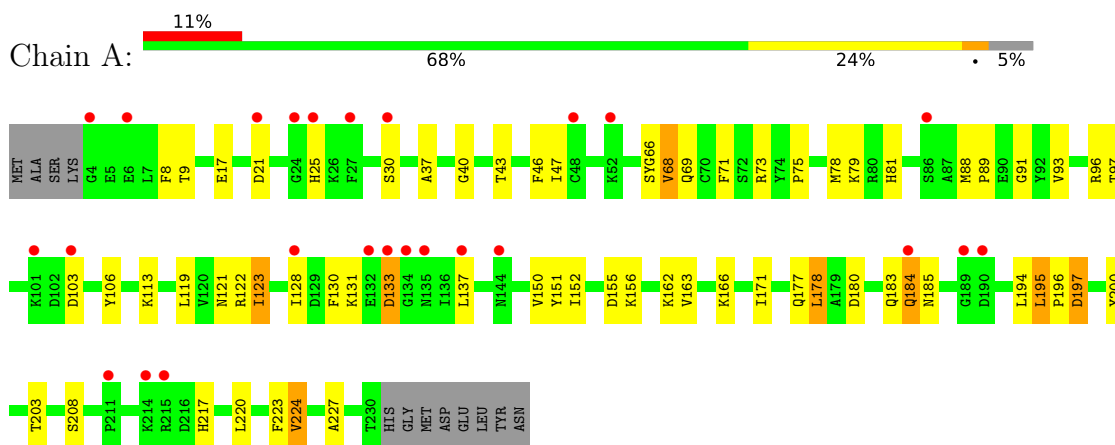
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total 40	O 40	0	0
2	B	42	Total 42	O 42	0	0
2	C	38	Total 38	O 38	0	0
2	D	38	Total 38	O 38	0	0

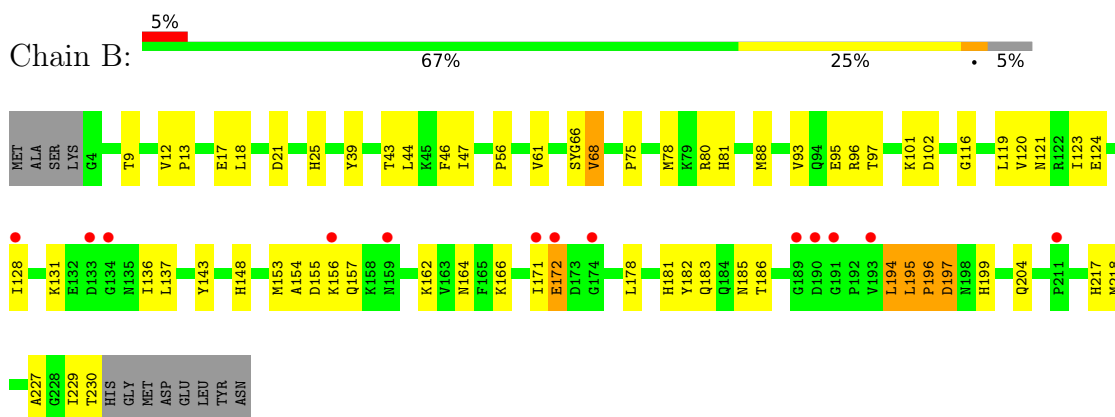
3 Residue-property plots

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

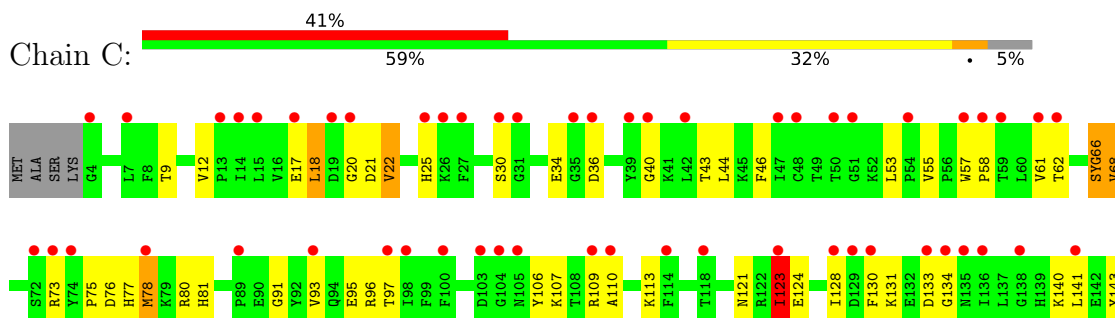
• Molecule 1: GREEN FLUORESCENT PROTEIN



• Molecule 1: GREEN FLUORESCENT PROTEIN

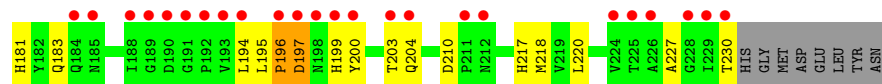
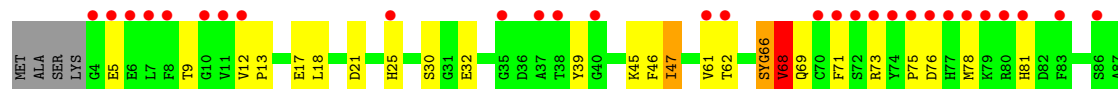


• Molecule 1: GREEN FLUORESCENT PROTEIN





● Molecule 1: GREEN FLUORESCENT PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.00Å 52.00Å 103.00Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	72.5 (10.00-2.30) 71.4 (10.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.28Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.205 , 0.288 0.298 , 0.340	Depositor DCC
R_{free} test set	2211 reflections (7.13%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 85.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7354	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5076e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.01	2/1817 (0.1%)	1.17	6/2458 (0.2%)
1	B	1.06	4/1817 (0.2%)	1.18	7/2458 (0.3%)
1	C	1.01	5/1834 (0.3%)	1.21	12/2480 (0.5%)
1	D	1.03	2/1817 (0.1%)	1.17	13/2458 (0.5%)
All	All	1.03	13/7285 (0.2%)	1.18	38/9854 (0.4%)

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	2
1	C	0	1
1	D	0	1
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	MET	SD-CE	-9.69	1.55	1.79
1	B	78	MET	SD-CE	-9.54	1.55	1.79
1	D	78	MET	SD-CE	-9.20	1.56	1.79
1	C	153	MET	SD-CE	7.74	1.99	1.79
1	B	61	VAL	CA-CB	7.31	1.62	1.54
1	C	22	VAL	CA-CB	6.73	1.62	1.53
1	C	230	THR	CA-CB	6.67	1.61	1.52
1	D	153	MET	SD-CE	6.47	1.95	1.79
1	C	78	MET	SD-CE	-6.16	1.64	1.79
1	B	153	MET	SD-CE	5.48	1.93	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	MET	SD-CE	-5.46	1.65	1.79
1	C	61	VAL	CA-CB	5.31	1.60	1.54
1	A	75	PRO	CA-C	-5.10	1.46	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	ASP	N-CA-C	-10.08	97.53	110.53
1	C	230	THR	N-CA-C	9.43	124.44	108.23
1	A	197	ASP	N-CA-C	-9.20	98.67	110.53
1	B	97	THR	N-CA-C	-8.98	93.61	108.34
1	B	197	ASP	N-CA-C	-7.99	99.76	110.55
1	D	97	THR	N-CA-C	-7.02	96.61	108.26
1	A	97	THR	N-CA-C	-6.54	97.61	108.34
1	D	123	ILE	N-CA-C	6.30	119.13	108.86
1	C	231	HIS	N-CA-C	6.27	128.57	111.00
1	A	123	ILE	N-CA-C	6.10	118.24	108.85
1	B	116	GLY	N-CA-C	-6.09	106.07	111.67
1	D	107	LYS	N-CA-C	-6.08	98.62	108.52
1	C	134	GLY	N-CA-C	-6.04	104.30	112.57
1	C	97	THR	N-CA-C	-5.92	98.63	108.34
1	C	216	ASP	N-CA-C	-5.85	100.99	109.59
1	A	119	LEU	N-CA-C	-5.83	99.73	109.24
1	B	196	PRO	N-CA-C	5.83	121.50	111.77
1	C	107	LYS	N-CA-C	-5.81	99.43	108.90
1	C	210	ASP	N-CA-C	-5.69	100.40	109.04
1	C	20	GLY	N-CA-C	5.63	119.36	111.14
1	D	152	ILE	N-CA-C	5.62	116.56	108.48
1	C	61	VAL	N-CA-C	5.52	116.16	110.36
1	D	210	ASP	N-CA-C	-5.51	101.58	109.24
1	D	69	GLN	N-CA-C	5.46	119.69	113.19
1	C	197	ASP	N-CA-C	-5.39	103.78	110.41
1	C	182	TYR	N-CA-C	-5.34	99.71	108.41
1	C	123	ILE	N-CA-C	5.30	117.50	108.86
1	B	172	GLU	N-CA-C	5.29	119.22	112.34
1	D	93	VAL	CB-CA-C	-5.29	103.97	111.21
1	D	220	LEU	N-CA-C	5.27	117.67	108.76
1	B	47	ILE	CB-CA-C	-5.24	102.44	110.50
1	A	220	LEU	N-CA-C	5.18	117.86	108.69
1	B	61	VAL	N-CA-C	5.18	115.80	110.36
1	D	61	VAL	N-CA-C	5.16	115.78	110.36
1	D	47	ILE	CB-CA-C	-5.09	102.55	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	68	VAL	N-CA-CB	-5.08	102.87	111.50
1	D	196	PRO	N-CA-C	5.06	120.22	111.77
1	A	79	LYS	N-CA-C	5.02	118.66	112.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	TYR	Sidechain
1	B	182	TYR	Sidechain
1	B	39	TYR	Sidechain
1	C	145	TYR	Sidechain
1	D	39	TYR	Sidechain

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	1795	0	1733	31	0
1	B	1795	0	1734	33	1
1	C	1811	0	1751	43	1
1	D	1795	0	1734	35	2
2	A	40	0	0	3	0
2	B	42	0	0	4	0
2	C	38	0	0	0	0
2	D	38	0	0	2	1
All	All	7354	0	6952	138	3

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 10.

All (138) 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:203[B]:THR:HG22	1:A:224:VAL:HG13	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:HIS:HD2	1:A:197:ASP:H	1.21	0.89
1:A:81:HIS:CD2	1:A:197:ASP:H	1.91	0.89
1:C:81:HIS:CD2	1:C:197:ASP:H	2.04	0.75
1:C:203[B]:THR:HG22	1:C:224:VAL:HG13	1.67	0.74
1:A:121:ASN:ND2	1:A:123:ILE:HD11	2.02	0.74
1:A:68:VAL:HG13	1:A:71:PHE:HD2	1.59	0.67
1:A:78:MET:HE1	1:A:227:ALA:HA	1.76	0.67
1:C:149:ASN:HD22	1:C:202:SER:HA	1.59	0.66
1:B:46:PHE:O	1:B:217:HIS:HB2	1.98	0.63
1:C:53:LEU:HD23	1:C:55:VAL:O	2.00	0.61
1:D:155:ASP:OD2	1:D:162:LYS:HE2	1.99	0.61
1:B:156:LYS:HG2	1:B:195:LEU:HD23	1.83	0.61
1:A:156:LYS:HG2	1:A:195:LEU:HD23	1.81	0.61
1:C:96:ARG:HG2	1:C:183:GLN:HB2	1.82	0.61
1:B:81:HIS:CD2	1:B:197:ASP:H	2.18	0.61
1:A:178:LEU:HB2	2:A:261:HOH:O	2.02	0.60
1:D:81:HIS:CD2	1:D:197:ASP:H	2.18	0.60
1:C:155:ASP:OD2	1:C:162:LYS:HE2	2.01	0.60
1:C:81:HIS:HD2	1:C:197:ASP:H	1.49	0.59
1:A:21:ASP:HA	1:A:25:HIS:O	2.02	0.59
1:B:68:VAL:HG13	1:B:68:VAL:O	2.03	0.58
1:A:81:HIS:HD2	1:A:197:ASP:N	1.98	0.58
1:B:155:ASP:OD2	1:B:162:LYS:HE2	2.03	0.58
1:A:133:ASP:O	1:C:80:ARG:NH2	2.37	0.57
1:C:46:PHE:O	1:C:217:HIS:HB2	2.06	0.56
1:A:155:ASP:OD2	1:A:162:LYS:HE2	2.06	0.56
1:C:75:PRO:HD2	1:C:78:MET:HE3	1.88	0.56
1:C:77:HIS:CD2	1:C:231:HIS:HA	2.40	0.56
1:D:45:LYS:HE2	1:D:47:ILE:HD11	1.88	0.56
1:D:121:ASN:ND2	1:D:123:ILE:HD11	2.21	0.55
1:D:203[B]:THR:HG21	2:D:241:HOH:O	2.05	0.55
1:C:21:ASP:HA	1:C:25:HIS:O	2.06	0.54
1:D:155:ASP:OD1	1:D:157:GLN:HB3	2.08	0.54
1:C:184:GLN:HG3	1:C:185:ASN:N	2.23	0.54
1:B:154:ALA:HB1	1:B:195:LEU:HG	1.88	0.54
1:C:149:ASN:ND2	1:C:202:SER:HA	2.23	0.54
1:B:204:GLN:NE2	2:B:259:HOH:O	2.41	0.53
1:A:91:GLY:HA3	1:A:113:LYS:HB3	1.89	0.53
1:C:68:VAL:O	1:C:68:VAL:HG13	2.09	0.53
1:A:68:VAL:HG13	1:A:71:PHE:CD2	2.40	0.53
1:D:68:VAL:O	1:D:68:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:HIS:HB3	1:B:229:ILE:HD11	1.90	0.52
1:C:140:LYS:O	1:C:172:GLU:HG3	2.09	0.52
1:D:18:LEU:C	1:D:18:LEU:HD23	2.34	0.52
1:D:96:ARG:HG2	1:D:183:GLN:HB2	1.90	0.52
1:D:142:GLU:HG2	1:D:172:GLU:OE2	2.10	0.52
1:C:123:ILE:HG22	1:C:124:GLU:N	2.25	0.52
1:A:152:ILE:HG12	1:A:163:VAL:HG22	1.91	0.52
1:B:155:ASP:OD1	1:B:157:GLN:HB3	2.10	0.52
1:B:148:HIS:HE1	2:B:252:HOH:O	1.92	0.51
1:A:73:ARG:HH22	1:B:124:GLU:CD	2.18	0.51
1:A:150:VAL:O	1:A:200:TYR:HA	2.10	0.51
1:B:81:HIS:HD2	1:B:197:ASP:H	1.57	0.51
1:D:46:PHE:O	1:D:217:HIS:HB2	2.11	0.51
1:A:96:ARG:HG2	1:A:183:GLN:HB2	1.92	0.51
1:D:142:GLU:OE2	1:D:172:GLU:HA	2.10	0.51
1:C:201:LEU:HD23	1:C:226:ALA:HA	1.93	0.51
1:D:149:ASN:HD22	1:D:200:TYR:HD2	1.59	0.50
1:A:46:PHE:O	1:A:217:HIS:HB2	2.12	0.50
1:C:95:GLU:HG2	1:C:109:ARG:HG3	1.93	0.49
1:C:141:LEU:N	1:C:141:LEU:HD12	2.28	0.49
1:D:143:TYR:OH	1:D:218:MET:HG3	2.13	0.48
1:A:131:LYS:O	1:A:137:LEU:HD12	2.13	0.48
1:D:68:VAL:HG13	1:D:71:PHE:HD2	1.78	0.48
1:D:123:ILE:HG22	1:D:124:GLU:N	2.29	0.48
1:A:197:ASP:HB3	2:A:270:HOH:O	2.13	0.48
1:B:102:ASP:O	1:B:131:LYS:HE3	2.13	0.48
1:A:184:GLN:HG3	1:A:185:ASN:N	2.28	0.48
1:D:171:ILE:HD11	1:D:177:GLN:HB2	1.95	0.47
1:C:62:THR:O	1:C:96:ARG:NH1	2.44	0.47
1:D:157:GLN:HE22	1:D:158:LYS:HE3	1.79	0.47
1:C:143:TYR:CZ	1:C:209:LYS:HE2	2.48	0.47
1:D:125:LEU:C	1:D:125:LEU:HD23	2.39	0.47
1:B:96:ARG:HG2	1:B:183:GLN:HB2	1.96	0.47
1:B:95:GLU:O	1:B:183:GLN:HA	2.15	0.47
1:A:106:TYR:CE1	1:A:130:PHE:CZ	3.02	0.47
1:D:21:ASP:HA	1:D:25:HIS:O	2.15	0.47
1:C:110:ALA:HB2	1:C:123:ILE:HG23	1.96	0.46
1:A:93:VAL:O	1:A:185:ASN:HA	2.14	0.46
1:D:164:ASN:HA	1:D:181:HIS:O	2.16	0.46
1:C:156:LYS:HG2	1:C:195:LEU:HD23	1.97	0.46
1:C:91:GLY:HA3	1:C:113:LYS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:VAL:O	1:B:185:ASN:HA	2.17	0.45
1:B:199:HIS:HB2	1:B:227:ALA:O	2.17	0.45
1:A:171:ILE:HD11	1:A:177:GLN:HB2	1.98	0.45
1:B:121:ASN:ND2	1:B:123:ILE:HD11	2.31	0.45
1:A:166:LYS:HE3	1:A:166:LYS:HB2	1.78	0.44
1:C:36:ASP:OD2	1:D:107:LYS:NZ	2.49	0.44
1:C:66:GYS:N2	1:C:66:GYS:HD1	2.32	0.44
1:D:204:GLN:NE2	2:D:255:HOH:O	2.50	0.44
1:B:131:LYS:O	1:B:137:LEU:HD12	2.18	0.44
1:B:166:LYS:HE3	1:B:166:LYS:HB2	1.80	0.44
1:C:73:ARG:HH22	1:D:124:GLU:CD	2.26	0.44
1:C:149:ASN:HA	1:C:201:LEU:O	2.18	0.44
1:C:40:GLY:O	1:C:223:PHE:HA	2.17	0.44
1:A:69:GLN:HG2	2:A:240:HOH:O	2.18	0.43
1:D:149:ASN:ND2	1:D:200:TYR:CD2	2.86	0.43
1:D:149:ASN:ND2	1:D:200:TYR:CE2	2.86	0.43
1:C:155:ASP:HB2	1:C:162:LYS:HG3	2.01	0.43
1:B:12:VAL:HA	1:B:13:PRO:HD3	1.92	0.43
1:B:123:ILE:HG22	1:B:124:GLU:N	2.34	0.43
1:C:57:TRP:N	1:C:58:PRO:CD	2.82	0.43
1:D:62:THR:HG22	1:D:66:GYS:CG2	2.48	0.43
1:B:21:ASP:HA	1:B:25:HIS:O	2.19	0.42
1:C:93:VAL:O	1:C:185:ASN:HA	2.19	0.42
1:C:150:VAL:O	1:C:200:TYR:HA	2.19	0.42
1:C:171:ILE:HG22	1:C:172:GLU:N	2.34	0.42
1:D:73:ARG:HG2	1:D:73:ARG:NH1	2.34	0.42
1:D:155:ASP:HB2	1:D:162:LYS:HG3	2.01	0.42
1:C:121:ASN:ND2	1:C:123:ILE:HD11	2.35	0.42
1:B:199:HIS:HB3	1:B:229:ILE:CD1	2.49	0.42
1:D:12:VAL:HA	1:D:13:PRO:HD3	1.92	0.42
1:D:91:GLY:HA3	1:D:113:LYS:HB3	2.02	0.42
1:B:80:ARG:O	1:B:194:LEU:HG	2.18	0.42
1:B:68:VAL:HG22	1:B:119:LEU:HD11	2.02	0.42
1:D:73:ARG:HG2	1:D:73:ARG:HH11	1.86	0.41
1:A:21:ASP:OD1	1:A:21:ASP:C	2.63	0.41
1:B:18:LEU:C	1:B:18:LEU:HD23	2.45	0.41
1:B:68:VAL:O	1:B:68:VAL:CG1	2.68	0.41
1:C:106:TYR:CE1	1:C:130:PHE:CZ	3.08	0.41
1:A:8:PHE:HB3	1:A:37:ALA:CB	2.50	0.41
1:B:164:ASN:HA	1:B:181:HIS:O	2.21	0.41
1:A:47:ILE:HD13	1:A:217:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:HIS:HB3	1:C:229:ILE:HD11	2.01	0.41
1:C:22:VAL:HG21	1:C:55:VAL:HG11	2.03	0.41
1:A:40:GLY:O	1:A:223:PHE:HA	2.20	0.41
1:B:197:ASP:HB3	2:B:275:HOH:O	2.19	0.41
1:D:81:HIS:HD2	1:D:196:PRO:HA	1.84	0.41
1:C:81:HIS:HD2	1:C:196:PRO:HA	1.85	0.41
1:C:12:VAL:O	1:C:34:GLU:HA	2.20	0.40
1:D:199:HIS:HB2	1:D:227:ALA:O	2.21	0.40
1:B:143:TYR:OH	1:B:218:MET:HG3	2.22	0.40
1:B:148:HIS:CE1	2:B:252:HOH:O	2.71	0.40
1:C:18:LEU:C	1:C:18:LEU:HD23	2.47	0.40
1:C:171:ILE:HD11	1:C:177:GLN:HB2	2.03	0.40
1:D:166:LYS:HE3	1:D:166:LYS:HB2	1.81	0.40
1:B:171:ILE:HD13	1:B:171:ILE:HG21	1.85	0.40

All (3) 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)
1:D:32:GLU:OE2	1:D:76:ASP:N[2_646]	1.91	0.29
1:D:117:ASP:OD1	2:D:260:HOH:O[2_646]	2.06	0.14
1:B:101:LYS:NZ	1:C:131:LYS:NZ[1_564]	2.10	0.10

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	221/237 (93%)	214 (97%)	7 (3%)	0	100	100
1	B	221/237 (93%)	211 (96%)	9 (4%)	1 (0%)	24	31
1	C	222/237 (94%)	215 (97%)	7 (3%)	0	100	100
1	D	221/237 (93%)	215 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	885/948 (93%)	855 (97%)	29 (3%)	1 (0%)	48 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	ILE

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	195/206 (95%)	177 (91%)	18 (9%)	8 11
1	B	195/206 (95%)	179 (92%)	16 (8%)	10 14
1	C	197/206 (96%)	179 (91%)	18 (9%)	9 11
1	D	195/206 (95%)	183 (94%)	12 (6%)	16 24
All	All	782/824 (95%)	718 (92%)	64 (8%)	10 14

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	17	GLU
1	A	30	SER
1	A	43	THR
1	A	68	VAL
1	A	89	PRO
1	A	103	ASP
1	A	122	ARG
1	A	128	ILE
1	A	133	ASP
1	A	178	LEU
1	A	180	ASP
1	A	184	GLN
1	A	194	LEU

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Mol	Chain	Res	Type
1	A	195	LEU
1	A	196	PRO
1	A	208	SER
1	A	224	VAL
1	B	9	THR
1	B	17	GLU
1	B	43	THR
1	B	44	LEU
1	B	56	PRO
1	B	68	VAL
1	B	75	PRO
1	B	120	VAL
1	B	128	ILE
1	B	172	GLU
1	B	178	LEU
1	B	186	THR
1	B	194	LEU
1	B	195	LEU
1	B	196	PRO
1	B	230	THR
1	C	9	THR
1	C	17	GLU
1	C	18	LEU
1	C	30	SER
1	C	43	THR
1	C	44	LEU
1	C	68	VAL
1	C	76	ASP
1	C	123	ILE
1	C	128	ILE
1	C	133	ASP
1	C	178	LEU
1	C	186	THR
1	C	194	LEU
1	C	195	LEU
1	C	196	PRO
1	C	205	SER
1	C	230	THR
1	D	5	GLU
1	D	9	THR
1	D	17	GLU
1	D	30	SER

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Mol	Chain	Res	Type
1	D	68	VAL
1	D	75	PRO
1	D	105	ASN
1	D	128	ILE
1	D	178	LEU
1	D	194	LEU
1	D	195	LEU
1	D	230	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	204	GLN
1	B	81	HIS
1	B	105	ASN
1	B	149	ASN
1	B	198	ASN
1	B	204	GLN
1	C	69	GLN
1	C	81	HIS
1	C	149	ASN
1	C	183	GLN
1	C	185	ASN
1	D	81	HIS
1	D	149	ASN
1	D	157	GLN
1	D	184	GLN
1	D	204	GLN

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	GYS	D	66	1	20,22,23	1.28	3 (15%)	25,30,32	1.45	5 (20%)
1	GYS	B	66	1	20,22,23	1.27	2 (10%)	25,30,32	1.69	6 (24%)
1	GYS	A	66	1	20,22,23	1.21	4 (20%)	25,30,32	1.14	2 (8%)
1	GYS	C	66	1	20,22,23	1.50	3 (15%)	25,30,32	1.18	3 (12%)

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	GYS	D	66	1	-	1/10/29/30	0/2/2/2
1	GYS	B	66	1	-	1/10/29/30	0/2/2/2
1	GYS	A	66	1	-	1/10/29/30	0/2/2/2
1	GYS	C	66	1	-	1/10/29/30	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	GYS	CE1-CD1	4.14	1.45	1.38
1	C	66	GYS	CE2-CD2	3.22	1.44	1.38
1	B	66	GYS	C2-N3	-3.04	1.33	1.40
1	B	66	GYS	CB2-CA2	-2.56	1.32	1.35
1	A	66	GYS	CB2-CA2	-2.55	1.32	1.35
1	D	66	GYS	C2-N3	-2.51	1.34	1.40
1	D	66	GYS	CB2-CA2	-2.46	1.32	1.35
1	A	66	GYS	CE1-CD1	2.45	1.42	1.38
1	C	66	GYS	C2-N3	-2.31	1.34	1.40
1	A	66	GYS	CE2-CD2	2.18	1.42	1.38
1	A	66	GYS	C2-N3	-2.11	1.35	1.40
1	D	66	GYS	CE2-CD2	2.09	1.42	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GYS	O2-C2-CA2	4.00	133.57	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	GYS	N3-C1-N2	3.43	114.19	111.48
1	D	66	GYS	O2-C2-CA2	3.28	133.11	131.02
1	B	66	GYS	CA2-N2-C1	-3.24	103.27	105.80
1	B	66	GYS	CA1-C1-N3	-3.14	120.75	124.84
1	B	66	GYS	N3-C1-N2	3.11	113.94	111.48
1	A	66	GYS	N3-C1-N2	3.11	113.93	111.48
1	D	66	GYS	N3-C1-N2	2.83	113.72	111.48
1	B	66	GYS	C2-N3-C1	2.81	109.37	108.07
1	D	66	GYS	CA2-N2-C1	-2.65	103.73	105.80
1	C	66	GYS	CA2-N2-C1	-2.64	103.74	105.80
1	D	66	GYS	C2-N3-C1	2.41	109.18	108.07
1	A	66	GYS	CA2-N2-C1	-2.27	104.03	105.80
1	D	66	GYS	CA1-C1-N3	-2.24	121.93	124.84
1	B	66	GYS	CG2-CB2-CA2	2.09	132.35	129.87
1	C	66	GYS	CA1-C1-N3	-2.01	122.22	124.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	GYS	N1-CA1-CB1-OG1
1	B	66	GYS	N1-CA1-CB1-OG1
1	C	66	GYS	N1-CA1-CB1-OG1
1	D	66	GYS	N1-CA1-CB1-OG1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	66	GYS	1	0
1	C	66	GYS	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

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	224/237 (94%)	1.05	25 (11%)	10 11	3, 14, 41, 56	1 (0%)
1	B	224/237 (94%)	0.69	13 (5%)	29 31	2, 10, 39, 59	1 (0%)
1	C	225/237 (94%)	1.89	96 (42%)	0 0	3, 13, 40, 60	1 (0%)
1	D	224/237 (94%)	1.77	78 (34%)	1 1	2, 11, 40, 61	1 (0%)
All	All	897/948 (94%)	1.35	212 (23%)	2 2	2, 12, 41, 61	4 (0%)

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	191	GLY	9.3
1	D	4	GLY	5.4
1	D	155	ASP	5.2
1	A	103	ASP	5.0
1	D	35	GLY	5.0
1	C	174	GLY	4.9
1	D	157	GLN	4.8
1	C	133	ASP	4.8
1	A	214	LYS	4.8
1	D	116	GLY	4.7
1	C	118	THR	4.5
1	C	31	GLY	4.5
1	D	156	LYS	4.3
1	D	192	PRO	4.3
1	C	227	ALA	4.3
1	D	197	ASP	4.3
1	D	38	THR	4.3
1	C	104	GLY	4.3
1	D	196	PRO	4.2
1	C	138	GLY	4.1
1	D	189	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	134	GLY	4.0
1	A	4	GLY	4.0
1	C	48	CYS	3.9
1	D	86	SER	3.9
1	D	193	VAL	3.9
1	B	190	ASP	3.9
1	C	208	SER	3.9
1	C	74	TYR	3.8
1	D	163	VAL	3.8
1	A	190	ASP	3.8
1	D	203[A]	THR	3.8
1	D	159	ASN	3.8
1	D	76	ASP	3.7
1	C	211	PRO	3.7
1	D	10	GLY	3.7
1	D	190	ASP	3.6
1	D	184	GLN	3.5
1	C	158	LYS	3.5
1	A	211	PRO	3.4
1	C	224	VAL	3.4
1	A	30	SER	3.4
1	C	165	PHE	3.3
1	C	103	ASP	3.3
1	A	133	ASP	3.3
1	B	172	GLU	3.3
1	B	128	ILE	3.3
1	B	133	ASP	3.2
1	D	89	PRO	3.2
1	D	229	ILE	3.2
1	D	160	GLY	3.2
1	C	203[A]	THR	3.2
1	C	54	PRO	3.2
1	C	25	HIS	3.1
1	D	117	ASP	3.1
1	D	83	PHE	3.1
1	C	98	ILE	3.1
1	C	168	ARG	3.1
1	C	157	GLN	3.1
1	D	7	LEU	3.1
1	C	47	ILE	3.0
1	C	164	ASN	3.0
1	D	226	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	24	GLY	3.0
1	C	35	GLY	3.0
1	C	212	ASN	3.0
1	C	114	PHE	3.0
1	C	152	ILE	3.0
1	D	92	TYR	3.0
1	C	17	GLU	3.0
1	C	213	GLU	3.0
1	D	37	ALA	2.9
1	A	134	GLY	2.9
1	C	100	PHE	2.9
1	C	128	ILE	2.9
1	B	189	GLY	2.9
1	C	4	GLY	2.9
1	C	180	ASP	2.9
1	A	27	PHE	2.9
1	A	128	ILE	2.9
1	D	88	MET	2.9
1	D	200	TYR	2.9
1	C	123	ILE	2.9
1	A	215	ARG	2.8
1	D	161	ILE	2.8
1	B	193	VAL	2.8
1	C	230	THR	2.8
1	D	77	HIS	2.8
1	C	145	TYR	2.8
1	D	61	VAL	2.8
1	A	101	LYS	2.7
1	B	134	GLY	2.7
1	C	57	TRP	2.7
1	D	194	LEU	2.7
1	D	150	VAL	2.7
1	A	135	ASN	2.7
1	D	91	GLY	2.7
1	D	80	ARG	2.7
1	D	153	MET	2.7
1	C	219	VAL	2.7
1	C	14	ILE	2.7
1	D	118	THR	2.6
1	C	58	PRO	2.6
1	D	114	PHE	2.6
1	C	163	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	211	PRO	2.6
1	D	6	GLU	2.6
1	C	105	ASN	2.6
1	C	30	SER	2.6
1	A	52	LYS	2.6
1	C	141	LEU	2.6
1	D	70	CYS	2.6
1	C	149	ASN	2.6
1	C	39	TYR	2.6
1	C	231	HIS	2.6
1	A	25	HIS	2.5
1	C	171	ILE	2.5
1	C	192	PRO	2.5
1	D	225	THR	2.5
1	C	188	ILE	2.5
1	D	75	PRO	2.5
1	D	188	ILE	2.5
1	C	155	ASP	2.5
1	D	11	VAL	2.4
1	A	137	LEU	2.4
1	C	214	LYS	2.4
1	C	40	GLY	2.4
1	C	228	GLY	2.4
1	D	5	GLU	2.4
1	C	61	VAL	2.4
1	C	93	VAL	2.4
1	D	8	PHE	2.4
1	D	78	MET	2.4
1	C	19	ASP	2.4
1	A	6	GLU	2.4
1	C	15	LEU	2.4
1	C	181	HIS	2.4
1	C	159	ASN	2.4
1	B	174	GLY	2.4
1	D	62	THR	2.4
1	C	72	SER	2.4
1	B	171	ILE	2.4
1	C	109	ARG	2.4
1	D	204	GLN	2.4
1	D	212	ASN	2.3
1	B	191	GLY	2.3
1	D	154	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	72	SER	2.3
1	C	182	TYR	2.3
1	C	223	PHE	2.3
1	D	228	GLY	2.3
1	C	204	GLN	2.3
1	D	71	PHE	2.3
1	D	93	VAL	2.3
1	C	129	ASP	2.3
1	C	78	MET	2.3
1	D	167	THR	2.3
1	C	199	HIS	2.3
1	D	81	HIS	2.3
1	C	42	LEU	2.2
1	C	130	PHE	2.2
1	C	135	ASN	2.2
1	D	146	ASN	2.2
1	A	189	GLY	2.2
1	D	40	GLY	2.2
1	A	132	GLU	2.2
1	C	148	HIS	2.2
1	C	184	GLN	2.2
1	B	159	ASN	2.2
1	D	211	PRO	2.2
1	B	156	LYS	2.2
1	C	110	ALA	2.2
1	C	156	LYS	2.2
1	D	224	VAL	2.2
1	D	149	ASN	2.2
1	A	48	CYS	2.2
1	C	51	GLY	2.2
1	D	230	THR	2.2
1	A	144	ASN	2.2
1	C	36	ASP	2.2
1	C	175	SER	2.2
1	C	73	ARG	2.1
1	C	136	ILE	2.1
1	C	221	LEU	2.1
1	C	173	ASP	2.1
1	A	184	GLN	2.1
1	A	86	SER	2.1
1	D	74	TYR	2.1
1	D	151	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	79	LYS	2.1
1	D	198	ASN	2.1
1	C	20	GLY	2.1
1	C	59	THR	2.1
1	C	97	THR	2.1
1	D	12	VAL	2.1
1	C	27	PHE	2.1
1	C	50	THR	2.1
1	C	226	ALA	2.1
1	A	21	ASP	2.1
1	D	25	HIS	2.1
1	D	185	ASN	2.1
1	D	73	ARG	2.1
1	C	62	THR	2.0
1	D	199	HIS	2.0
1	D	125	LEU	2.0
1	C	13	PRO	2.0
1	C	160	GLY	2.0
1	C	7	LEU	2.0
1	C	194	LEU	2.0
1	C	89	PRO	2.0
1	D	152	ILE	2.0
1	C	26	LYS	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	GYS	D	66	21/22	0.75	0.15	2,2,7,10	0
1	GYS	C	66	21/22	0.79	0.13	2,4,9,13	0
1	GYS	B	66	21/22	0.86	0.11	2,4,7,9	0
1	GYS	A	66	21/22	0.87	0.09	2,3,12,16	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.