



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:57 AM UTC

PDB ID : 2AHA / pdb_00002aha
Title : Crystal structure analysis of a rate-enhanced variant of redox-sensitive green fluorescent protein in the reduced form, roGFP1-R8.
Authors : Cannon, M.B.; Remington, S.J.
Deposited on : 2005-07-27
Resolution : 1.98 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

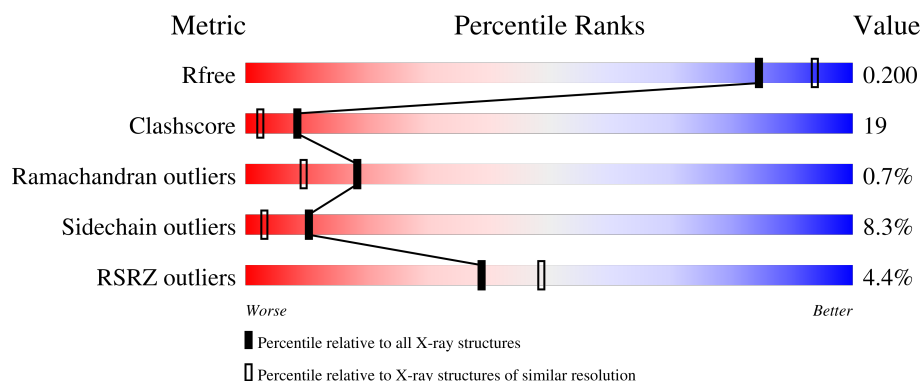
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	236	5% 58% 28% 9% • •
1	B	236	4% 58% 28% 9% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3667 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	226	Total	C	N	O	S	0	0	0
			1725	1096	287	335	7			
1	B	226	Total	C	N	O	S	0	0	0
			1731	1101	287	336	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ASP	LYS	engineered mutation	UNP P42212
A	48	SER	CYS	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	engineered mutation	UNP P42212
A	147	CYS	SER	engineered mutation	UNP P42212
A	204	CYS	GLN	engineered mutation	UNP P42212
A	223	ARG	PHE	engineered mutation	UNP P42212
B	41	ASP	LYS	engineered mutation	UNP P42212
B	48	SER	CYS	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	engineered mutation	UNP P42212
B	147	CYS	SER	engineered mutation	UNP P42212
B	204	CYS	GLN	engineered mutation	UNP P42212
B	223	ARG	PHE	engineered mutation	UNP P42212

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

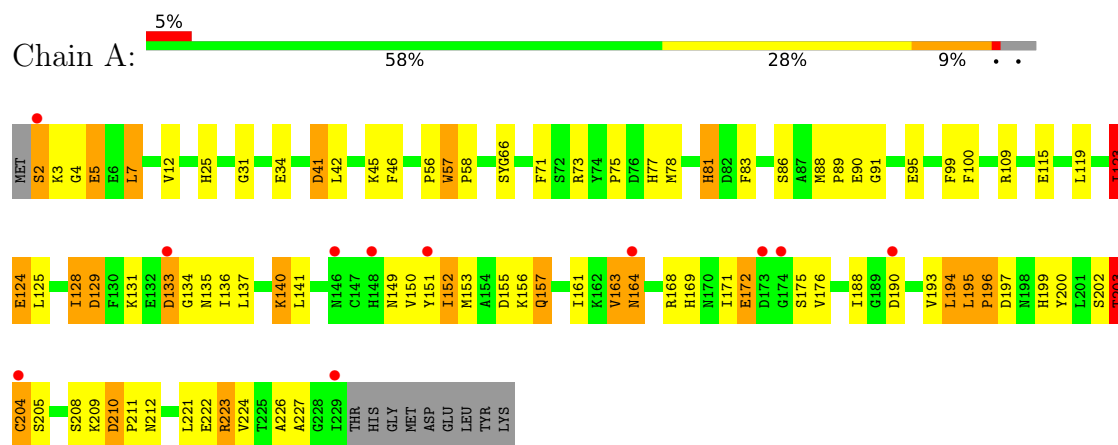
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	96	Total	O	0	0
			96	96		
3	B	95	Total	O	0	0
			95	95		

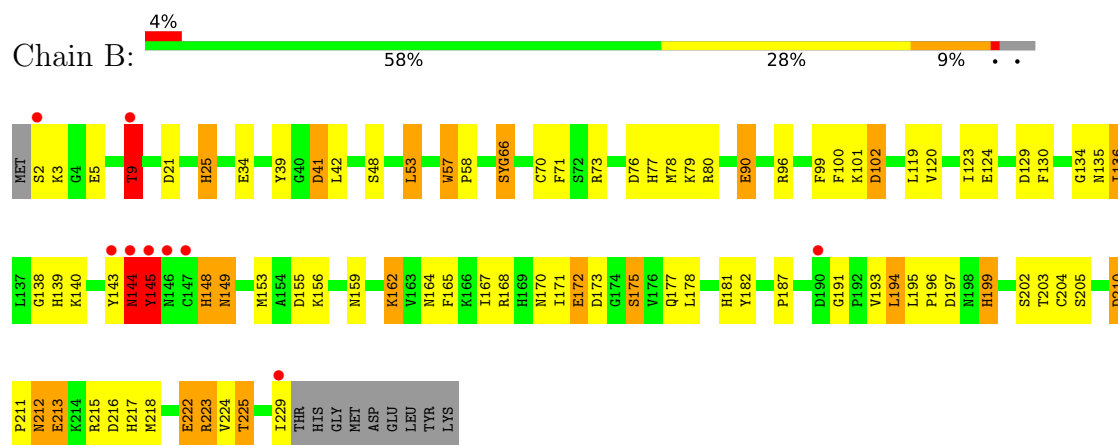
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.69Å 79.69Å 166.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.98 50.00 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.98) 99.5 (50.00-1.98)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.57 (at 1.95Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.199 , 0.275 0.203 , 0.200	Depositor DCC
R_{free} test set	2293 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 90.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3667	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GYS, SO4

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	1.30	2/1744 (0.1%)	1.92	36/2370 (1.5%)
1	B	1.35	6/1750 (0.3%)	1.90	38/2380 (1.6%)
All	All	1.33	8/3494 (0.2%)	1.91	74/4750 (1.6%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	LEU	C-N	-6.45	1.27	1.33
1	A	5	GLU	CD-OE2	5.93	1.36	1.25
1	B	129	ASP	CG-OD2	5.86	1.36	1.25
1	B	156	LYS	CA-C	-5.50	1.45	1.52
1	B	149	ASN	CA-C	-5.21	1.46	1.52
1	B	99	PHE	CA-CB	5.17	1.60	1.53
1	B	213	GLU	CD-OE2	5.04	1.34	1.25
1	A	129	ASP	CG-OD2	5.04	1.34	1.25

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	ASN	CA-CB-CG	-12.04	100.56	112.60
1	A	71	PHE	CA-CB-CG	-9.31	104.48	113.80
1	A	81	HIS	CA-CB-CG	-8.70	105.10	113.80
1	A	100	PHE	CA-CB-CG	-8.21	105.59	113.80
1	A	25	HIS	CA-CB-CG	-7.79	106.01	113.80
1	B	191	GLY	CA-C-N	7.38	127.97	119.99
1	B	191	GLY	C-N-CA	7.38	127.97	119.99
1	B	197	ASP	N-CA-C	-7.26	101.16	110.53
1	B	3	LYS	N-CA-CB	7.21	120.47	110.01
1	A	203	THR	N-CA-C	7.20	120.14	108.41
1	A	204	CYS	N-CA-CB	7.18	122.12	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	PHE	CA-CB-CG	-7.07	106.73	113.80
1	A	163	VAL	CB-CA-C	-6.91	101.16	111.80
1	A	90	GLU	N-CA-CB	6.83	120.16	110.12
1	A	199	HIS	N-CA-C	6.65	116.64	107.73
1	B	25	HIS	CA-CB-CG	-6.61	107.19	113.80
1	A	172	GLU	CA-C-N	-6.53	112.23	122.49
1	A	172	GLU	C-N-CA	-6.53	112.23	122.49
1	B	145	TYR	N-CA-CB	6.47	121.51	110.57
1	B	145	TYR	O-C-N	6.42	130.75	123.42
1	A	124	GLU	CA-CB-CG	6.41	126.92	114.10
1	B	144	ASN	CB-CA-C	-6.39	98.99	110.36
1	A	150	VAL	CB-CA-C	-6.28	101.80	110.96
1	B	149	ASN	CA-CB-CG	-6.26	106.34	112.60
1	B	71	PHE	CA-CB-CG	-6.25	107.55	113.80
1	B	130	PHE	CA-CB-CG	-6.22	107.58	113.80
1	B	77	HIS	CA-CB-CG	-6.17	107.63	113.80
1	B	9	THR	CA-CB-OG1	-6.11	100.44	109.60
1	A	196	PRO	CB-CA-C	-6.09	101.34	110.17
1	B	144	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	B	191	GLY	O-C-N	6.05	127.82	121.77
1	B	172	GLU	N-CA-C	6.02	117.51	111.07
1	B	216	ASP	N-CA-C	-6.02	101.13	110.10
1	A	199	HIS	CA-C-N	-5.85	112.73	122.21
1	A	199	HIS	C-N-CA	-5.85	112.73	122.21
1	B	21	ASP	CA-C-N	-5.85	115.31	123.10
1	B	21	ASP	C-N-CA	-5.85	115.31	123.10
1	A	128	ILE	CB-CA-C	-5.85	101.70	111.29
1	A	73	ARG	CA-CB-CG	-5.84	102.43	114.10
1	A	223	ARG	CD-NE-CZ	-5.79	116.29	124.40
1	B	120	VAL	N-CA-C	5.78	116.27	108.17
1	B	156	LYS	O-C-N	5.69	128.69	122.20
1	B	156	LYS	N-CA-CB	5.68	119.11	110.14
1	A	115	GLU	N-CA-C	-5.62	98.02	108.02
1	A	124	GLU	N-CA-CB	-5.57	101.96	110.65
1	B	196	PRO	CB-CA-C	-5.55	102.95	110.60
1	A	150	VAL	N-CA-CB	-5.54	104.48	111.46
1	A	99	PHE	CA-CB-CG	5.51	119.31	113.80
1	B	187	PRO	CB-CA-C	-5.51	103.75	110.98
1	B	41	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	155	ASP	CA-CB-CG	-5.45	107.15	112.60
1	B	199	HIS	CA-CB-CG	-5.42	108.38	113.80
1	A	12	VAL	CA-C-O	5.39	122.85	119.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	HIS	CA-CB-CG	5.37	119.17	113.80
1	A	190	ASP	CB-CA-C	5.37	119.00	109.65
1	B	168	ARG	CA-C-N	-5.37	115.62	122.77
1	B	168	ARG	C-N-CA	-5.37	115.62	122.77
1	A	95	GLU	CA-C-N	-5.31	113.87	122.36
1	A	95	GLU	C-N-CA	-5.31	113.87	122.36
1	B	70	CYS	N-CA-C	-5.20	106.77	113.01
1	B	181	HIS	N-CA-C	5.19	118.27	109.76
1	B	148	HIS	CA-CB-CG	-5.17	108.64	113.80
1	A	57	TRP	CA-C-O	5.16	123.08	118.33
1	B	123	ILE	N-CA-CB	-5.13	102.43	111.93
1	A	46	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	140	LYS	CA-C-N	-5.12	114.51	122.09
1	A	140	LYS	C-N-CA	-5.12	114.51	122.09
1	A	73	ARG	CB-CA-C	-5.11	102.24	110.77
1	B	162	LYS	N-CA-C	-5.11	101.07	109.40
1	B	217	HIS	CA-CB-CG	-5.09	108.71	113.80
1	A	41	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	123	ILE	N-CA-C	5.08	116.68	108.85
1	B	57	TRP	CA-C-O	5.08	123.30	118.63
1	A	129	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1725	0	1567	70	0
1	B	1731	0	1580	66	0
2	A	5	0	0	1	0
2	B	15	0	0	1	0
3	A	96	0	0	3	0
3	B	95	0	0	2	0
All	All	3667	0	3147	126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (126) 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:149:ASN:HD21	1:B:212:ASN:HD21	1.05	0.99
1:B:135:ASN:HA	1:B:140:LYS:HG3	1.48	0.95
1:A:75:PRO:HD2	1:A:78:MET:HE3	1.55	0.87
1:A:203:THR:HB	1:A:224:VAL:HG22	1.55	0.86
1:A:151:TYR:CD1	1:A:200:TYR:HB3	2.13	0.82
1:B:193:VAL:HG23	1:B:195:LEU:HD21	1.64	0.79
1:A:2:SER:HB2	1:A:5:GLU:HB2	1.65	0.78
1:A:211:PRO:HG2	1:B:202:SER:OG	1.87	0.75
1:A:78:MET:HE1	1:A:226:ALA:C	2.12	0.73
1:B:2:SER:HB3	1:B:5:GLU:OE2	1.88	0.73
1:B:90:GLU:H	1:B:90:GLU:CD	1.97	0.73
1:A:193:VAL:HG23	1:A:195:LEU:HD21	1.69	0.72
1:A:194:LEU:C	1:A:195:LEU:HD23	2.13	0.72
1:B:213:GLU:OE2	1:B:215:ARG:HG3	1.89	0.71
1:B:194:LEU:C	1:B:195:LEU:HD23	2.17	0.70
1:B:48:SER:HB3	1:B:53:LEU:HD13	1.76	0.68
1:A:209:LYS:NZ	3:A:312:HOH:O	2.27	0.68
1:A:149:ASN:HD21	1:B:212:ASN:ND2	1.87	0.68
1:B:80:ARG:O	1:B:194:LEU:HG	1.95	0.66
1:B:143:TYR:OH	1:B:218:MET:HG3	1.96	0.66
1:A:75:PRO:HD2	1:A:78:MET:CE	2.26	0.66
1:A:195:LEU:HD23	1:A:195:LEU:N	2.10	0.65
1:B:66:GYS:OH	1:B:148:HIS:HE1	1.78	0.65
1:B:144:ASN:OD1	1:B:145:TYR:N	2.30	0.65
1:A:210:ASP:C	1:A:210:ASP:OD1	2.39	0.64
1:A:2:SER:O	1:A:5:GLU:N	2.30	0.64
1:B:101:LYS:O	1:B:177:GLN:NE2	2.30	0.63
1:A:193:VAL:HG23	1:A:195:LEU:CD2	2.28	0.63
1:A:163:VAL:HG12	1:A:164:ASN:N	2.14	0.62
1:B:210:ASP:OD1	1:B:210:ASP:C	2.43	0.61
1:B:193:VAL:HG23	1:B:195:LEU:CD2	2.31	0.60
1:B:193:VAL:CG2	1:B:195:LEU:HD21	2.32	0.59
1:B:173:ASP:OD1	1:B:175:SER:HB2	2.02	0.59
1:B:171:ILE:HG22	1:B:172:GLU:N	2.18	0.58
1:A:149:ASN:ND2	1:B:212:ASN:HD21	1.89	0.57
1:A:135:ASN:HA	1:A:140:LYS:HG3	1.87	0.56
1:A:151:TYR:C	1:A:152:ILE:HD13	2.30	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASP:OD1	1:A:133:ASP:N	2.35	0.56
1:A:41:ASP:OD2	1:B:34:GLU:OE2	2.24	0.56
1:B:148:HIS:N	1:B:148:HIS:ND1	2.52	0.55
1:A:152:ILE:HD13	1:A:152:ILE:N	2.22	0.55
1:A:4:GLY:O	1:A:7:LEU:HB2	2.07	0.54
1:B:194:LEU:O	1:B:195:LEU:HD23	2.05	0.54
1:B:153:MET:HE2	1:B:162:LYS:HB2	1.89	0.54
1:A:205:SER:HA	1:A:222:GLU:HG2	1.90	0.54
1:B:145:TYR:OH	1:B:167:ILE:HD12	2.09	0.53
1:B:73:ARG:HB3	1:B:225:THR:HB	1.91	0.51
1:A:56:PRO:HA	2:A:239:SO4:O3	2.10	0.51
1:B:78:MET:O	1:B:79:LYS:C	2.52	0.51
1:B:159:ASN:OD1	1:B:195:LEU:HD11	2.11	0.50
1:B:138:GLY:O	1:B:139:HIS:C	2.47	0.50
1:A:152:ILE:HD12	1:A:163:VAL:HG22	1.94	0.49
1:A:210:ASP:OD1	1:A:212:ASN:N	2.42	0.49
1:A:42:LEU:HD12	1:A:42:LEU:C	2.37	0.49
1:A:78:MET:HE1	1:A:226:ALA:O	2.12	0.49
1:B:2:SER:HB3	1:B:5:GLU:CD	2.37	0.49
1:A:168:ARG:HB2	3:A:330:HOH:O	2.12	0.49
1:B:42:LEU:C	1:B:42:LEU:HD12	2.37	0.49
1:A:156:LYS:O	1:A:157:GLN:C	2.55	0.49
1:B:25:HIS:HD2	2:B:241:SO4:O2	1.95	0.49
1:A:81:HIS:HB3	1:A:196:PRO:CB	2.42	0.49
1:A:208:SER:HB3	1:B:204:CYS:SG	2.52	0.49
1:A:163:VAL:CG1	1:A:164:ASN:N	2.76	0.48
1:B:66:GYS:N2	1:B:66:GYS:HD1	2.28	0.48
1:B:171:ILE:CG2	1:B:172:GLU:N	2.76	0.48
1:B:195:LEU:HD23	1:B:195:LEU:N	2.28	0.48
1:A:141:LEU:HD13	1:A:169:HIS:HB3	1.96	0.48
1:A:171:ILE:HD12	1:A:176:VAL:CA	2.44	0.47
1:A:34:GLU:OE2	1:B:41:ASP:OD2	2.32	0.47
1:B:223:ARG:NH2	3:B:273:HOH:O	2.30	0.47
1:B:41:ASP:OD1	1:B:223:ARG:HD3	2.14	0.47
1:B:57:TRP:N	1:B:58:PRO:CD	2.78	0.47
1:A:78:MET:HE1	1:A:227:ALA:HA	1.97	0.47
1:A:119:LEU:C	1:A:119:LEU:HD13	2.40	0.47
1:B:144:ASN:ND2	1:B:170:ASN:H	2.13	0.47
1:A:81:HIS:CE1	1:A:197:ASP:H	2.33	0.47
1:B:42:LEU:HD11	1:B:222:GLU:HG3	1.97	0.47
1:B:135:ASN:ND2	1:B:171:ILE:HD13	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLY:O	1:B:138:GLY:N	2.47	0.46
1:B:135:ASN:ND2	1:B:171:ILE:CD1	2.79	0.46
1:B:149:ASN:HD22	1:B:202:SER:HA	1.81	0.46
1:A:57:TRP:HB2	1:A:58:PRO:HD3	1.97	0.45
1:A:137:LEU:HA	1:A:137:LEU:HD23	1.65	0.45
1:A:223:ARG:NH2	1:B:34:GLU:OE2	2.45	0.45
1:B:205:SER:HB2	1:B:222:GLU:OE2	2.16	0.45
1:B:171:ILE:HD12	1:B:175:SER:HB3	1.99	0.45
1:B:177:GLN:HG3	1:B:178:LEU:N	2.30	0.45
1:A:78:MET:HE1	1:A:227:ALA:N	2.31	0.45
1:A:131:LYS:O	1:A:134:GLY:N	2.43	0.45
1:B:9:THR:N	3:B:316:HOH:O	2.49	0.44
1:A:2:SER:CB	1:A:5:GLU:HB2	2.40	0.44
1:A:136:ILE:HD12	1:A:136:ILE:N	2.32	0.44
1:A:171:ILE:HD12	1:A:176:VAL:N	2.32	0.44
1:B:101:LYS:N	1:B:177:GLN:HE21	2.15	0.44
1:B:164:ASN:O	1:B:165:PHE:HB3	2.18	0.44
1:B:90:GLU:OE1	1:B:90:GLU:N	2.43	0.43
1:B:136:ILE:N	1:B:136:ILE:HD13	2.33	0.43
1:A:195:LEU:N	1:A:195:LEU:CD2	2.79	0.43
1:B:144:ASN:HD22	1:B:170:ASN:H	1.67	0.43
1:A:202:SER:OG	1:B:211:PRO:HG2	2.18	0.43
1:B:57:TRP:HB2	1:B:58:PRO:HD3	2.00	0.43
1:B:119:LEU:C	1:B:119:LEU:HD13	2.44	0.43
1:A:128:ILE:HG13	1:A:129:ASP:CG	2.44	0.43
1:A:171:ILE:O	1:A:172:GLU:C	2.61	0.43
1:B:96:ARG:HA	1:B:182:TYR:O	2.18	0.43
1:A:81:HIS:HB3	1:A:196:PRO:HB3	2.01	0.42
1:B:203:THR:HG22	1:B:224:VAL:HG13	2.01	0.42
1:A:2:SER:O	1:A:4:GLY:N	2.53	0.42
1:A:155:ASP:OD1	1:A:155:ASP:C	2.60	0.42
1:A:78:MET:HE1	1:A:227:ALA:CA	2.50	0.41
1:B:199:HIS:HB3	1:B:229:ILE:HG13	2.02	0.41
1:A:34:GLU:OE1	1:B:39:TYR:CD1	2.74	0.41
1:A:57:TRP:N	1:A:58:PRO:CD	2.83	0.41
1:A:123:ILE:HG22	1:A:124:GLU:N	2.35	0.41
1:A:212:ASN:HB2	3:A:320:HOH:O	2.20	0.41
1:A:81:HIS:HB3	1:A:196:PRO:HB2	2.03	0.41
1:A:88:MET:HB3	1:A:89:PRO:HA	2.03	0.41
1:A:86:SER:HB3	1:A:194:LEU:HD22	2.03	0.40
1:A:125:LEU:HD23	1:A:125:LEU:C	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:O	1:A:172:GLU:HG2	2.20	0.40
1:B:101:LYS:HG3	1:B:102:ASP:N	2.34	0.40
1:A:83:PHE:CD2	1:A:83:PHE:C	2.98	0.40
1:A:31:GLY:HA2	1:A:45:LYS:O	2.21	0.40
1:A:91:GLY:O	1:A:188:ILE:HB	2.21	0.40
1:A:81:HIS:ND1	1:A:197:ASP:N	2.60	0.40
1:B:57:TRP:N	1:B:58:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/236 (94%)	213 (96%)	5 (2%)	3 (1%)	9	2
1	B	221/236 (94%)	211 (96%)	10 (4%)	0	100	100
All	All	442/472 (94%)	424 (96%)	15 (3%)	3 (1%)	18	9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	157	GLN
1	A	175	SER

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	174/206 (84%)	159 (91%)	15 (9%)	10	3
1	B	176/206 (85%)	162 (92%)	14 (8%)	11	3
All	All	350/412 (85%)	321 (92%)	29 (8%)	10	3

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	7	LEU
1	A	109	ARG
1	A	123	ILE
1	A	133	ASP
1	A	152	ILE
1	A	153	MET
1	A	161	ILE
1	A	164	ASN
1	A	194	LEU
1	A	195	LEU
1	A	203	THR
1	A	204	CYS
1	A	210	ASP
1	A	221	LEU
1	B	9	THR
1	B	76	ASP
1	B	90	GLU
1	B	102	ASP
1	B	124	GLU
1	B	136	ILE
1	B	144	ASN
1	B	145	TYR
1	B	175	SER
1	B	194	LEU
1	B	210	ASP
1	B	222	GLU
1	B	223	ARG
1	B	225	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	148	HIS
1	B	25	HIS
1	B	135	ASN
1	B	148	HIS
1	B	149	ASN
1	B	177	GLN
1	B	212	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	B	66	1	20,22,23	2.58	7 (35%)	25,30,32	2.18	9 (36%)
1	GYS	A	66	1	20,22,23	2.11	6 (30%)	25,30,32	2.15	9 (36%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	GYS	OH-CZ	-5.68	1.24	1.37
1	B	66	GYS	CA3-N3	-5.13	1.37	1.47
1	B	66	GYS	CE1-CZ	4.85	1.48	1.39
1	B	66	GYS	CG2-CB2	-4.82	1.38	1.46
1	A	66	GYS	CE1-CZ	4.41	1.47	1.39
1	A	66	GYS	OH-CZ	-4.40	1.27	1.37
1	A	66	GYS	CG2-CB2	-3.95	1.39	1.46
1	A	66	GYS	CA3-N3	-2.81	1.42	1.47
1	A	66	GYS	C1-N3	2.51	1.41	1.37
1	B	66	GYS	CE2-CD2	-2.34	1.35	1.38
1	B	66	GYS	CB2-CA2	2.28	1.37	1.35
1	A	66	GYS	CE2-CZ	2.20	1.43	1.39
1	B	66	GYS	CE2-CZ	2.15	1.43	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GYS	O2-C2-CA2	6.10	134.91	131.02
1	A	66	GYS	CA1-C1-N3	-4.02	119.60	124.84
1	B	66	GYS	CA1-C1-N3	-3.97	119.68	124.84
1	A	66	GYS	C3-CA3-N3	3.76	120.98	112.43
1	A	66	GYS	C2-N3-C1	-3.76	106.33	108.07
1	B	66	GYS	N3-C1-N2	3.67	114.37	111.48
1	A	66	GYS	N3-C1-N2	3.64	114.35	111.48
1	A	66	GYS	CE2-CZ-CE1	-3.29	114.53	119.77
1	A	66	GYS	CD1-CE1-CZ	3.16	123.22	119.88
1	B	66	GYS	C3-CA3-N3	3.12	119.52	112.43
1	B	66	GYS	CE2-CZ-CE1	-2.91	115.14	119.77
1	A	66	GYS	CG2-CB2-CA2	2.90	133.32	129.87
1	A	66	GYS	CE2-CD2-CG2	2.56	124.52	121.22
1	B	66	GYS	CD1-CE1-CZ	2.43	122.44	119.88
1	B	66	GYS	CG2-CB2-CA2	2.36	132.68	129.87
1	B	66	GYS	CE2-CD2-CG2	2.24	124.11	121.22
1	B	66	GYS	O3-C3-CA3	-2.22	115.50	125.47
1	A	66	GYS	CB2-CA2-C2	-2.13	119.77	122.36

There are no chirality outliers.

All (2) 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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	GYS	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z > 2$
2	SO4	A	239	-	4,4,4	0.72	0	6,6,6	0.94	0
2	SO4	B	241	-	4,4,4	0.49	0	6,6,6	1.03	0
2	SO4	B	239	-	4,4,4	0.57	0	6,6,6	1.05	0
2	SO4	B	240	-	4,4,4	0.69	0	6,6,6	0.92	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	239	SO4	1	0
2	B	241	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	225/236 (95%)	0.20	11 (4%) 35 44	23, 35, 59, 93	0
1	B	225/236 (95%)	0.09	9 (4%) 42 52	22, 33, 56, 79	0
All	All	450/472 (95%)	0.15	20 (4%) 39 49	22, 34, 57, 93	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	ASN	5.7
1	A	2	SER	4.6
1	B	143	TYR	3.6
1	A	146	ASN	3.4
1	A	174	GLY	3.3
1	B	144	ASN	3.1
1	A	151	TYR	2.9
1	B	2	SER	2.7
1	B	9	THR	2.6
1	B	145	TYR	2.6
1	A	148	HIS	2.5
1	B	147	CYS	2.4
1	A	133	ASP	2.4
1	B	229	ILE	2.4
1	A	173	ASP	2.2
1	A	204	CYS	2.2
1	A	190	ASP	2.1
1	A	229	ILE	2.1
1	B	190	ASP	2.1
1	A	164	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	GYS	B	66	21/22	0.95	0.07	20,27,32,34	0
1	GYS	A	66	21/22	0.96	0.07	20,27,31,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
2	SO4	B	240	5/5	0.84	0.15	74,84,100,100	0
2	SO4	B	241	5/5	0.90	0.11	80,86,100,100	0
2	SO4	B	239	5/5	0.91	0.12	45,51,87,90	0
2	SO4	A	239	5/5	0.96	0.10	43,43,56,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.