Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:27 AM GMT

PDB ID	:	2AHA
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

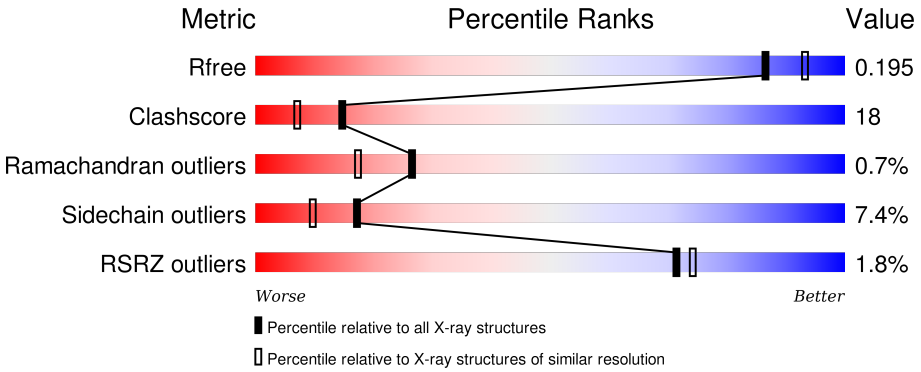
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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}	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	236	2% 59% 28% 8%
1	B	236	60% 28% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	240	-	-	-	X

2 Entry composition (i)

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.

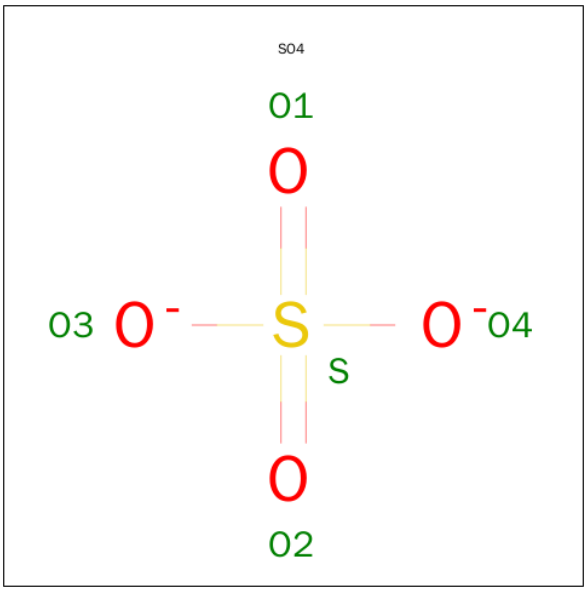
- Molecule 1 is a protein called Green fluorescent protein.

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	UNP P42212
A	48	SER	CYS	ENGINEERED	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	UNP P42212
A	147	CYS	SER	ENGINEERED	UNP P42212
A	204	CYS	GLN	ENGINEERED	UNP P42212
A	223	ARG	PHE	ENGINEERED	UNP P42212
B	41	ASP	LYS	ENGINEERED	UNP P42212
B	48	SER	CYS	ENGINEERED	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	UNP P42212
B	147	CYS	SER	ENGINEERED	UNP P42212
B	204	CYS	GLN	ENGINEERED	UNP P42212
B	223	ARG	PHE	ENGINEERED	UNP P42212

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

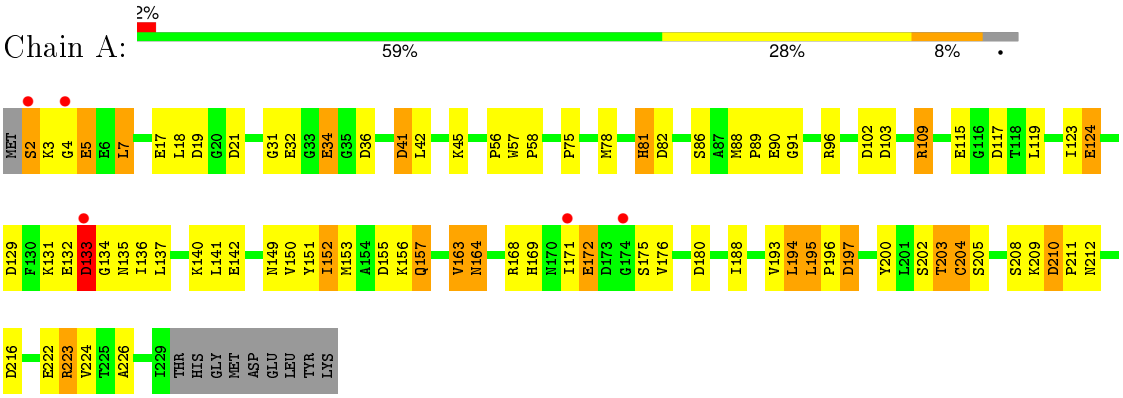
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	96	Total O 96 96	0	0
3	B	95	Total O 95 95	0	0

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.

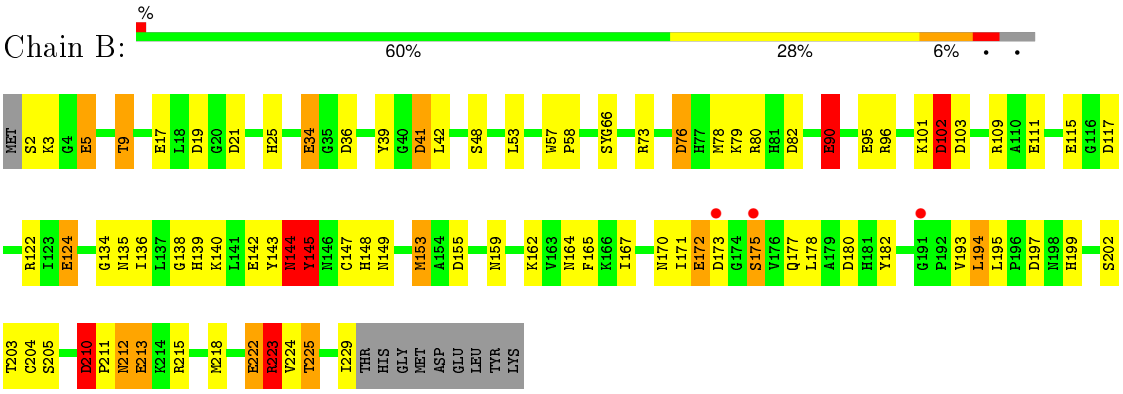
- Molecule 1: Green fluorescent protein

Chain A:



- Molecule 1: Green fluorescent protein

Chain B:



4 Data and refinement statistics (i)

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 39.85 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.98) 99.5 (39.85-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.57 (at 1.95Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.199 , 0.275 0.198 , 0.195	Depositor DCC
R_{free} test set	2172 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 104.6	EDS
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 45346 reflections	Xtriage
F_o,F_c correlation	0.96	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.*

[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: 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	1.09	10/1744 (0.6%)	1.65	36/2370 (1.5%)
1	B	1.11	11/1750 (0.6%)	1.64	33/2380 (1.4%)
All	All	1.10	21/3494 (0.6%)	1.64	69/4750 (1.5%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	GLU	CD-OE2	9.96	1.36	1.25
1	B	213	GLU	CD-OE2	8.44	1.34	1.25
1	A	90	GLU	CD-OE2	8.23	1.34	1.25
1	A	32	GLU	CD-OE2	7.69	1.34	1.25
1	B	124	GLU	CD-OE2	7.38	1.33	1.25
1	A	124	GLU	CD-OE2	7.26	1.33	1.25
1	A	132	GLU	CD-OE2	7.18	1.33	1.25
1	A	142	GLU	CD-OE2	6.93	1.33	1.25
1	A	172	GLU	CD-OE2	6.88	1.33	1.25
1	B	5	GLU	CD-OE2	6.51	1.32	1.25
1	B	142	GLU	CD-OE2	6.17	1.32	1.25
1	A	17	GLU	CD-OE2	5.99	1.32	1.25
1	B	111	GLU	CD-OE2	5.96	1.32	1.25
1	B	90	GLU	CD-OE2	5.90	1.32	1.25
1	A	115	GLU	CD-OE1	-5.88	1.19	1.25
1	B	34	GLU	CD-OE2	5.80	1.32	1.25
1	B	172	GLU	CD-OE2	5.56	1.31	1.25
1	B	115	GLU	CD-OE2	5.50	1.31	1.25
1	B	17	GLU	CD-OE2	5.38	1.31	1.25
1	B	115	GLU	CD-OE1	-5.12	1.20	1.25
1	A	34	GLU	CD-OE2	5.02	1.31	1.25

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	41	ASP	CB-CG-OD2	-11.94	107.55	118.30
1	B	36	ASP	CB-CG-OD2	-11.28	108.15	118.30
1	B	36	ASP	CB-CG-OD1	10.85	128.06	118.30
1	A	19	ASP	CB-CG-OD1	10.82	128.04	118.30
1	A	41	ASP	CB-CG-OD1	9.88	127.19	118.30
1	A	36	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	A	36	ASP	CB-CG-OD1	9.64	126.98	118.30
1	B	103	ASP	CB-CG-OD2	-9.25	109.97	118.30
1	A	210	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	A	19	ASP	CB-CG-OD2	-8.98	110.22	118.30
1	B	103	ASP	CB-CG-OD1	8.95	126.35	118.30
1	B	41	ASP	CB-CG-OD2	-8.94	110.26	118.30
1	B	102	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	B	197	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	B	82	ASP	CB-CG-OD1	8.29	125.76	118.30
1	A	21	ASP	CB-CG-OD1	8.11	125.60	118.30
1	A	103	ASP	CB-CG-OD1	8.05	125.55	118.30
1	B	82	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	180	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	21	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	A	210	ASP	CB-CG-OD1	7.38	124.95	118.30
1	A	103	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	B	155	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	B	210	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	B	76	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	102	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	B	180	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	21	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	A	82	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	133	ASP	CB-CG-OD1	6.74	124.37	118.30
1	B	197	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	197	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	133	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	A	204	CYS	N-CA-CB	6.40	122.12	110.60
1	B	41	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	76	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	223	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	96	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	A	124	GLU	CA-CB-CG	6.15	126.92	113.40
1	B	117	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	145	TYR	N-CA-CB	6.06	121.51	110.60
1	A	197	ASP	CB-CG-OD1	6.04	123.73	118.30
1	A	117	ASP	CB-CG-OD2	-6.00	112.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	153	MET	CB-CA-C	-5.85	98.71	110.40
1	B	21	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	212	ASN	CA-CB-CG	-5.83	100.56	113.40
1	B	144	ASN	CB-CA-C	-5.71	98.99	110.40
1	B	117	ASP	CB-CG-OD1	5.62	123.35	118.30
1	B	109	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	109	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	3	LYS	N-CA-CB	5.48	120.47	110.60
1	A	180	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	163	VAL	CB-CA-C	-5.39	101.16	111.40
1	A	82	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	102	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	90	GLU	N-CA-CB	5.31	120.16	110.60
1	A	132	GLU	CG-CD-OE2	-5.30	107.69	118.30
1	B	180	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	96	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	19	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	223	ARG	CD-NE-CZ	-5.22	116.29	123.60
1	B	95	GLU	CG-CD-OE2	-5.22	107.86	118.30
1	B	122	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	124	GLU	CB-CA-C	-5.06	100.28	110.40
1	A	129	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	150	VAL	CB-CA-C	-5.05	101.80	111.40
1	B	145	TYR	O-C-N	5.03	130.75	122.70
1	A	81	HIS	CA-CB-CG	-5.00	105.10	113.60

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	1571	62	0
1	B	1731	0	1584	66	0
2	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3155	118	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 18.

All (118) 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:A:75:PRO:HD2	1:A:78:MET:HE3	1.43	0.98
1:B:135:ASN:HA	1:B:140:LYS:HG3	1.48	0.95
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:B:2:SER:HB3	1:B:5:GLU:OE2	1.88	0.73
1:A:193:VAL:HG23	1:A:195:LEU:HD21	1.69	0.72
1:B:213:GLU:OE2	1:B:215:ARG:HG3	1.89	0.71
1:B:48:SER:HB3	1:B:53:LEU:HD13	1.76	0.68
1:B:90:GLU:CD	1:B:90:GLU:H	1.97	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:A:194:LEU:C	1:A:195:LEU:HD23	2.13	0.67
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:195:LEU:N	1:A:195:LEU:HD23	2.10	0.65
1:B:194:LEU:C	1:B:195:LEU:HD23	2.17	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:78:MET:HE1	1:A:226:ALA:C	2.18	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:A:75:PRO:HD2	1:A:78:MET:CE	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASP:OD1	1:B:175:SER:HB2	2.02	0.59
1:A:210:ASP:C	1:A:210:ASP:OD1	2.39	0.59
1:B:153:MET:HE2	1:B:162:LYS:HB2	1.84	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:133:ASP:N	1:A:133:ASP:OD1	2.35	0.56
1:B:210:ASP:C	1:B:210:ASP:OD1	2.43	0.56
1:A:41:ASP:OD2	1:B:34:GLU:OE2	2.24	0.56
1:B:148:HIS:ND1	1:B:148:HIS:N	2.52	0.55
1:A:152:ILE:N	1:A:152:ILE:HD13	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: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:A:151:TYR:C	1:A:152:ILE:HD13	2.30	0.52
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: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:168:ARG:HB2	3:A:330:HOH:O	2.12	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:171:ILE:CG2	1:B:172:GLU:N	2.76	0.48
1:B:66:GYS:HD1	1:B:66:GYS:N2	2.28	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:B:223:ARG:NH2	3:B:273:HOH:O	2.30	0.47
1:A:34:GLU:OE2	1:B:41:ASP:OD2	2.32	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: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
1:B:78:MET:O	1:B:79:LYS:C	2.52	0.46

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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:A:42:LEU:HD12	1:A:42:LEU:C	2.37	0.45
1:B:177:GLN:HG3	1:B:178:LEU:N	2.30	0.45
1:B:153:MET:HB2	1:B:153:MET:HE2	1.70	0.45
1:A:131:LYS:O	1:A:134:GLY:N	2.43	0.45
1:B:2:SER:HB3	1:B:5:GLU:CD	2.37	0.45
1:B:42:LEU:HD12	1:B:42:LEU:C	2.37	0.45
1:B:9:THR:N	3:B:316:HOH:O	2.49	0.44
1:A:156:LYS:O	1:A:157:GLN:C	2.55	0.44
1:A:2:SER:CB	1:A:5:GLU:HB2	2.40	0.44
1:A:171:ILE:HD12	1:A:176:VAL:N	2.32	0.44
1:A:136:ILE:HD12	1:A:136:ILE: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:N	1:B:90:GLU:OE1	2.43	0.43
1:B:136:ILE:HD13	1:B:136:ILE:N	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: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:119:LEU:HD13	1:A:119:LEU:C	2.40	0.42
1:A:2:SER:O	1:A:4:GLY:N	2.53	0.42
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:212:ASN:HB2	3:A:320:HOH:O	2.20	0.41
1:A:123:ILE:HG22	1:A:124:GLU:N	2.35	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:B:101:LYS:HG3	1:B:102:ASP:N	2.34	0.40

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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:A:91:GLY:O	1:A:188:ILE:HB	2.21	0.40
1:A:31:GLY:HA2	1:A:45:LYS:O	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
1:A:155:ASP:C	1:A:155:ASP:OD1	2.60	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	223/236 (94%)	214 (96%)	6 (3%)	3 (1%)	15 6
1	B	223/236 (94%)	212 (95%)	11 (5%)	0	100 100
All	All	446/472 (94%)	426 (96%)	17 (4%)	3 (1%)	26 17

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%)	162 (93%)	12 (7%)	19 12
1	B	176/206 (85%)	162 (92%)	14 (8%)	15 8
All	All	350/412 (85%)	324 (93%)	26 (7%)	17 10

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	7	LEU
1	A	18	LEU
1	A	109	ARG
1	A	133	ASP
1	A	152	ILE
1	A	153	MET
1	A	164	ASN
1	A	194	LEU
1	A	195	LEU
1	A	203	THR
1	A	204	CYS
1	B	9	THR
1	B	76	ASP
1	B	90	GLU
1	B	102	ASP
1	B	124	GLU
1	B	144	ASN
1	B	145	TYR
1	B	147	CYS
1	B	175	SER
1	B	194	LEU
1	B	210	ASP
1	B	222	GLU
1	B	223	ARG
1	B	225	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	B	25	HIS
1	B	135	ASN
1	B	148	HIS

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Mol	Chain	Res	Type
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	A	66	1	22,22,23	2.03	7 (31%)	27,30,32	1.78	6 (22%)
1	GYS	B	66	1	22,22,23	2.52	8 (36%)	27,30,32	2.08	6 (22%)

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	A	66	1	-	0/8/29/30	0/2/2/2
1	GYS	B	66	1	-	0/8/29/30	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	GYS	CA3-N3	-5.71	1.37	1.47
1	B	66	GYS	OH-CZ	-5.38	1.24	1.37
1	B	66	GYS	CG2-CB2	-4.38	1.38	1.46
1	A	66	GYS	OH-CZ	-4.18	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GYS	CG2-CB2	-3.59	1.39	1.46
1	B	66	GYS	CA1-C1	-3.30	1.46	1.51
1	A	66	GYS	CA3-N3	-3.14	1.42	1.47
1	A	66	GYS	CA1-C1	-2.63	1.47	1.51
1	B	66	GYS	CE2-CD2	-2.07	1.35	1.38
1	B	66	GYS	CE2-CZ	2.05	1.43	1.38
1	A	66	GYS	CE2-CZ	2.09	1.43	1.38
1	A	66	GYS	C1-N3	2.17	1.41	1.37
1	B	66	GYS	CB2-CA2	2.59	1.37	1.35
1	A	66	GYS	CE1-CZ	4.14	1.47	1.38
1	B	66	GYS	CE1-CZ	4.55	1.48	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	GYS	CE2-CZ-CE1	-3.69	114.53	119.79
1	B	66	GYS	CE2-CZ-CE1	-3.26	115.14	119.79
1	B	66	GYS	CD1-CE1-CZ	2.23	122.44	119.87
1	B	66	GYS	CE2-CD2-CG2	2.26	124.11	121.29
1	A	66	GYS	CG2-CB2-CA2	2.39	133.32	130.22
1	A	66	GYS	CE2-CD2-CG2	2.59	124.52	121.29
1	A	66	GYS	CD1-CE1-CZ	2.90	123.22	119.87
1	B	66	GYS	C-CA3-N3	2.98	119.52	113.00
1	A	66	GYS	N3-C1-N2	3.62	114.35	111.56
1	A	66	GYS	C-CA3-N3	3.64	120.98	113.00
1	B	66	GYS	N3-C1-N2	3.65	114.37	111.56
1	B	66	GYS	O2-C2-CA2	7.35	134.91	130.95

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates 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	1.67	1 (25%)	6,6,6	0.86	0
2	SO4	B	239	-	4,4,4	1.42	0	6,6,6	1.02	0
2	SO4	B	240	-	4,4,4	1.30	0	6,6,6	1.23	1 (16%)
2	SO4	B	241	-	4,4,4	1.28	0	6,6,6	0.95	0

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
2	SO4	A	239	-	-	0/0/0/0	0/0/0/0
2	SO4	B	239	-	-	0/0/0/0	0/0/0/0
2	SO4	B	240	-	-	0/0/0/0	0/0/0/0
2	SO4	B	241	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	239	SO4	O1-S	-2.77	1.37	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	240	SO4	O2-S-O1	-2.39	101.93	109.50

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

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	225/236 (95%)	-0.05	5 (2%)	65	68	23, 35, 59, 93	0
1	B	225/236 (95%)	-0.02	3 (1%)	79	82	22, 33, 56, 79	0
All	All	450/472 (95%)	-0.04	8 (1%)	71	74	22, 34, 57, 93	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	ASP	5.4
1	B	175	SER	3.7
1	A	133	ASP	2.9
1	A	2	SER	2.9
1	B	191	GLY	2.6
1	A	4	GLY	2.4
1	A	171	ILE	2.3
1	A	174	GLY	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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	GYS	A	66	21/22	0.96	0.10	-	20,27,31,44	0
1	GYS	B	66	21/22	0.96	0.11	-	20,27,32,34	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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
2	SO4	B	240	5/5	0.91	0.17	2.59	74,84,100,100	0
2	SO4	B	239	5/5	0.96	0.10	0.07	45,51,87,90	0
2	SO4	A	239	5/5	0.99	0.10	-0.01	43,43,56,60	0
2	SO4	B	241	5/5	0.96	0.11	-	80,86,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.