



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:45 PM UTC

PDB ID : 2ICR / pdb_00002icr
Title : Red fluorescent protein zRFP574 from Zoanthus sp.
Authors : Pletnev, S.; Pletneva, N.; Tikhonova, T.; Pletnev, V.
Deposited on : 2006-09-13
Resolution : 1.51 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

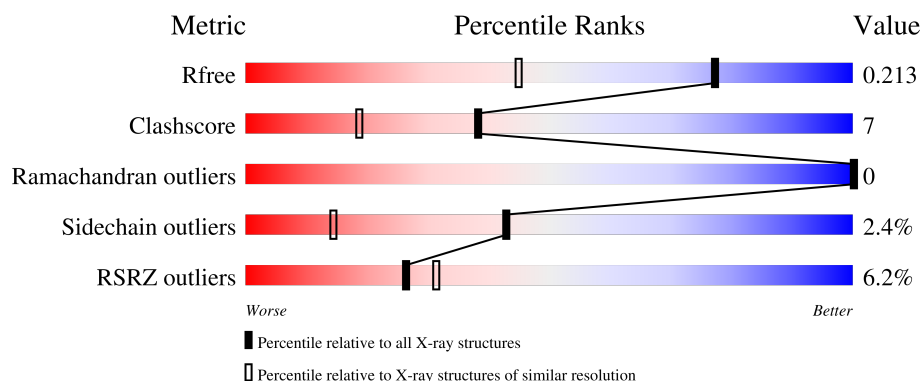
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	2% 80% 14% • 5%
1	B	237	2% 78% 16% • 5%
1	C	237	3% 79% 15% • •
1	D	237	16% 66% 27% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7857 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Red fluorescent protein zoanRFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	4	0
			1843	1173	314	339	17			
1	B	226	Total	C	N	O	S	0	6	0
			1853	1181	317	339	16			
1	C	227	Total	C	N	O	S	0	7	0
			1869	1194	318	340	17			
1	D	226	Total	C	N	O	S	0	4	0
			1845	1173	315	339	18			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q8T4U4
A	-6	ARG	-	expression tag	UNP Q8T4U4
A	-5	GLY	-	expression tag	UNP Q8T4U4
A	-4	SER	-	expression tag	UNP Q8T4U4
A	-3	HIS	-	expression tag	UNP Q8T4U4
A	-2	HIS	-	expression tag	UNP Q8T4U4
A	-1	HIS	-	expression tag	UNP Q8T4U4
A	0	HIS	-	expression tag	UNP Q8T4U4
A	1	HIS	-	expression tag	UNP Q8T4U4
A	2	HIS	-	expression tag	UNP Q8T4U4
A	3	GLY	-	expression tag	UNP Q8T4U4
A	5	ALA	LYS	engineered mutation	UNP Q8T4U4
A	66	XYG	ASP	chromophore	UNP Q8T4U4
A	66	XYG	TYR	chromophore	UNP Q8T4U4
A	66	XYG	GLY	chromophore	UNP Q8T4U4
B	-7	MET	-	expression tag	UNP Q8T4U4
B	-6	ARG	-	expression tag	UNP Q8T4U4
B	-5	GLY	-	expression tag	UNP Q8T4U4
B	-4	SER	-	expression tag	UNP Q8T4U4
B	-3	HIS	-	expression tag	UNP Q8T4U4
B	-2	HIS	-	expression tag	UNP Q8T4U4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	expression tag	UNP Q8T4U4
B	0	HIS	-	expression tag	UNP Q8T4U4
B	1	HIS	-	expression tag	UNP Q8T4U4
B	2	HIS	-	expression tag	UNP Q8T4U4
B	3	GLY	-	expression tag	UNP Q8T4U4
B	5	ALA	LYS	engineered mutation	UNP Q8T4U4
B	66	XYG	ASP	chromophore	UNP Q8T4U4
B	66	XYG	TYR	chromophore	UNP Q8T4U4
B	66	XYG	GLY	chromophore	UNP Q8T4U4
C	-7	MET	-	expression tag	UNP Q8T4U4
C	-6	ARG	-	expression tag	UNP Q8T4U4
C	-5	GLY	-	expression tag	UNP Q8T4U4
C	-4	SER	-	expression tag	UNP Q8T4U4
C	-3	HIS	-	expression tag	UNP Q8T4U4
C	-2	HIS	-	expression tag	UNP Q8T4U4
C	-1	HIS	-	expression tag	UNP Q8T4U4
C	0	HIS	-	expression tag	UNP Q8T4U4
C	1	HIS	-	expression tag	UNP Q8T4U4
C	2	HIS	-	expression tag	UNP Q8T4U4
C	3	GLY	-	expression tag	UNP Q8T4U4
C	5	ALA	LYS	engineered mutation	UNP Q8T4U4
C	66	XYG	ASP	chromophore	UNP Q8T4U4
C	66	XYG	TYR	chromophore	UNP Q8T4U4
C	66	XYG	GLY	chromophore	UNP Q8T4U4
D	-7	MET	-	expression tag	UNP Q8T4U4
D	-6	ARG	-	expression tag	UNP Q8T4U4
D	-5	GLY	-	expression tag	UNP Q8T4U4
D	-4	SER	-	expression tag	UNP Q8T4U4
D	-3	HIS	-	expression tag	UNP Q8T4U4
D	-2	HIS	-	expression tag	UNP Q8T4U4
D	-1	HIS	-	expression tag	UNP Q8T4U4
D	0	HIS	-	expression tag	UNP Q8T4U4
D	1	HIS	-	expression tag	UNP Q8T4U4
D	2	HIS	-	expression tag	UNP Q8T4U4
D	3	GLY	-	expression tag	UNP Q8T4U4
D	5	ALA	LYS	engineered mutation	UNP Q8T4U4
D	66	XYG	ASP	chromophore	UNP Q8T4U4
D	66	XYG	TYR	chromophore	UNP Q8T4U4
D	66	XYG	GLY	chromophore	UNP Q8T4U4

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



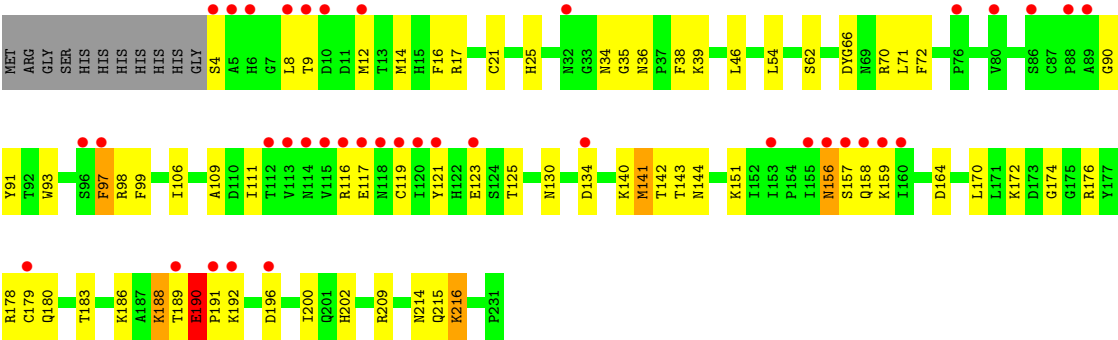
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		
3	B	113	Total	O	0	0
			113	113		
3	C	115	Total	O	0	0
			115	115		
3	D	66	Total	O	0	0
			66	66		

- Molecule 1: Red fluorescent protein zoanRFP





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	115.19Å 146.74Å 122.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.51 30.00 – 1.51	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-1.51) 99.5 (30.00-1.51)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.46Å)	Xtriage
Refinement program	SHELX, SHELXL-97	Depositor
R, R_{free}	0.178 , 0.225 0.177 , 0.213	Depositor DCC
R_{free} test set	1737 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7857	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: SO4, XYG

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	0.73	0/1880	1.61	23/2535 (0.9%)
1	B	0.65	0/1899	1.58	21/2561 (0.8%)
1	C	0.71	1/1919 (0.1%)	1.54	20/2590 (0.8%)
1	D	0.67	2/1882 (0.1%)	1.70	40/2537 (1.6%)
All	All	0.69	3/7580 (0.0%)	1.61	104/10223 (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	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	MET	SD-CE	-7.59	1.60	1.79
1	D	141[A]	MET	SD-CE	-6.16	1.64	1.79
1	D	141[B]	MET	SD-CE	-6.16	1.64	1.79

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	214	ASN	CA-CB-CG	11.97	124.57	112.60
1	B	117	GLU	CB-CG-CD	10.30	130.11	112.60
1	D	117	GLU	CB-CG-CD	10.21	129.96	112.60
1	C	97	PHE	CA-CB-CG	9.50	123.30	113.80
1	B	71	LEU	N-CA-C	-8.70	101.73	111.82
1	D	71	LEU	N-CA-C	-8.55	101.91	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	178	ARG	CD-NE-CZ	8.06	135.68	124.40
1	A	202	HIS	CA-CB-CG	8.02	121.81	113.80
1	D	188	LYS	N-CA-C	-7.67	103.39	112.89
1	B	214	ASN	CA-CB-CG	7.64	120.24	112.60
1	A	71	LEU	N-CA-C	-7.42	103.22	111.82
1	B	202	HIS	CA-CB-CG	7.37	121.17	113.80
1	A	62	SER	N-CA-C	7.37	120.24	111.33
1	C	5	ALA	CA-C-O	-7.35	112.45	120.24
1	B	62	SER	CA-C-O	-7.29	112.76	120.63
1	B	181	PHE	CA-CB-CG	7.26	121.06	113.80
1	A	200	ILE	N-CA-CB	7.08	121.44	111.82
1	C	97	PHE	O-C-N	7.03	131.25	123.52
1	C	200	ILE	N-CA-CB	7.02	121.37	111.82
1	B	200	ILE	N-CA-CB	7.02	121.46	112.34
1	C	71	LEU	N-CA-C	-6.85	103.83	111.71
1	D	38	PHE	CA-CB-CG	-6.83	106.97	113.80
1	D	178	ARG	N-CA-C	6.69	120.78	110.20
1	D	202	HIS	CA-CB-CG	6.66	120.46	113.80
1	D	72	PHE	CA-CB-CG	-6.65	107.15	113.80
1	C	62	SER	N-CA-C	6.60	119.32	111.33
1	C	202	HIS	CA-CB-CG	6.58	120.38	113.80
1	C	178	ARG	N-CA-C	6.53	120.93	109.96
1	D	178	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	B	38	PHE	CA-CB-CG	-6.47	107.33	113.80
1	C	181	PHE	CA-CB-CG	6.43	120.23	113.80
1	D	214	ASN	N-CA-C	6.36	119.08	109.23
1	A	129	VAL	CA-C-O	6.21	127.59	121.19
1	C	144	ASN	CA-CB-CG	6.20	118.80	112.60
1	D	97	PHE	O-C-N	5.98	130.10	123.52
1	A	130	ASN	N-CA-CB	-5.97	102.83	111.91
1	B	130	ASN	N-CA-C	5.89	119.77	111.52
1	A	181	PHE	CA-CB-CG	5.88	119.68	113.80
1	C	130	ASN	N-CA-C	5.86	119.72	111.52
1	D	130	ASN	CA-CB-CG	-5.77	106.83	112.60
1	C	164	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	97	PHE	CA-CB-CG	5.76	119.56	113.80
1	D	215	GLN	CA-C-O	-5.75	113.98	120.43
1	D	156	ASN	N-CA-C	5.74	118.00	111.11
1	A	178	ARG	N-CA-C	5.72	119.23	110.20
1	D	130	ASN	N-CA-C	5.70	119.50	111.52
1	B	69	ASN	OD1-CG-ND2	5.67	128.28	122.60
1	A	196	ASP	N-CA-C	-5.67	102.37	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ASN	N-CA-C	5.63	117.87	111.11
1	C	52	GLY	O-C-N	-5.62	116.15	121.77
1	D	116	ARG	CD-NE-CZ	5.59	132.23	124.40
1	D	209	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	B	130	ASN	N-CA-CB	-5.50	103.55	111.91
1	A	129	VAL	CA-C-N	5.49	129.97	122.34
1	A	129	VAL	C-N-CA	5.49	129.97	122.34
1	D	16	PHE	CA-CB-CG	5.49	119.28	113.80
1	C	186	LYS	N-CA-C	5.42	117.22	108.34
1	C	38	PHE	CA-CB-CG	-5.40	108.40	113.80
1	D	97	PHE	N-CA-CB	5.40	119.73	110.77
1	D	125	THR	CA-C-O	-5.39	114.46	120.66
1	D	46	LEU	N-CA-C	5.38	118.33	109.72
1	D	183	THR	N-CA-C	5.36	117.98	109.50
1	A	213	LYS	CA-C-O	5.36	125.46	119.41
1	C	72	PHE	CA-CB-CG	-5.35	108.45	113.80
1	D	190	GLU	N-CA-C	5.34	117.29	109.71
1	D	196	ASP	N-CA-C	-5.32	102.11	110.36
1	A	197	TRP	CG-CD2-CE3	-5.32	128.58	133.90
1	C	179	CYS	CA-C-O	-5.30	114.90	121.11
1	A	205	ASN	O-C-N	5.30	129.74	123.27
1	B	116	ARG	CD-NE-CZ	5.28	131.79	124.40
1	D	98	ARG	O-C-N	5.28	129.39	123.27
1	D	178	ARG	CA-C-O	-5.27	115.04	121.05
1	D	200	ILE	N-CA-CB	5.27	119.19	112.34
1	D	186	LYS	N-CA-C	5.25	116.96	108.34
1	D	216	LYS	CB-CG-CD	5.25	123.37	111.30
1	B	179	CYS	CA-C-O	-5.25	113.83	120.28
1	D	144	ASN	CB-CA-C	-5.24	101.02	110.03
1	B	197	TRP	CG-CD2-CE3	-5.21	128.69	133.90
1	D	62	SER	N-CA-C	5.17	117.58	111.33
1	A	17	ARG	N-CA-CB	5.16	119.11	110.59
1	B	209	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	D	62	SER	CA-C-O	-5.14	115.07	120.63
1	C	178	ARG	CA-C-O	-5.14	115.01	120.92
1	B	98	ARG	CA-C-O	-5.14	114.96	120.46
1	A	148	SER	N-CA-C	5.11	116.43	109.18
1	D	14	MET	CA-C-O	-5.10	115.63	121.40
1	D	164	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	25	HIS	CA-CB-CG	-5.10	108.70	113.80
1	D	196	ASP	CA-C-O	-5.09	115.66	121.82
1	D	35	GLY	CA-C-N	5.09	129.93	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	35	GLY	C-N-CA	5.09	129.93	122.66
1	D	174	GLY	CA-C-N	-5.08	114.40	121.67
1	D	174	GLY	C-N-CA	-5.08	114.40	121.67
1	B	196	ASP	N-CA-C	-5.08	102.48	110.36
1	C	45	ASN	OD1-CG-ND2	5.08	127.68	122.60
1	C	130	ASN	N-CA-CB	-5.05	104.23	111.91
1	A	164	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	211	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	52	GLY	O-C-N	-5.03	116.75	121.77
1	A	24	GLY	CA-C-N	-5.01	115.75	122.42
1	A	24	GLY	C-N-CA	-5.01	115.75	122.42
1	A	144	ASN	CB-CA-C	-5.01	102.01	110.43
1	B	131	PHE	N-CA-C	-5.00	102.01	109.42
1	A	220	ILE	CA-C-O	-5.00	115.22	120.27

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	17[A]	ARG	Sidechain
1	B	17[B]	ARG	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	1843	0	1768	14	0
1	B	1853	0	1789	16	0
1	C	1869	0	1808	27	0
1	D	1845	0	1766	50	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	133	0	0	1	0
3	B	113	0	0	3	0
3	C	115	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	66	0	0	1	0
All	All	7857	0	7131	100	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 7.

All (100) 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:97:PHE:HE1	1:A:107[A]:CYS:SG	1.36	1.48
1:A:97:PHE:CE1	1:A:107[A]:CYS:SG	2.07	1.47
1:D:97:PHE:CD2	1:D:179:CYS:SG	2.15	1.39
1:D:8:LEU:CD2	1:D:12[B]:MET:HE1	1.62	1.29
1:C:97:PHE:CD2	1:C:179:CYS:SG	2.42	1.12
1:A:97:PHE:CZ	1:A:107[A]:CYS:SG	2.45	1.09
1:C:98:ARG:HB3	3:C:354:HOH:O	1.52	1.09
1:C:97:PHE:HD2	1:C:179:CYS:SG	1.77	1.06
1:D:8:LEU:HD23	1:D:12[B]:MET:HE1	1.02	1.01
1:D:8:LEU:CD2	1:D:12[B]:MET:CE	2.40	0.98
1:D:97:PHE:HD2	1:D:179:CYS:SG	1.68	0.98
1:D:8:LEU:HD22	1:D:12[B]:MET:CE	2.06	0.85
1:D:97:PHE:CG	1:D:179:CYS:SG	2.75	0.80
1:B:77:GLU:HG3	3:B:322:HOH:O	1.86	0.75
1:D:17:ARG:HB3	1:D:123:GLU:OE1	1.90	0.71
1:D:97:PHE:HE2	1:D:99:PHE:CZ	2.10	0.69
1:D:97:PHE:CB	1:D:180:GLN:O	2.40	0.69
1:D:119:CYS:SG	1:D:121:TYR:HE1	2.17	0.67
1:D:97:PHE:HB3	1:D:180:GLN:O	1.95	0.66
1:B:97:PHE:HB2	1:B:105:CYS:HB2	1.77	0.65
1:C:162:LYS:HG2	1:C:184[B]:ILE:HD13	1.78	0.65
1:D:97:PHE:HB2	1:D:179:CYS:SG	2.36	0.64
1:A:127:TYR:HB2	1:D:106:ILE:HD11	1.80	0.64
1:D:119:CYS:SG	1:D:121:TYR:CE1	2.90	0.64
1:C:17:ARG:NH2	1:D:156:ASN:HB3	2.15	0.62
1:D:97:PHE:HA	1:D:180:GLN:O	2.01	0.61
1:A:97:PHE:HB2	1:A:105:CYS:HB2	1.83	0.60
1:D:8:LEU:HD22	1:D:12[B]:MET:HE3	1.82	0.60
1:A:97:PHE:HZ	1:A:107[A]:CYS:SG	2.21	0.60
1:D:9:THR:H	1:D:12[B]:MET:HE2	1.66	0.60
1:C:151:LYS:HE3	1:C:153[A]:ILE:HD11	1.86	0.58
1:B:106:ILE:HD11	1:C:127:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:HD23	1:D:176:ARG:HG2	1.86	0.57
1:D:97:PHE:HA	3:D:281:HOH:O	2.05	0.56
1:B:162:LYS:HD2	1:B:184:ILE:CD1	2.35	0.56
1:D:97:PHE:HE2	1:D:99:PHE:CE1	2.24	0.55
1:D:143:THR:CG2	1:D:172:LYS:HG3	2.36	0.55
1:C:41:LYS:HE2	1:C:43:PHE:CZ	2.42	0.54
1:B:106:ILE:HD11	1:C:127:TYR:CB	2.38	0.54
1:D:97:PHE:CE2	1:D:99:PHE:CE1	2.96	0.53
1:C:97:PHE:HB2	1:C:179:CYS:SG	2.49	0.53
1:C:162:LYS:HG2	1:C:184[B]:ILE:CD1	2.37	0.53
1:D:97:PHE:CE2	1:D:99:PHE:CZ	2.94	0.53
1:D:142:THR:O	1:D:172:LYS:HE3	2.07	0.52
1:A:5:ALA:O	1:A:6:HIS:HB2	2.10	0.52
1:B:189:THR:HG21	3:B:303:HOH:O	2.10	0.52
1:A:127:TYR:CB	1:D:106:ILE:HD11	2.39	0.51
1:C:151:LYS:CE	1:C:153[A]:ILE:HD11	2.40	0.51
1:D:97:PHE:CB	1:D:179:CYS:SG	2.99	0.50
1:D:54:LEU:O	1:D:140:LYS:HE2	2.12	0.50
1:C:17:ARG:HH22	1:D:156:ASN:HB3	1.75	0.50
1:D:159:LYS:HD2	1:D:190:GLU:OE2	2.11	0.50
1:C:97:PHE:HA	3:C:293:HOH:O	2.12	0.49
1:D:93:TRP:NE1	1:D:109:ALA:HB3	2.26	0.49
1:B:162:LYS:HD2	1:B:184:ILE:HD13	1.95	0.49
1:D:12[A]:MET:O	1:D:34:ASN:HA	2.14	0.47
1:A:59:ASP:HB3	1:A:169:LEU:HD21	1.97	0.46
1:C:98:ARG:CB	3:C:354:HOH:O	2.33	0.46
1:A:222:HIS:HE1	3:A:333:HOH:O	1.99	0.45
1:C:87:CYS:HB3	1:C:88:PRO:HA	1.98	0.45
1:C:184[B]:ILE:CG2	1:C:186:LYS:HE2	2.46	0.45
1:D:141[B]:MET:HA	1:D:172:LYS:HD2	1.99	0.44
1:D:8:LEU:HB3	1:D:12[B]:MET:HE2	1.98	0.44
1:D:36:ASN:ND2	1:D:39:LYS:HG3	2.32	0.44
1:A:4:SER:HB3	1:A:7:GLY:HA2	1.99	0.44
1:B:162:LYS:HD2	1:B:184:ILE:HD11	1.99	0.44
1:C:97:PHE:HA	1:C:180:GLN:O	2.17	0.44
1:C:97:PHE:CB	1:C:180:GLN:O	2.65	0.43
1:B:5:ALA:O	1:B:6:HIS:HB2	2.18	0.43
1:B:98:ARG:HH21	1:B:98:ARG:HD2	1.65	0.43
1:D:97:PHE:CA	1:D:180:GLN:O	2.67	0.43
1:D:190:GLU:HA	1:D:191:PRO:HD3	1.72	0.43
1:D:90:GLY:HA3	1:D:111:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:THR:HG21	3:B:348:HOH:O	2.18	0.42
1:C:77:GLU:HG3	3:C:328:HOH:O	2.20	0.42
1:C:184[B]:ILE:HG21	1:C:186:LYS:HE2	2.00	0.42
1:D:91:TYR:HA	1:D:188:LYS:HG3	2.01	0.42
1:B:221:GLU:HG2	1:B:222:HIS:N	2.33	0.42
1:B:4:SER:HA	1:B:8:LEU:O	2.20	0.42
1:B:19:GLU:O	1:B:125:THR:HA	2.20	0.42
1:C:70:ARG:NE	1:C:70:ARG:HA	2.35	0.42
1:D:111:ILE:N	1:D:111:ILE:HD12	2.34	0.42
1:D:141[A]:MET:HA	1:D:172:LYS:HD2	2.02	0.42
1:D:106:ILE:HD13	1:D:106:ILE:HG21	1.84	0.41
1:D:70:ARG:NE	1:D:70:ARG:HA	2.35	0.41
1:B:227:ARG:HA	1:B:227:ARG:HD2	1.85	0.41
1:C:93:TRP:NE1	1:C:109:ALA:HB3	2.36	0.41
1:D:21:CYS:HA	1:D:25:HIS:O	2.20	0.41
1:A:221:GLU:HG2	1:A:222:HIS:N	2.36	0.41
1:C:17:ARG:NH1	1:D:157:SER:HA	2.36	0.41
1:D:9:THR:N	1:D:12[B]:MET:HE2	2.33	0.41
1:D:141[A]:MET:HA	1:D:141[A]:MET:HE2	2.02	0.41
1:A:114:ASN:HD22	1:A:117:GLU:H	1.69	0.40
1:C:41:LYS:HG3	1:C:42:GLN:N	2.37	0.40
1:B:62:SER:HB3	1:B:204:LEU:HD21	2.04	0.40
1:D:8:LEU:HB3	1:D:12[B]:MET:CE	2.52	0.40
1:D:8:LEU:HA	1:D:12[B]:MET:CE	2.52	0.40
1:B:184:ILE:HG21	1:B:186:LYS:HE2	2.02	0.40
1:C:97:PHE:HB3	1:C:180:GLN:O	2.21	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	225/237 (95%)	222 (99%)	3 (1%)	0	100	100
1	B	227/237 (96%)	224 (99%)	3 (1%)	0	100	100
1	C	230/237 (97%)	226 (98%)	4 (2%)	0	100	100
1	D	225/237 (95%)	222 (99%)	3 (1%)	0	100	100
All	All	907/948 (96%)	894 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	200/205 (98%)	197 (98%)	3 (2%)	57	29
1	B	202/205 (98%)	198 (98%)	4 (2%)	48	19
1	C	204/205 (100%)	200 (98%)	4 (2%)	48	19
1	D	200/205 (98%)	192 (96%)	8 (4%)	28	5
All	All	806/820 (98%)	787 (98%)	19 (2%)	43	14

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	213	LYS
1	A	216	LYS
1	B	158	GLN
1	B	162	LYS
1	B	189	THR
1	B	230	LEU
1	C	98	ARG
1	C	134	ASP
1	C	193	GLU
1	C	216	LYS
1	D	4	SER
1	D	134	ASP

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Mol	Chain	Res	Type
1	D	151	LYS
1	D	158	GLN
1	D	189	THR
1	D	190	GLU
1	D	192	LYS
1	D	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	114	ASN
1	A	156	ASN
1	A	218	GLN
1	A	222	HIS
1	B	45	ASN
1	B	158	GLN
1	B	218	GLN
1	B	222	HIS
1	C	214	ASN
1	C	218	GLN
1	D	158	GLN
1	D	214	ASN
1	D	218	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	XYG	C	66	1	21,21,22	1.97	3 (14%)	23,29,31	2.26	9 (39%)
1	XYG	D	66	1	21,21,22	1.89	3 (14%)	23,29,31	2.43	9 (39%)
1	XYG	A	66	1	21,21,22	1.84	3 (14%)	23,29,31	1.72	5 (21%)
1	XYG	B	66	1	21,21,22	1.93	3 (14%)	23,29,31	1.99	6 (26%)

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	XYG	C	66	1	-	0/7/27/28	0/2/2/2
1	XYG	D	66	1	-	0/7/27/28	0/2/2/2
1	XYG	A	66	1	-	0/7/27/28	0/2/2/2
1	XYG	B	66	1	-	0/7/27/28	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	XYG	C1-CA1	-7.41	1.37	1.48
1	C	66	XYG	C1-CA1	-7.17	1.37	1.48
1	A	66	XYG	C1-CA1	-6.87	1.38	1.48
1	D	66	XYG	C1-CA1	-6.76	1.38	1.48
1	A	66	XYG	CA1-N1	3.37	1.33	1.27
1	D	66	XYG	CA1-N1	3.33	1.33	1.27
1	B	66	XYG	CA1-N1	2.89	1.32	1.27
1	C	66	XYG	CB1-CA1	2.80	1.54	1.50
1	C	66	XYG	CA1-N1	2.69	1.32	1.27
1	B	66	XYG	CB1-CA1	2.53	1.54	1.50
1	D	66	XYG	CB1-CA1	2.30	1.54	1.50
1	A	66	XYG	CB1-CA1	2.24	1.53	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	XYG	C3-CA3-N3	5.77	125.56	112.43
1	D	66	XYG	CB2-CA2-N2	4.90	135.41	128.76
1	C	66	XYG	C3-CA3-N3	4.85	123.46	112.43
1	D	66	XYG	C3-CA3-N3	4.82	123.40	112.43
1	C	66	XYG	CB2-CA2-N2	4.42	134.76	128.76
1	D	66	XYG	O2-C2-CA2	-4.14	128.38	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	XYG	CB2-CA2-C2	-3.71	117.86	122.36
1	A	66	XYG	C3-CA3-N3	3.65	120.73	112.43
1	D	66	XYG	CA2-N2-C1	3.51	110.56	104.09
1	A	66	XYG	N3-C1-N2	-3.45	108.53	112.62
1	C	66	XYG	CA2-N2-C1	3.41	110.37	104.09
1	B	66	XYG	N3-C1-N2	-3.40	108.58	112.62
1	D	66	XYG	N3-C1-N2	-3.34	108.65	112.62
1	C	66	XYG	CB2-CA2-C2	-3.27	118.39	122.36
1	D	66	XYG	C2-CA2-N2	-3.27	106.61	108.95
1	C	66	XYG	N3-C1-N2	-3.26	108.75	112.62
1	B	66	XYG	CB2-CA2-C2	-3.08	118.63	122.36
1	C	66	XYG	C2-CA2-N2	-3.04	106.77	108.95
1	A	66	XYG	CA2-N2-C1	2.95	109.52	104.09
1	B	66	XYG	CB2-CA2-N2	2.85	132.63	128.76
1	A	66	XYG	CB2-CA2-N2	2.85	132.63	128.76
1	B	66	XYG	CA2-N2-C1	2.70	109.07	104.09
1	C	66	XYG	CE1-CD1-CG2	-2.47	118.03	121.22
1	A	66	XYG	C2-CA2-N2	-2.35	107.27	108.95
1	B	66	XYG	CA2-C2-N3	-2.26	101.60	103.50
1	C	66	XYG	O3-C3-CA3	-2.22	115.49	125.47
1	C	66	XYG	CD2-CE2-CZ	-2.10	117.66	119.88
1	D	66	XYG	O3-C3-CA3	-2.10	116.04	125.47
1	D	66	XYG	CE1-CD1-CG2	-2.02	118.61	121.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	C	250	-	4,4,4	0.41	0	6,6,6	0.20	0
2	SO4	A	250	-	4,4,4	0.30	0	6,6,6	0.28	0
2	SO4	D	250	-	4,4,4	0.37	0	6,6,6	0.23	0
2	SO4	B	250	-	4,4,4	0.46	0	6,6,6	0.32	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.

No monomer is involved in short contacts.

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	225/237 (94%)	-0.11	5 (2%) 62 68	9, 19, 32, 56	4 (1%)
1	B	225/237 (94%)	0.08	4 (1%) 67 73	12, 22, 35, 60	6 (2%)
1	C	226/237 (95%)	0.14	8 (3%) 47 54	7, 22, 36, 57	7 (3%)
1	D	225/237 (94%)	1.17	39 (17%) 4 4	17, 31, 54, 81	4 (1%)
All	All	901/948 (95%)	0.32	56 (6%) 26 31	7, 23, 44, 81	21 (2%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	119	CYS	13.2
1	D	113	VAL	8.0
1	D	120	ILE	7.5
1	D	156	ASN	7.4
1	D	115	VAL	6.8
1	D	117	GLU	6.7
1	A	4	SER	6.6
1	D	97	PHE	6.6
1	D	116	ARG	6.3
1	D	160	ILE	5.9
1	A	5	ALA	5.7
1	C	97	PHE	5.6
1	D	114	ASN	5.5
1	D	155	ILE	5.4
1	D	112	THR	5.3
1	D	189	THR	5.3
1	D	157	SER	5.0
1	D	118	ASN	4.6
1	D	5	ALA	4.4
1	D	159	LYS	4.3
1	D	4	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	4	SER	3.9
1	A	97	PHE	3.9
1	B	97	PHE	3.8
1	D	158	GLN	3.8
1	C	98	ARG	3.6
1	D	88	PRO	3.3
1	D	12[A]	MET	3.3
1	D	179	CYS	3.2
1	C	3	GLY	3.2
1	A	212	ALA	3.1
1	A	98	ARG	3.0
1	B	5	ALA	3.0
1	C	5	ALA	3.0
1	D	32	ASN	3.0
1	D	89	ALA	2.9
1	C	179	CYS	2.9
1	D	96	SER	2.7
1	D	121	TYR	2.6
1	C	231	PRO	2.6
1	D	123	GLU	2.5
1	D	10	ASP	2.5
1	D	6	HIS	2.4
1	D	86	SER	2.4
1	D	191	PRO	2.4
1	C	15[A]	HIS	2.3
1	D	9	THR	2.3
1	C	170	LEU	2.3
1	D	8	LEU	2.3
1	D	192	LYS	2.2
1	D	134	ASP	2.1
1	D	153	ILE	2.1
1	B	98	ARG	2.1
1	D	76	PRO	2.1
1	D	80	VAL	2.0
1	D	196	ASP	2.0

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. 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	XYG	D	66	20/21	0.96	0.06	22,26,30,32	0
1	XYG	B	66	20/21	0.97	0.06	17,18,22,24	0
1	XYG	C	66	20/21	0.97	0.06	17,18,22,25	0
1	XYG	A	66	20/21	0.97	0.05	13,16,18,21	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($\text{\AA}^2$)	Q<0.9
2	SO4	D	250	5/5	0.95	0.08	44,45,48,56	0
2	SO4	A	250	5/5	0.96	0.07	32,33,42,44	0
2	SO4	B	250	5/5	0.97	0.07	32,33,37,38	0
2	SO4	C	250	5/5	0.98	0.07	25,27,32,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.