Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2024 – 02:14 PM JST

PDB ID	:	8JL5
Title	:	Crystal structure of the Green fluorescent protein SEA227D variant at pH 4.5
Authors	:	Shin, S.C.
Deposited on	:	2023-06-02
Resolution	:	1.80 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:

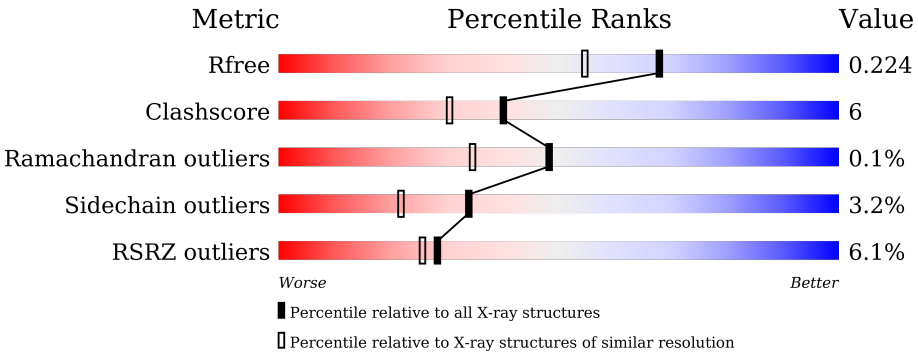
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 <=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	8% 81% 11% • • 5%
1	B	236	4% 83% 11% • 5%
1	C	236	5% 83% 11% • •
1	D	236	6% 82% 11% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8115 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	224	Total	C	N	O	S	0	0	0
			1802	1148	303	345	6			
1	B	225	Total	C	N	O	S	0	0	0
			1810	1154	304	346	6			
1	C	226	Total	C	N	O	S	0	0	0
			1818	1158	306	348	6			
1	D	224	Total	C	N	O	S	0	0	0
			1803	1148	303	346	6			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	147	ASP	SER	engineered mutation	UNP P42212
A	149	GLN	ASN	engineered mutation	UNP P42212
A	163	ALA	VAL	engineered mutation	UNP P42212
A	175	GLY	SER	engineered mutation	UNP P42212
A	202	PHE	SER	engineered mutation	UNP P42212
A	204	THR	GLN	engineered mutation	UNP P42212
A	206	THR	ALA	engineered mutation	UNP P42212
A	227	ASP	ALA	engineered mutation	UNP P42212
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	CRO	SER	chromophore	UNP P42212
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
B	147	ASP	SER	engineered mutation	UNP P42212
B	149	GLN	ASN	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	175	GLY	SER	engineered mutation	UNP P42212
B	202	PHE	SER	engineered mutation	UNP P42212
B	204	THR	GLN	engineered mutation	UNP P42212
B	206	THR	ALA	engineered mutation	UNP P42212
B	227	ASP	ALA	engineered mutation	UNP P42212
C	64	LEU	PHE	engineered mutation	UNP P42212
C	66	CRO	SER	chromophore	UNP P42212
C	66	CRO	TYR	chromophore	UNP P42212
C	66	CRO	GLY	chromophore	UNP P42212
C	80	ARG	GLN	engineered mutation	UNP P42212
C	147	ASP	SER	engineered mutation	UNP P42212
C	149	GLN	ASN	engineered mutation	UNP P42212
C	163	ALA	VAL	engineered mutation	UNP P42212
C	175	GLY	SER	engineered mutation	UNP P42212
C	202	PHE	SER	engineered mutation	UNP P42212
C	204	THR	GLN	engineered mutation	UNP P42212
C	206	THR	ALA	engineered mutation	UNP P42212
C	227	ASP	ALA	engineered mutation	UNP P42212
D	64	LEU	PHE	engineered mutation	UNP P42212
D	66	CRO	SER	chromophore	UNP P42212
D	66	CRO	TYR	chromophore	UNP P42212
D	66	CRO	GLY	chromophore	UNP P42212
D	80	ARG	GLN	engineered mutation	UNP P42212
D	147	ASP	SER	engineered mutation	UNP P42212
D	149	GLN	ASN	engineered mutation	UNP P42212
D	163	ALA	VAL	engineered mutation	UNP P42212
D	175	GLY	SER	engineered mutation	UNP P42212
D	202	PHE	SER	engineered mutation	UNP P42212
D	204	THR	GLN	engineered mutation	UNP P42212
D	206	THR	ALA	engineered mutation	UNP P42212
D	227	ASP	ALA	engineered mutation	UNP P42212

- Molecule 2 is water.

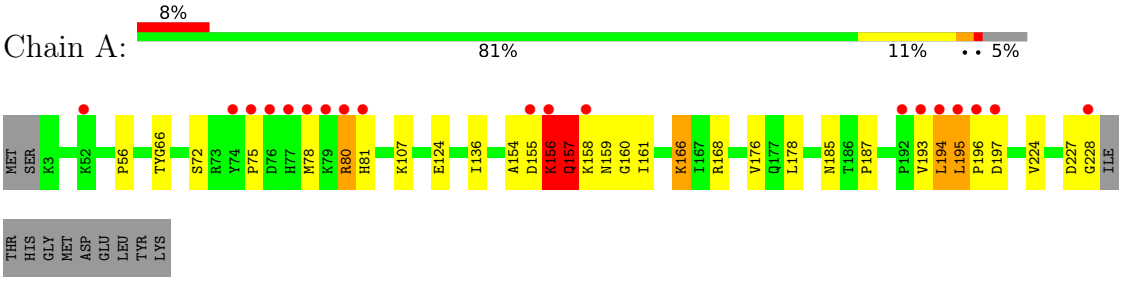
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	207	Total O 207 207	0	0
2	B	223	Total O 223 223	0	0
2	C	237	Total O 237 237	0	0
2	D	215	Total O 215 215	0	0

3 Residue-property plots (i)

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

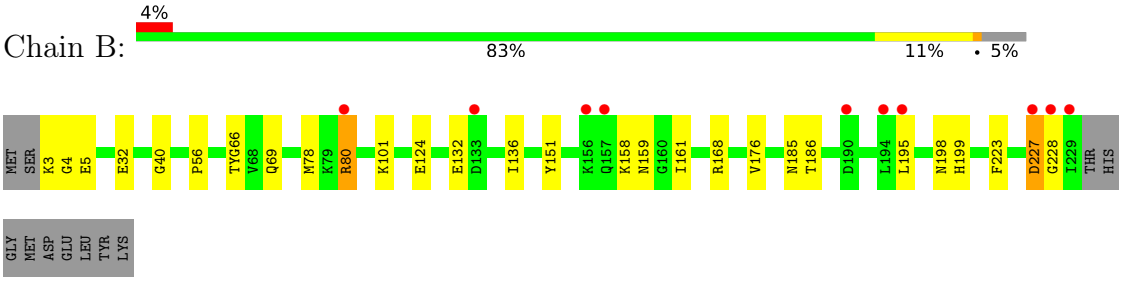
• Molecule 1: Green fluorescent protein

Chain A:



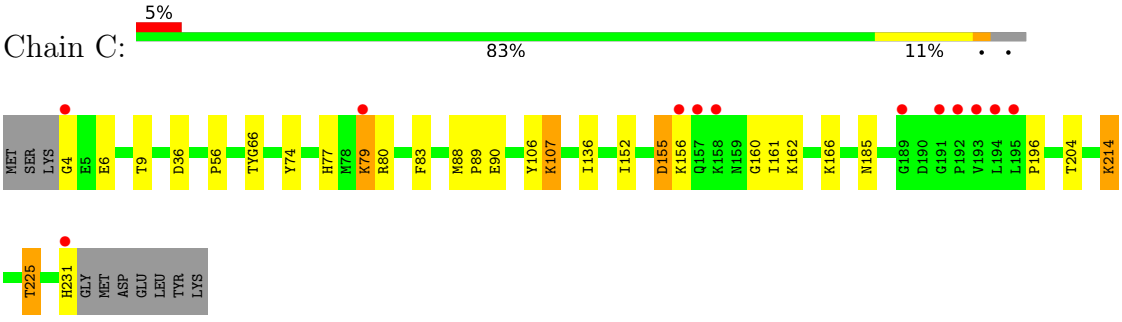
• Molecule 1: Green fluorescent protein

Chain B:



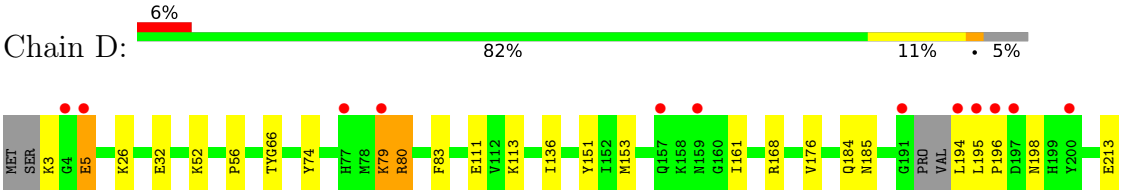
• Molecule 1: Green fluorescent protein

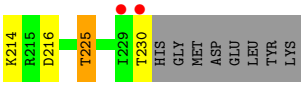
Chain C:



• Molecule 1: Green fluorescent protein

Chain D:




K214
R215
D216
T225
I229
T230
HIS
GLY
MET
ASP
GLU
LEU
TYR
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.94Å 82.95Å 180.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.47 – 1.80 41.47 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.47-1.80) 99.2 (41.47-1.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.185 , 0.222 0.190 , 0.224	Depositor DCC
R_{free} test set	101325 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8115	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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, 0.333 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: CRO

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	0.41	0/1821	0.67	2/2460 (0.1%)
1	B	0.40	0/1829	0.63	0/2471
1	C	0.41	0/1838	0.66	1/2485 (0.0%)
1	D	0.40	0/1820	0.62	0/2456
All	All	0.41	0/7308	0.64	3/9872 (0.0%)

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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	157	GLN	CB-CA-C	-9.05	92.30	110.40
1	C	155	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	157	GLN	N-CA-C	6.18	127.68	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	227	ASP	Peptide

5.2 Too-close contacts (i)

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	1802	0	1734	26	0
1	B	1810	0	1745	21	0
1	C	1818	0	1746	26	0
1	D	1803	0	1735	21	0
2	A	207	0	0	1	0
2	B	223	0	0	5	0
2	C	237	0	0	5	0
2	D	215	0	0	3	0
All	All	8115	0	6960	92	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 6.

All (92) 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:B:3:LYS:HE2	1:B:5:GLU:HG3	1.63	0.81
1:A:159:ASN:HD21	1:A:193:VAL:HG21	1.49	0.77
1:D:168:ARG:HG3	1:D:176:VAL:CG1	2.17	0.75
1:B:80:ARG:O	1:B:80:ARG:HG2	1.86	0.75
1:D:168:ARG:HG3	1:D:176:VAL:HG11	1.73	0.71
2:B:318:HOH:O	1:C:225:THR:HG22	1.93	0.67
1:A:75:PRO:HG2	1:A:78:MET:HG3	1.76	0.67
1:A:78:MET:HE1	1:A:228:GLY:HA2	1.77	0.65
1:D:5:GLU:HG2	1:D:79:LYS:HB3	1.79	0.64
1:A:155:ASP:O	1:A:157:GLN:N	2.30	0.64
1:D:83:PHE:HB2	1:D:196:PRO:HB3	1.81	0.63
1:C:107:LYS:N	1:C:107:LYS:HD3	2.14	0.62
1:A:168:ARG:HG2	1:A:176:VAL:HG11	1.85	0.59
1:C:79:LYS:HD3	1:C:79:LYS:N	2.18	0.59
1:C:79:LYS:HD3	1:C:79:LYS:H	1.68	0.59
1:C:4:GLY:N	2:C:307:HOH:O	2.35	0.59
1:D:168:ARG:HG3	1:D:176:VAL:HG13	1.85	0.58
1:A:166:LYS:HB3	1:A:178:LEU:HD11	1.84	0.58
1:C:4:GLY:N	2:C:309:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LYS:NZ	1:D:184:GLN:HE22	2.04	0.56
1:B:101:LYS:NZ	2:B:303:HOH:O	2.22	0.54
1:A:154:ALA:O	1:A:156:LYS:N	2.39	0.53
1:A:72:SER:HA	1:A:224:VAL:HG13	1.90	0.53
1:D:32:GLU:HG3	2:D:468:HOH:O	2.09	0.52
1:A:155:ASP:C	1:A:157:GLN:H	2.12	0.52
1:C:79:LYS:HZ1	1:C:80:ARG:HH21	1.57	0.52
1:C:79:LYS:NZ	1:C:80:ARG:HH21	2.08	0.52
1:A:161:ILE:HG13	1:A:185:ASN:HB2	1.92	0.52
1:A:160:GLY:H	1:A:195:LEU:HD21	1.76	0.51
1:A:187:PRO:HG3	1:A:193:VAL:HG21	1.92	0.51
1:D:80:ARG:H	1:D:80:ARG:HD2	1.76	0.51
1:D:225:THR:HG21	2:D:435:HOH:O	2.11	0.50
1:A:78:MET:CE	1:A:228:GLY:HA2	2.41	0.50
1:C:90:GLU:HB3	2:C:488:HOH:O	2.12	0.50
1:B:3:LYS:HE2	1:B:5:GLU:H	1.76	0.50
1:D:151:TYR:CE2	1:D:153:MET:HG2	2.47	0.50
1:C:231:HIS:O	2:C:301:HOH:O	2.20	0.49
1:B:158:LYS:HE3	1:B:186:THR:HG21	1.94	0.49
1:A:155:ASP:C	1:A:157:GLN:N	2.66	0.49
1:C:6:GLU:O	1:C:9:THR:HG23	2.12	0.48
1:C:106:TYR:C	1:C:107:LYS:HD3	2.33	0.48
1:B:151:TYR:CZ	1:B:198:ASN:HB3	2.48	0.48
1:B:124:GLU:OE1	2:B:301:HOH:O	2.20	0.47
1:B:168:ARG:HB3	1:B:176:VAL:HG11	1.96	0.47
1:C:36:ASP:OD2	2:C:302:HOH:O	2.20	0.47
1:B:159:ASN:OD1	1:B:195:LEU:HD11	2.15	0.47
1:D:5:GLU:CG	1:D:79:LYS:HB3	2.44	0.47
1:C:155:ASP:O	1:C:155:ASP:OD1	2.32	0.47
1:D:161:ILE:HG13	1:D:185:ASN:HB2	1.96	0.47
1:B:3:LYS:HE3	1:B:4:GLY:H	1.79	0.47
1:C:79:LYS:H	1:C:79:LYS:CD	2.26	0.47
1:C:166:LYS:HZ2	1:D:184:GLN:HE22	1.62	0.47
1:D:111:GLU:OE1	1:D:113:LYS:NZ	2.34	0.46
1:C:214:LYS:H	1:C:214:LYS:HE2	1.80	0.46
1:A:157:GLN:CG	1:A:158:LYS:H	2.28	0.46
1:A:227:ASP:OD1	1:A:228:GLY:N	2.48	0.46
1:B:78:MET:SD	1:B:228:GLY:HA2	2.56	0.45
1:B:69:GLN:HA	2:B:458:HOH:O	2.16	0.45
1:D:168:ARG:CG	1:D:176:VAL:HG11	2.43	0.45
1:A:80:ARG:HA	1:A:80:ARG:HD3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:MET:CE	1:B:228:GLY:HA2	2.47	0.45
1:D:26:LYS:NZ	2:D:302:HOH:O	2.39	0.45
1:A:124:GLU:OE1	2:A:301:HOH:O	2.21	0.44
1:D:52:LYS:HD2	1:D:216:ASP:OD2	2.17	0.44
1:A:81:HIS:O	1:A:196:PRO:HB3	2.17	0.44
1:B:80:ARG:O	1:B:80:ARG:CG	2.60	0.44
1:D:198:ASN:HB2	1:D:230:THR:OG1	2.17	0.44
1:C:214:LYS:N	1:C:214:LYS:HD3	2.33	0.44
1:D:56:PRO:HD3	1:D:136:ILE:O	2.16	0.43
1:C:161:ILE:HG13	1:C:185:ASN:HB2	2.00	0.43
1:C:77:HIS:HA	1:C:79:LYS:NZ	2.32	0.43
1:A:159:ASN:OD1	1:A:193:VAL:HB	2.19	0.43
1:C:152:ILE:HG23	1:C:161:ILE:HD13	2.01	0.43
1:B:3:LYS:HE2	1:B:5:GLU:CG	2.43	0.43
1:A:56:PRO:HD3	1:A:136:ILE:O	2.19	0.42
1:A:194:LEU:HD23	1:A:194:LEU:N	2.33	0.42
1:B:161:ILE:HG13	1:B:185:ASN:HB2	2.01	0.42
1:A:155:ASP:O	1:A:157:GLN:HG2	2.20	0.42
1:C:56:PRO:HD3	1:C:136:ILE:O	2.20	0.42
1:A:195:LEU:HD22	1:A:195:LEU:HA	1.66	0.41
1:C:160:GLY:HA3	1:C:185:ASN:O	2.20	0.41
1:D:213:GLU:C	1:D:214:LYS:HE2	2.39	0.41
1:B:132:GLU:OE2	2:B:302:HOH:O	2.22	0.41
1:D:3:LYS:HE2	1:D:3:LYS:HB2	1.88	0.41
1:A:78:MET:HE2	1:A:78:MET:HB3	1.96	0.41
1:A:168:ARG:HG2	1:A:176:VAL:CG1	2.50	0.41
1:B:40:GLY:O	1:B:223:PHE:HA	2.21	0.41
1:B:227:ASP:OD1	1:B:228:GLY:N	2.47	0.41
1:B:56:PRO:HD3	1:B:136:ILE:O	2.21	0.40
1:C:83:PHE:HB2	1:C:196:PRO:HB3	2.03	0.40
1:C:88:MET:HB3	1:C:89:PRO:HA	2.03	0.40
1:B:199:HIS:HB2	1:B:227:ASP:O	2.22	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	219/236 (93%)	214 (98%)	4 (2%)	1 (0%)	25 14
1	B	220/236 (93%)	217 (99%)	3 (1%)	0	100 100
1	C	221/236 (94%)	217 (98%)	4 (2%)	0	100 100
1	D	217/236 (92%)	213 (98%)	4 (2%)	0	100 100
All	All	877/944 (93%)	861 (98%)	15 (2%)	1 (0%)	48 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	LYS

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	193/206 (94%)	185 (96%)	8 (4%)	26 14
1	B	194/206 (94%)	192 (99%)	2 (1%)	73 68
1	C	195/206 (95%)	187 (96%)	8 (4%)	26 14
1	D	193/206 (94%)	186 (96%)	7 (4%)	30 18
All	All	775/824 (94%)	750 (97%)	25 (3%)	34 22

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	107	LYS
1	A	156	LYS
1	A	157	GLN
1	A	166	LYS

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Mol	Chain	Res	Type
1	A	194	LEU
1	A	195	LEU
1	A	197	ASP
1	B	32	GLU
1	B	80	ARG
1	C	74	TYR
1	C	79	LYS
1	C	107	LYS
1	C	156	LYS
1	C	162	LYS
1	C	204	THR
1	C	214	LYS
1	C	225	THR
1	D	5	GLU
1	D	74	TYR
1	D	79	LYS
1	D	80	ARG
1	D	194	LEU
1	D	195	LEU
1	D	225	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	184	GLN
1	D	184	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	CRO	C	66	1	23,23,24	6.03	8 (34%)	30,32,34	3.43	10 (33%)
1	CRO	B	66	1	23,23,24	5.40	9 (39%)	30,32,34	3.14	9 (30%)
1	CRO	D	66	1	23,23,24	5.53	9 (39%)	30,32,34	4.31	10 (33%)
1	CRO	A	66	1	23,23,24	5.36	8 (34%)	30,32,34	3.51	12 (40%)

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	CRO	C	66	1	-	2/12/31/32	0/2/2/2
1	CRO	B	66	1	-	0/12/31/32	0/2/2/2
1	CRO	D	66	1	-	1/12/31/32	0/2/2/2
1	CRO	A	66	1	-	1/12/31/32	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CRO	CB2-CA2	22.54	1.54	1.35
1	D	66	CRO	CB2-CA2	20.56	1.52	1.35
1	A	66	CRO	CB2-CA2	18.61	1.50	1.35
1	B	66	CRO	CB2-CA2	18.61	1.50	1.35
1	A	66	CRO	CA2-C2	-11.15	1.37	1.48
1	C	66	CRO	OG1-CB1	-10.72	1.13	1.43
1	B	66	CRO	OG1-CB1	-10.10	1.15	1.43
1	C	66	CRO	CA2-C2	-10.10	1.38	1.48
1	B	66	CRO	CA2-C2	-9.88	1.38	1.48
1	A	66	CRO	OG1-CB1	-9.48	1.17	1.43
1	D	66	CRO	CA2-C2	-9.37	1.39	1.48
1	D	66	CRO	OG1-CB1	-9.33	1.17	1.43
1	C	66	CRO	O2-C2	5.86	1.35	1.23
1	D	66	CRO	O2-C2	5.72	1.35	1.23
1	B	66	CRO	O2-C2	5.49	1.34	1.23
1	C	66	CRO	C2-N3	-4.93	1.28	1.39
1	A	66	CRO	C1-N3	-4.91	1.28	1.37
1	B	66	CRO	C1-N3	-4.76	1.29	1.37
1	B	66	CRO	C2-N3	-4.69	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	CRO	C2-N3	-4.65	1.28	1.39
1	A	66	CRO	C2-N3	-4.65	1.28	1.39
1	A	66	CRO	O2-C2	4.60	1.32	1.23
1	B	66	CRO	CA2-N2	-4.57	1.28	1.38
1	C	66	CRO	C1-N3	-4.31	1.29	1.37
1	D	66	CRO	C1-N3	-3.69	1.30	1.37
1	D	66	CRO	CA2-N2	-3.47	1.31	1.38
1	C	66	CRO	CA2-N2	-3.11	1.31	1.38
1	A	66	CRO	CA2-N2	-3.10	1.31	1.38
1	A	66	CRO	CG2-CB2	3.07	1.52	1.46
1	C	66	CRO	CG2-CB2	3.06	1.52	1.46
1	B	66	CRO	CG2-CB2	2.98	1.52	1.46
1	D	66	CRO	CG2-CB2	2.94	1.52	1.46
1	B	66	CRO	C1-N2	-2.09	1.29	1.32
1	D	66	CRO	CA3-N3	-2.03	1.43	1.47

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	66	CRO	O2-C2-CA2	-15.09	122.48	130.96
1	D	66	CRO	CA2-C2-N3	13.01	109.52	103.37
1	A	66	CRO	CA2-C2-N3	12.34	109.21	103.37
1	C	66	CRO	CA2-C2-N3	11.30	108.72	103.37
1	C	66	CRO	O2-C2-CA2	-9.85	125.43	130.96
1	B	66	CRO	O2-C2-CA2	-9.45	125.66	130.96
1	B	66	CRO	CA2-C2-N3	8.75	107.51	103.37
1	A	66	CRO	O2-C2-CA2	-7.47	126.76	130.96
1	C	66	CRO	CG2-CB2-CA2	-6.43	122.07	129.94
1	D	66	CRO	CG2-CB2-CA2	-6.38	122.12	129.94
1	B	66	CRO	CG2-CB2-CA2	-6.02	122.57	129.94
1	A	66	CRO	CG2-CB2-CA2	-5.89	122.72	129.94
1	A	66	CRO	C2-CA2-N2	-5.78	104.89	108.93
1	C	66	CRO	C2-CA2-N2	-5.28	105.23	108.93
1	D	66	CRO	C2-N3-C1	-5.22	105.32	107.97
1	D	66	CRO	C2-CA2-N2	-5.03	105.41	108.93
1	B	66	CRO	O3-C3-CA3	-4.72	112.13	126.39
1	A	66	CRO	CB2-CA2-N2	4.37	134.89	128.83
1	A	66	CRO	C1-CA1-N1	3.91	116.32	109.96
1	B	66	CRO	C2-CA2-N2	-3.77	106.29	108.93
1	D	66	CRO	CB2-CA2-N2	3.60	133.82	128.83
1	B	66	CRO	C1-CA1-N1	3.41	115.49	109.96
1	D	66	CRO	O3-C3-CA3	-3.34	116.32	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	66	CRO	CB2-CA2-N2	3.31	133.41	128.83
1	C	66	CRO	CA1-C1-N3	-3.07	121.07	124.75
1	A	66	CRO	O3-C3-CA3	-3.02	117.27	126.39
1	A	66	CRO	C2-N3-C1	-2.87	106.51	107.97
1	D	66	CRO	CG1-CB1-CA1	-2.73	105.73	112.16
1	A	66	CRO	CA3-N3-C1	2.64	130.33	127.16
1	B	66	CRO	CA2-N2-C1	2.43	107.56	105.77
1	A	66	CRO	CG1-CB1-CA1	-2.38	106.56	112.16
1	A	66	CRO	OG1-CB1-CA1	2.35	114.08	109.04
1	B	66	CRO	C2-N3-C1	-2.33	106.79	107.97
1	C	66	CRO	C1-CA1-N1	2.33	113.74	109.96
1	B	66	CRO	CA1-C1-N3	-2.32	121.96	124.75
1	A	66	CRO	CA2-N2-C1	2.31	107.48	105.77
1	D	66	CRO	CD2-CE2-CZ	2.29	122.38	119.88
1	C	66	CRO	CA1-C1-N2	2.25	127.04	123.89
1	C	66	CRO	CA2-N2-C1	2.17	107.37	105.77
1	C	66	CRO	C2-N3-C1	-2.15	106.88	107.97
1	D	66	CRO	OG1-CB1-CA1	2.06	113.45	109.04

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	66	CRO	N2-CA2-CB2-CG2
1	D	66	CRO	N2-CA2-CB2-CG2
1	C	66	CRO	C3-CA3-N3-C2
1	A	66	CRO	C1-CA1-CB1-CG1

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (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, 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	223/236 (94%)	-0.04	19 (8%)	18	16	12, 20, 56, 68	0
1	B	224/236 (94%)	-0.19	10 (4%)	39	36	11, 18, 42, 54	0
1	C	225/236 (95%)	-0.20	12 (5%)	33	30	11, 19, 41, 63	0
1	D	223/236 (94%)	-0.06	14 (6%)	27	24	11, 19, 45, 58	0
All	All	895/944 (94%)	-0.12	55 (6%)	28	26	11, 19, 47, 68	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	ILE	5.8
1	A	194	LEU	5.3
1	D	191	GLY	5.2
1	A	193	VAL	5.0
1	C	192	PRO	4.6
1	D	79	LYS	4.6
1	A	195	LEU	4.5
1	D	194	LEU	4.5
1	C	193	VAL	4.3
1	C	157	GLN	3.7
1	A	79	LYS	3.7
1	D	77	HIS	3.5
1	D	195	LEU	3.3
1	A	77	HIS	3.3
1	C	194	LEU	3.3
1	B	80	ARG	3.2
1	B	228	GLY	3.2
1	D	230	THR	3.2
1	D	157	GLN	3.1
1	B	157	GLN	3.1
1	C	231	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	155	ASP	2.9
1	A	81	HIS	2.9
1	C	156	LYS	2.8
1	A	228	GLY	2.8
1	B	156	LYS	2.7
1	D	5	GLU	2.7
1	C	191	GLY	2.7
1	C	158	LYS	2.7
1	A	74	TYR	2.6
1	D	229	ILE	2.6
1	A	192	PRO	2.6
1	A	197	ASP	2.6
1	A	78	MET	2.6
1	A	196	PRO	2.6
1	A	75	PRO	2.5
1	C	195	LEU	2.5
1	A	52	LYS	2.4
1	A	158	LYS	2.4
1	C	4	GLY	2.4
1	B	194	LEU	2.3
1	B	133	ASP	2.3
1	A	156	LYS	2.3
1	A	76	ASP	2.3
1	C	189	GLY	2.3
1	D	4	GLY	2.2
1	D	196	PRO	2.2
1	D	200	TYR	2.2
1	B	227	ASP	2.2
1	B	190	ASP	2.1
1	D	159	ASN	2.1
1	A	80	ARG	2.1
1	D	197	ASP	2.0
1	B	195	LEU	2.0
1	C	79	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, 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	B-factors(Å^2)	Q<0.9
1	CRO	A	66	22/23	0.94	0.08	17,22,24,25	0
1	CRO	C	66	22/23	0.94	0.08	17,22,24,25	0
1	CRO	D	66	22/23	0.94	0.09	17,22,24,25	0
1	CRO	B	66	22/23	0.95	0.09	17,22,24,25	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.