Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 07:53 PM EDT

PDB ID	:	2B3Q
Title	:	Crystal structure of a well-folded variant of green fluorescent protein
Authors	:	Pedelacq, J.D.; Cabantous, S.; Tran, T.H.; Terwilliger, T.C.; Waldo, G.S.
Deposited on	:	2005-09-20
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

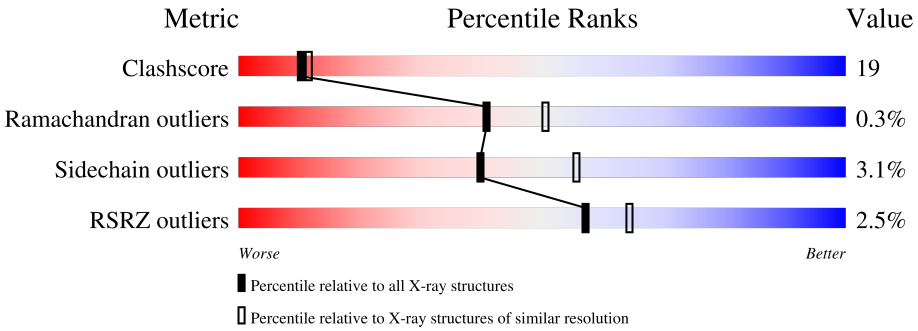
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	244	66% 25% • 7%
1	B	244	3% 59% 31% • 7%
1	C	244	5% 53% 35% • • 7%
1	D	244	2% 66% 26% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7676 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	227	Total	C	N	O	S	0	0	0
			1806	1145	309	347	5			
1	B	227	Total	C	N	O	S	0	0	0
			1792	1136	304	347	5			
1	C	227	Total	C	N	O	S	0	0	0
			1806	1144	308	349	5			
1	D	227	Total	C	N	O	S	0	0	0
			1814	1150	310	349	5			

There are 64 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	99	SER	PHE	engineered mutation	UNP P42212
A	153	THR	MET	engineered mutation	UNP P42212
A	163	ALA	VAL	engineered mutation	UNP P42212
A	239	GLY	-	expression tag	UNP P42212
A	240	SER	-	expression tag	UNP P42212
A	241	HIS	-	expression tag	UNP P42212
A	242	HIS	-	expression tag	UNP P42212
A	243	HIS	-	expression tag	UNP P42212
A	244	HIS	-	expression tag	UNP P42212
A	245	HIS	-	expression tag	UNP P42212
A	246	HIS	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	99	SER	PHE	engineered mutation	UNP P42212
B	153	THR	MET	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212
B	239	GLY	-	expression tag	UNP P42212
B	240	SER	-	expression tag	UNP P42212
B	241	HIS	-	expression tag	UNP P42212
B	242	HIS	-	expression tag	UNP P42212
B	243	HIS	-	expression tag	UNP P42212
B	244	HIS	-	expression tag	UNP P42212
B	245	HIS	-	expression tag	UNP P42212
B	246	HIS	-	expression tag	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	99	SER	PHE	engineered mutation	UNP P42212
C	153	THR	MET	engineered mutation	UNP P42212
C	163	ALA	VAL	engineered mutation	UNP P42212
C	239	GLY	-	expression tag	UNP P42212
C	240	SER	-	expression tag	UNP P42212
C	241	HIS	-	expression tag	UNP P42212
C	242	HIS	-	expression tag	UNP P42212
C	243	HIS	-	expression tag	UNP P42212
C	244	HIS	-	expression tag	UNP P42212
C	245	HIS	-	expression tag	UNP P42212
C	246	HIS	-	expression tag	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	99	SER	PHE	engineered mutation	UNP P42212
D	153	THR	MET	engineered mutation	UNP P42212
D	163	ALA	VAL	engineered mutation	UNP P42212
D	239	GLY	-	expression tag	UNP P42212
D	240	SER	-	expression tag	UNP P42212
D	241	HIS	-	expression tag	UNP P42212
D	242	HIS	-	expression tag	UNP P42212
D	243	HIS	-	expression tag	UNP P42212
D	244	HIS	-	expression tag	UNP P42212
D	245	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	246	HIS	-	expression tag	UNP P42212

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0

- Molecule 3 is water.

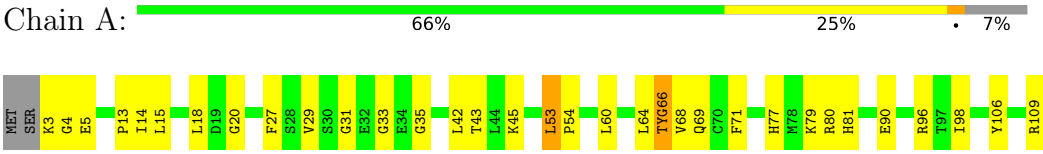
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	152	Total O 152 152	0	0
3	B	120	Total O 120 120	0	0
3	C	67	Total O 67 67	0	0
3	D	116	Total O 116 116	0	0

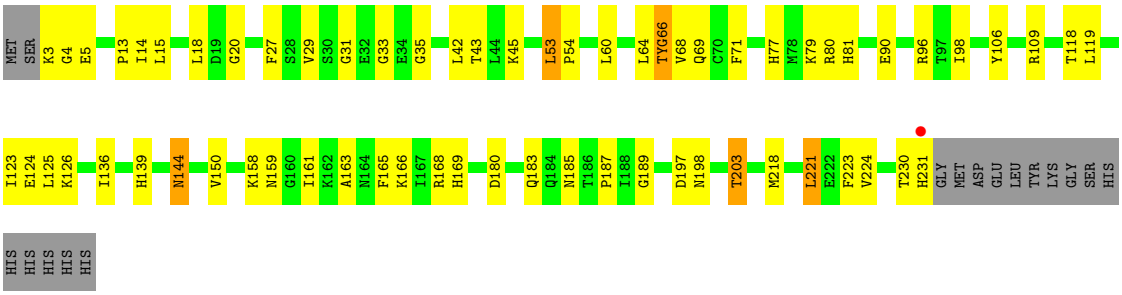
3 Residue-property plots (i)

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

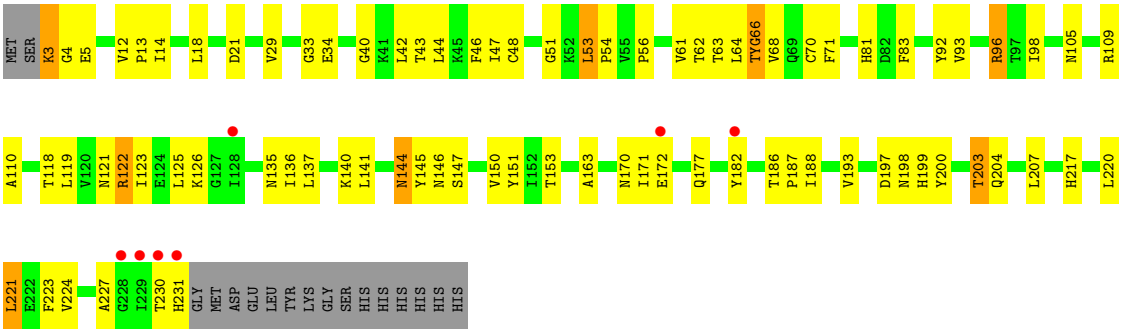
Chain A:





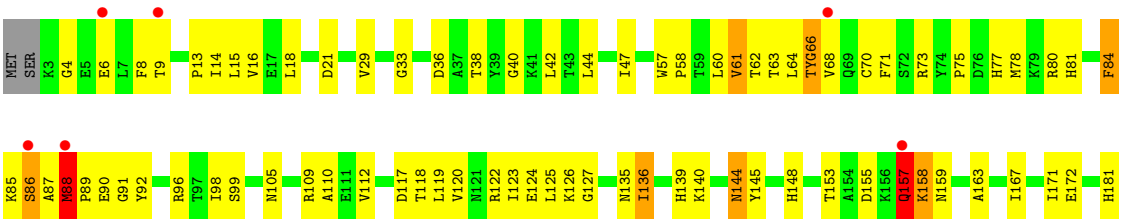
• Molecule 1: green fluorescent protein

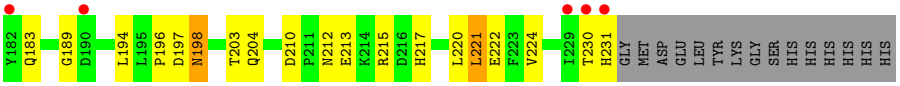
Chain B:



• Molecule 1: green fluorescent protein

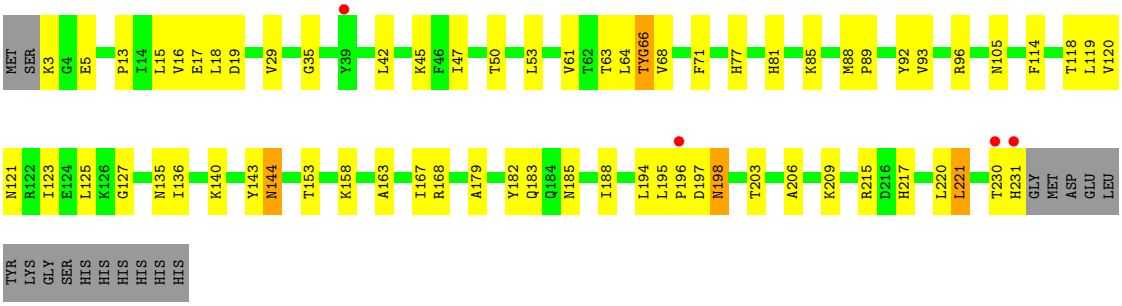
Chain C:





• Molecule 1: green fluorescent protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.41Å 87.16Å 145.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 24.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	81.8 (20.00-2.30) 80.3 (24.93-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.259 0.204 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.927	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7676	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% 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, MG

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	0.58	0/1824	0.87	4/2467 (0.2%)
1	B	0.53	1/1810 (0.1%)	0.76	2/2452 (0.1%)
1	C	0.62	3/1824 (0.2%)	0.91	10/2468 (0.4%)
1	D	0.54	0/1832	0.79	1/2476 (0.0%)
All	All	0.57	4/7290 (0.1%)	0.83	17/9863 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	D	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	92	TYR	C-N	9.12	1.55	1.34
1	C	204	GLN	C-N	-5.64	1.21	1.34
1	C	198	ASN	C-N	-5.19	1.22	1.34
1	B	40	GLY	C-N	5.02	1.45	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	88	MET	O-C-N	-13.29	95.85	121.10
1	C	84	PHE	O-C-N	-9.54	107.44	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	88	MET	CA-C-N	9.49	143.67	117.10
1	B	122	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	C	109	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	A	109	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	A	168	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	B	96	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	C	96	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	A	96	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	D	168	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	C	212	ASN	O-C-N	-6.78	111.85	122.70
1	C	84	PHE	C-N-CA	6.48	137.90	121.70
1	C	88	MET	CG-SD-CE	6.41	110.45	100.20
1	C	86	SER	O-C-N	6.38	132.91	122.70
1	A	218	MET	CG-SD-CE	6.15	110.04	100.20
1	C	84	PHE	CA-C-N	5.38	129.03	117.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	ASN	Mainchain
1	A	221	LEU	Mainchain
1	C	84	PHE	Mainchain
1	C	88	MET	Mainchain
1	D	198	ASN	Mainchain
1	D	50	THR	Mainchain

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	1806	0	1747	59	0
1	B	1792	0	1714	67	0
1	C	1806	0	1738	85	0
1	D	1814	0	1762	61	0
2	A	3	0	0	0	0
3	A	152	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	120	0	0	1	0
3	C	67	0	0	4	0
3	D	116	0	0	1	0
All	All	7676	0	6961	267	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 (267) 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:D:13:PRO:HB2	1:D:118:THR:HG22	1.41	0.97
1:D:64:LEU:C	1:D:66:CRO:H2	1.72	0.93
1:D:71:PHE:CE2	1:D:119:LEU:HD22	2.06	0.91
1:A:163:ALA:HB3	1:A:183:GLN:HB3	1.54	0.89
1:C:81:HIS:HD2	1:C:197:ASP:H	1.19	0.88
1:D:71:PHE:HE2	1:D:119:LEU:HD22	1.39	0.88
1:C:88:MET:HE1	1:C:112:VAL:HG12	1.56	0.88
1:D:153:THR:HG22	1:D:198:ASN:OD1	1.75	0.87
1:D:81:HIS:HD2	1:D:197:ASP:H	1.25	0.85
1:A:64:LEU:C	1:A:66:CRO:H2	1.79	0.85
1:C:18:LEU:HB3	1:C:29:VAL:HG22	1.62	0.81
1:D:64:LEU:C	1:D:66:CRO:N1	2.33	0.80
1:A:66:CRO:HA31	1:A:68:VAL:N	1.96	0.79
1:B:66:CRO:CA3	1:B:68:VAL:N	2.46	0.79
1:D:194:LEU:O	1:D:196:PRO:HD3	1.83	0.78
1:A:13:PRO:HB2	1:A:118:THR:HG22	1.65	0.78
1:B:66:CRO:HA31	1:B:68:VAL:N	1.96	0.78
1:C:86:SER:O	3:C:301:HOH:O	2.02	0.78
1:B:64:LEU:C	1:B:66:CRO:H2	1.88	0.78
1:D:81:HIS:CD2	1:D:197:ASP:H	2.02	0.77
1:B:71:PHE:CE2	1:B:119:LEU:HD22	2.19	0.76
1:D:163:ALA:HB3	1:D:183:GLN:HB3	1.68	0.75
1:D:66:CRO:HA31	1:D:68:VAL:N	2.03	0.74
1:B:66:CRO:C3	1:B:68:VAL:N	2.52	0.73
1:A:64:LEU:C	1:A:66:CRO:N1	2.41	0.72
1:B:146:ASN:HD21	1:B:170:ASN:ND2	1.87	0.72
1:B:71:PHE:HE2	1:B:119:LEU:HD22	1.54	0.71
1:B:47:ILE:HD13	1:B:217:HIS:HB3	1.72	0.70
1:A:166:LYS:HE2	1:A:180:ASP:OD2	1.92	0.69
1:D:66:CRO:C3	1:D:68:VAL:N	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:CRO:O3	1:B:68:VAL:N	2.26	0.69
1:D:66:CRO:CA3	1:D:68:VAL:N	2.55	0.69
1:A:66:CRO:CA3	1:A:68:VAL:N	2.56	0.68
1:D:71:PHE:HE2	1:D:119:LEU:CD2	2.07	0.68
1:C:70:CYS:O	1:C:85:LYS:HE3	1.93	0.68
1:D:47:ILE:HD13	1:D:217:HIS:HB3	1.74	0.68
1:D:81:HIS:HB3	1:D:196:PRO:HB3	1.75	0.67
1:B:203:THR:HB	1:B:224:VAL:HG22	1.75	0.67
1:A:81:HIS:HD2	1:A:197:ASP:H	1.43	0.67
1:A:159:ASN:ND2	1:A:187:PRO:HG2	2.10	0.67
1:C:215:ARG:HG3	1:C:215:ARG:HH11	1.60	0.67
1:C:66:CRO:HA31	1:C:68:VAL:N	2.10	0.66
1:B:3:LYS:HD3	1:B:5:GLU:HB2	1.78	0.66
1:B:64:LEU:C	1:B:66:CRO:N1	2.49	0.65
1:D:66:CRO:O3	1:D:68:VAL:N	2.29	0.65
1:D:42:LEU:HD11	1:D:68:VAL:HG23	1.78	0.64
1:C:4:GLY:HA3	1:C:85:LYS:O	1.97	0.64
1:C:15:LEU:HD13	1:C:16:VAL:N	2.13	0.64
1:C:64:LEU:C	1:C:66:CRO:H2	2.01	0.64
1:C:88:MET:O	1:C:89:PRO:C	2.35	0.63
1:A:230:THR:O	1:A:231:HIS:HB2	1.97	0.63
1:B:18:LEU:HB3	1:B:29:VAL:HG22	1.80	0.63
1:C:153:THR:HG22	1:C:198:ASN:OD1	1.98	0.63
1:B:53:LEU:HD23	1:B:54:PRO:HD2	1.80	0.63
1:B:135:ASN:HD22	1:B:140:LYS:HD2	1.64	0.63
1:C:81:HIS:CD2	1:C:197:ASP:H	2.10	0.62
1:C:220:LEU:HD23	1:C:221:LEU:N	2.14	0.62
1:A:81:HIS:CD2	1:A:197:ASP:HB2	2.35	0.62
1:D:77:HIS:CD2	1:D:231:HIS:HB3	2.35	0.61
1:B:153:THR:HG22	1:B:198:ASN:OD1	2.00	0.61
1:C:66:CRO:CA3	1:C:68:VAL:N	2.63	0.61
1:D:18:LEU:C	1:D:18:LEU:HD23	2.21	0.61
1:C:157:GLN:CD	1:C:157:GLN:H	2.03	0.61
1:A:64:LEU:O	1:A:66:CRO:N1	2.34	0.60
1:C:122:ARG:HG2	1:C:122:ARG:HH11	1.66	0.60
1:B:146:ASN:HD21	1:B:170:ASN:HD21	1.47	0.60
1:A:81:HIS:HD2	1:A:197:ASP:N	1.98	0.60
1:D:81:HIS:HD2	1:D:197:ASP:N	1.98	0.60
1:C:64:LEU:C	1:C:66:CRO:N1	2.55	0.60
1:B:81:HIS:HD2	1:B:197:ASP:H	1.50	0.59
1:B:171:ILE:HD11	1:B:177:GLN:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:LEU:HD11	1:D:17:GLU:HG2	1.85	0.59
1:C:90:GLU:OE1	1:C:189:GLY:HA3	2.03	0.59
1:A:144:ASN:C	1:A:144:ASN:HD22	2.06	0.59
1:D:88:MET:HE2	1:D:89:PRO:HA	1.84	0.59
1:C:42:LEU:HD21	1:C:71:PHE:CG	2.38	0.58
1:A:90:GLU:OE1	1:A:189:GLY:HA3	2.04	0.58
1:B:47:ILE:HD13	1:B:217:HIS:CB	2.33	0.58
1:D:135:ASN:HD22	1:D:140:LYS:HD2	1.69	0.58
1:D:121:ASN:ND2	1:D:123:ILE:HD11	2.18	0.57
1:B:18:LEU:C	1:B:18:LEU:HD23	2.24	0.57
1:C:230:THR:O	1:C:231:HIS:HB2	2.03	0.57
1:A:163:ALA:HB3	1:A:183:GLN:CB	2.33	0.57
1:A:203:THR:HB	1:A:224:VAL:HG22	1.84	0.56
1:C:6:GLU:O	1:C:9:THR:HG23	2.05	0.56
1:C:77:HIS:CD2	1:C:231:HIS:HB3	2.40	0.56
1:C:81:HIS:HB3	1:C:196:PRO:HB3	1.87	0.56
1:D:144:ASN:C	1:D:144:ASN:HD22	2.08	0.56
1:B:46:PHE:O	1:B:217:HIS:HB2	2.06	0.56
1:A:81:HIS:CD2	1:A:197:ASP:H	2.22	0.56
1:A:169:HIS:HD2	3:A:713:HOH:O	1.89	0.55
1:C:135:ASN:HD22	1:C:140:LYS:HD2	1.72	0.55
1:C:8:PHE:CZ	1:C:88:MET:HG3	2.42	0.55
1:D:42:LEU:HD11	1:D:68:VAL:CG2	2.36	0.55
1:D:125:LEU:C	1:D:125:LEU:HD23	2.27	0.55
1:C:18:LEU:HD13	1:C:123:ILE:HB	1.87	0.55
1:C:148:HIS:CD2	1:C:167:ILE:HA	2.42	0.55
1:D:220:LEU:C	1:D:220:LEU:HD23	2.27	0.55
1:C:125:LEU:C	1:C:125:LEU:HD23	2.27	0.54
1:A:18:LEU:C	1:A:18:LEU:HD23	2.28	0.54
1:A:125:LEU:C	1:A:125:LEU:HD23	2.28	0.54
1:D:230:THR:O	1:D:231:HIS:HB2	2.07	0.54
1:D:15:LEU:CD1	1:D:17:GLU:HG2	2.38	0.54
1:A:69:GLN:HA	3:A:751:HOH:O	2.06	0.54
1:C:8:PHE:CE2	1:C:88:MET:HG3	2.43	0.53
1:D:81:HIS:O	1:D:196:PRO:HB3	2.09	0.53
1:C:163:ALA:HB3	1:C:183:GLN:HB3	1.91	0.53
1:D:47:ILE:HG21	1:D:215:ARG:HE	1.73	0.53
1:B:144:ASN:HD22	1:B:144:ASN:C	2.12	0.53
1:D:81:HIS:O	1:D:196:PRO:HG3	2.08	0.53
1:D:167:ILE:HB	1:D:179:ALA:HB3	1.89	0.53
1:B:136:ILE:N	1:B:136:ILE:HD12	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ASP:OD1	1:C:38:THR:HB	2.08	0.52
1:C:86:SER:OG	1:C:87:ALA:N	2.42	0.52
1:C:136:ILE:HD12	1:C:136:ILE:N	2.24	0.52
1:A:98:ILE:HB	1:A:106:TYR:HB2	1.91	0.52
1:C:29:VAL:HG21	1:C:64:LEU:HD21	1.92	0.52
1:C:91:GLY:HA3	1:C:112:VAL:O	2.09	0.52
1:A:14:ILE:CD1	1:A:42:LEU:HD22	2.40	0.52
1:B:48:CYS:SG	1:B:51:GLY:O	2.66	0.52
1:A:118:THR:HG21	3:C:260:HOH:O	2.10	0.52
1:B:92:TYR:HA	1:B:188:ILE:HG13	1.92	0.51
1:C:80:ARG:O	1:C:194:LEU:HD13	2.11	0.51
1:A:53:LEU:HD11	1:A:60:LEU:HD12	1.93	0.51
1:B:140:LYS:O	1:B:172:GLU:HG2	2.10	0.51
1:A:203:THR:HG21	3:A:744:HOH:O	2.11	0.51
1:A:31:GLY:HA2	1:A:45:LYS:O	2.11	0.50
1:A:77:HIS:CD2	1:A:231:HIS:HB3	2.46	0.50
1:C:88:MET:CE	1:C:112:VAL:HG12	2.34	0.50
1:C:98:ILE:HG12	1:C:181:HIS:CD2	2.46	0.50
1:B:110:ALA:HB2	1:B:123:ILE:HG23	1.94	0.50
1:C:125:LEU:HD23	1:C:126:LYS:N	2.26	0.50
1:C:122:ARG:HG2	1:C:122:ARG:NH1	2.25	0.50
1:A:3:LYS:HD3	1:A:4:GLY:N	2.27	0.50
1:A:66:CRO:C3	1:A:68:VAL:N	2.75	0.49
1:C:123:ILE:HG22	1:C:124:GLU:N	2.27	0.49
1:B:121:ASN:ND2	1:B:123:ILE:HD11	2.26	0.49
1:A:71:PHE:CE2	1:A:119:LEU:HD22	2.47	0.49
1:A:125:LEU:HD23	1:A:126:LYS:N	2.27	0.49
1:B:33:GLY:HA3	1:B:44:LEU:HD23	1.93	0.49
1:C:215:ARG:HG3	1:C:215:ARG:NH1	2.26	0.49
1:A:118:THR:HG21	1:C:215:ARG:NH1	2.28	0.49
1:C:210:ASP:HB3	1:C:213:GLU:HB3	1.95	0.49
1:C:88:MET:CE	1:C:119:LEU:HD11	2.43	0.49
1:B:81:HIS:CD2	1:B:197:ASP:H	2.29	0.49
1:C:15:LEU:HB3	1:C:120:VAL:HG22	1.94	0.49
1:D:18:LEU:HD23	1:D:19:ASP:N	2.27	0.49
1:A:42:LEU:HD21	1:A:71:PHE:CG	2.48	0.48
1:A:203:THR:HG22	1:A:224:VAL:HG13	1.95	0.48
1:B:98:ILE:O	1:B:105:ASN:HA	2.14	0.48
1:A:221:LEU:CD2	1:D:221:LEU:HD13	2.43	0.48
1:B:3:LYS:HE2	1:B:4:GLY:N	2.28	0.48
1:B:135:ASN:ND2	1:B:140:LYS:HD2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LYS:O	1:C:159:ASN:HB3	2.14	0.48
1:D:15:LEU:HB3	1:D:120:VAL:HG22	1.95	0.48
1:B:207:LEU:CD2	1:B:220:LEU:HD12	2.43	0.48
1:D:88:MET:HE2	1:D:114:PHE:HD1	1.77	0.48
1:D:93:VAL:O	1:D:185:ASN:HA	2.13	0.48
1:D:64:LEU:CA	1:D:66:CRO:H2	2.27	0.47
1:B:14:ILE:CD1	1:B:42:LEU:HD22	2.45	0.47
1:B:64:LEU:O	1:B:66:CRO:N1	2.47	0.47
1:B:230:THR:O	1:B:231:HIS:HB2	2.14	0.47
1:B:42:LEU:HD11	1:B:68:VAL:HG23	1.96	0.47
1:B:83:PHE:HE1	1:B:193:VAL:HG21	1.80	0.47
1:A:123:ILE:HG22	1:A:124:GLU:N	2.29	0.47
1:C:42:LEU:HD11	1:C:68:VAL:HG23	1.96	0.47
1:C:220:LEU:HD23	1:C:220:LEU:C	2.34	0.47
1:B:151:TYR:O	1:B:163:ALA:HA	2.15	0.47
1:A:159:ASN:CG	1:A:159:ASN:O	2.53	0.47
1:D:45:LYS:HE2	1:D:47:ILE:HD11	1.97	0.47
1:C:171:ILE:HG22	1:C:172:GLU:N	2.30	0.47
1:B:46:PHE:CD1	1:B:64:LEU:HD13	2.50	0.46
1:C:33:GLY:HA3	1:C:44:LEU:HD23	1.96	0.46
1:D:63:THR:CG2	1:D:123:ILE:HG21	2.45	0.46
1:A:118:THR:HG21	1:C:215:ARG:HH11	1.80	0.46
1:C:73:ARG:HG2	1:C:73:ARG:HH21	1.80	0.46
1:C:57:TRP:N	1:C:58:PRO:CD	2.78	0.46
1:C:71:PHE:CE2	1:C:119:LEU:HD22	2.50	0.46
1:B:231:HIS:O	1:B:231:HIS:ND1	2.49	0.46
1:B:171:ILE:HG22	1:B:172:GLU:N	2.31	0.46
1:B:62:THR:HG23	1:B:145:TYR:OH	2.16	0.46
1:C:62:THR:HG23	1:C:145:TYR:OH	2.16	0.46
1:C:42:LEU:HD12	1:C:222:GLU:OE2	2.15	0.46
1:C:157:GLN:CD	1:C:157:GLN:N	2.69	0.45
1:B:125:LEU:HD23	1:B:125:LEU:C	2.37	0.45
1:C:75:PRO:HD2	1:C:78:MET:CG	2.46	0.45
1:C:13:PRO:HB2	1:C:118:THR:HG22	1.98	0.45
1:D:35:GLY:CA	1:D:42:LEU:HD23	2.45	0.45
1:B:21:ASP:C	1:B:21:ASP:OD2	2.55	0.45
1:C:144:ASN:C	1:C:144:ASN:HD22	2.19	0.45
1:D:81:HIS:CB	1:D:196:PRO:HB3	2.44	0.45
1:D:15:LEU:HD13	1:D:16:VAL:N	2.32	0.45
1:B:68:VAL:C	1:B:70:CYS:H	2.20	0.45
1:B:221:LEU:HD21	1:B:223:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD11	1:A:68:VAL:HG23	1.99	0.44
1:B:199:HIS:HB2	1:B:227:ALA:O	2.17	0.44
1:D:47:ILE:HD13	1:D:217:HIS:CB	2.44	0.44
1:A:223:PHE:HD2	1:D:206:ALA:HB1	1.83	0.44
1:C:194:LEU:O	1:C:196:PRO:HD3	2.18	0.44
1:A:81:HIS:NE2	1:A:197:ASP:HB2	2.33	0.44
1:D:92:TYR:HA	1:D:188:ILE:HG13	1.99	0.44
1:B:93:VAL:HG11	1:B:109:ARG:NH1	2.33	0.44
1:D:81:HIS:CD2	1:D:197:ASP:HB2	2.53	0.44
1:B:96:ARG:HA	1:B:182:TYR:O	2.18	0.43
1:A:33:GLY:HA3	1:A:43:THR:O	2.18	0.43
1:A:221:LEU:HD22	1:D:221:LEU:HD13	2.00	0.43
1:C:105:ASN:O	1:C:127:GLY:HA2	2.17	0.43
1:A:161:ILE:HG12	1:A:185:ASN:HB2	2.00	0.43
1:B:56:PRO:HD3	1:B:136:ILE:O	2.19	0.43
1:D:143:TYR:CZ	1:D:209:LYS:HE2	2.54	0.43
1:B:122:ARG:HG2	1:B:122:ARG:HH11	1.84	0.43
1:C:42:LEU:HD21	1:C:71:PHE:CB	2.49	0.43
1:B:186:THR:HG23	1:B:187:PRO:HD2	2.00	0.43
1:C:61:VAL:O	1:C:66:CRO:N1	2.51	0.43
1:A:136:ILE:HD12	1:A:136:ILE:H	1.84	0.43
1:C:68:VAL:HG23	1:C:68:VAL:O	2.19	0.43
1:C:155:ASP:OD2	1:C:158:LYS:HB2	2.19	0.43
1:A:136:ILE:HD12	1:A:136:ILE:N	2.34	0.43
1:C:14:ILE:HD11	1:C:42:LEU:HD22	2.01	0.43
1:C:47:ILE:HD13	1:C:217:HIS:HB3	2.00	0.43
1:C:63:THR:CG2	1:C:123:ILE:HG21	2.49	0.43
1:D:3:LYS:HB3	1:D:5:GLU:HB3	2.00	0.42
1:B:147:SER:OG	1:B:204:GLN:HG2	2.19	0.42
1:C:40:GLY:HA2	1:C:71:PHE:O	2.19	0.42
1:D:68:VAL:HG23	1:D:68:VAL:O	2.19	0.42
1:A:80:ARG:HG3	1:A:80:ARG:HH11	1.85	0.42
1:C:13:PRO:HB2	1:C:118:THR:CG2	2.50	0.42
1:B:150:VAL:O	1:B:200:TYR:HA	2.19	0.42
1:D:61:VAL:O	1:D:66:CRO:N1	2.53	0.42
1:C:66:CRO:C3	1:C:68:VAL:N	2.83	0.42
1:D:85:LYS:NZ	3:D:263:HOH:O	2.52	0.42
1:D:136:ILE:N	1:D:136:ILE:HD12	2.34	0.42
1:A:150:VAL:HG13	1:A:165:PHE:CD1	2.55	0.42
1:B:12:VAL:HA	1:B:13:PRO:HD3	1.89	0.42
1:B:93:VAL:HG11	1:B:109:ARG:HH12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:THR:CG2	1:C:231:HIS:N	2.84	0.41
1:A:35:GLY:HA3	1:A:42:LEU:HD23	2.02	0.41
1:B:61:VAL:O	1:B:66:CRO:N1	2.52	0.41
1:D:35:GLY:HA2	1:D:42:LEU:HD23	2.01	0.41
1:A:5:GLU:OE1	1:A:79:LYS:HD3	2.20	0.41
1:C:110:ALA:HA	1:C:122:ARG:O	2.21	0.41
1:C:203:THR:HG22	1:C:224:VAL:HG22	2.02	0.41
1:D:96:ARG:HA	1:D:182:TYR:O	2.20	0.41
1:A:54:PRO:O	1:A:139:HIS:HE1	2.03	0.41
1:A:139:HIS:HD2	3:A:841:HOH:O	2.03	0.41
1:B:34:GLU:HB3	3:B:345:HOH:O	2.21	0.41
1:A:144:ASN:C	1:A:144:ASN:ND2	2.74	0.41
1:A:20:GLY:HA3	1:A:27:PHE:CZ	2.56	0.41
1:A:42:LEU:HD21	1:A:71:PHE:CD2	2.56	0.41
1:C:99:SER:HB3	3:C:276:HOH:O	2.21	0.41
1:C:139:HIS:HD2	3:C:297:HOH:O	2.04	0.41
1:C:90:GLU:OE1	1:C:189:GLY:CA	2.69	0.41
1:C:123:ILE:HD12	1:C:123:ILE:N	2.36	0.41
1:C:230:THR:HG22	1:C:231:HIS:N	2.36	0.40
1:B:63:THR:HG22	1:B:123:ILE:HD13	2.03	0.40
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.94	0.40
1:D:105:ASN:O	1:D:127:GLY:HA2	2.22	0.40
1:A:90:GLU:CD	1:A:189:GLY:HA3	2.41	0.40
1:B:3:LYS:HD3	1:B:5:GLU:CB	2.48	0.40
1:C:13:PRO:HD2	1:C:117:ASP:O	2.21	0.40
1:C:60:LEU:O	1:C:61:VAL:C	2.59	0.40
1:D:81:HIS:CA	1:D:196:PRO:HB3	2.51	0.40
1:A:230:THR:O	1:A:231:HIS:CB	2.66	0.40
1:B:125:LEU:HD23	1:B:126:LYS:N	2.37	0.40
1:B:141:LEU:HD12	1:B:141:LEU:N	2.36	0.40
1:B:33:GLY:HA3	1:B:43:THR:O	2.20	0.40
1:C:21:ASP:O	1:C:126:LYS:HA	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	222/244 (91%)	217 (98%)	5 (2%)	0	100 100
1	B	222/244 (91%)	205 (92%)	17 (8%)	0	100 100
1	C	222/244 (91%)	205 (92%)	14 (6%)	3 (1%)	11 11
1	D	222/244 (91%)	217 (98%)	5 (2%)	0	100 100
All	All	888/976 (91%)	844 (95%)	41 (5%)	3 (0%)	41 50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	157	GLN
1	C	136	ILE
1	C	61	VAL

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	195/212 (92%)	189 (97%)	6 (3%)	40 55
1	B	192/212 (91%)	186 (97%)	6 (3%)	40 55
1	C	195/212 (92%)	190 (97%)	5 (3%)	46 63
1	D	197/212 (93%)	190 (96%)	7 (4%)	35 49
All	All	779/848 (92%)	755 (97%)	24 (3%)	40 55

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	29	VAL
1	A	53	LEU

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Mol	Chain	Res	Type
1	A	144	ASN
1	A	158	LYS
1	A	203	THR
1	B	3	LYS
1	B	53	LEU
1	B	118	THR
1	B	144	ASN
1	B	203	THR
1	B	221	LEU
1	C	88	MET
1	C	144	ASN
1	C	157	GLN
1	C	158	LYS
1	C	221	LEU
1	D	29	VAL
1	D	53	LEU
1	D	144	ASN
1	D	158	LYS
1	D	195	LEU
1	D	203	THR
1	D	221	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	135	ASN
1	A	139	HIS
1	A	144	ASN
1	A	149	ASN
1	A	157	GLN
1	A	159	ASN
1	A	169	HIS
1	B	81	HIS
1	B	135	ASN
1	B	144	ASN
1	B	149	ASN
1	B	157	GLN
1	B	170	ASN
1	C	81	HIS
1	C	135	ASN
1	C	139	HIS

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Mol	Chain	Res	Type
1	C	144	ASN
1	C	149	ASN
1	C	169	HIS
1	D	81	HIS
1	D	135	ASN
1	D	139	HIS
1	D	144	ASN
1	D	149	ASN
1	D	169	HIS
1	D	212	ASN

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	A	66	-	23,23,24	2.81	8 (34%)	30,32,34	2.13	12 (40%)
1	CRO	D	66	-	23,23,24	2.67	8 (34%)	30,32,34	1.91	10 (33%)
1	CRO	C	66	-	23,23,24	2.76	9 (39%)	30,32,34	2.11	11 (36%)
1	CRO	B	66	-	23,23,24	2.86	8 (34%)	30,32,34	2.09	11 (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	CRO	A	66	-	-	2/12/31/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRO	D	66	-	-	2/12/31/32	0/2/2/2
1	CRO	C	66	-	-	2/12/31/32	0/2/2/2
1	CRO	B	66	-	-	2/12/31/32	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRO	CB2-CA2	6.44	1.40	1.35
1	B	66	CRO	CE1-CZ	6.37	1.51	1.38
1	C	66	CRO	CB2-CA2	6.17	1.40	1.35
1	A	66	CRO	CB2-CA2	6.04	1.40	1.35
1	C	66	CRO	CE1-CZ	5.92	1.50	1.38
1	A	66	CRO	CE1-CZ	5.90	1.50	1.38
1	D	66	CRO	CE1-CZ	5.73	1.49	1.38
1	A	66	CRO	CE2-CZ	5.33	1.49	1.38
1	B	66	CRO	CE2-CZ	5.17	1.48	1.38
1	D	66	CRO	CE2-CZ	5.14	1.48	1.38
1	C	66	CRO	CE2-CZ	4.89	1.48	1.38
1	D	66	CRO	OH-CZ	-4.70	1.26	1.37
1	A	66	CRO	CD1-CG2	4.69	1.48	1.39
1	B	66	CRO	CD1-CG2	4.65	1.48	1.39
1	D	66	CRO	CB2-CA2	4.61	1.39	1.35
1	C	66	CRO	CD1-CG2	4.54	1.48	1.39
1	B	66	CRO	OH-CZ	-4.35	1.26	1.37
1	D	66	CRO	CD1-CG2	4.30	1.47	1.39
1	A	66	CRO	OH-CZ	-4.18	1.27	1.37
1	C	66	CRO	OH-CZ	-4.11	1.27	1.37
1	A	66	CRO	CD2-CG2	4.08	1.47	1.39
1	B	66	CRO	CD2-CG2	4.06	1.47	1.39
1	D	66	CRO	CD2-CG2	3.64	1.46	1.39
1	C	66	CRO	CD2-CG2	3.53	1.46	1.39
1	D	66	CRO	C1-N3	3.02	1.42	1.37
1	C	66	CRO	C1-N3	3.01	1.42	1.37
1	B	66	CRO	C1-N3	2.61	1.41	1.37
1	C	66	CRO	CG2-CB2	-2.53	1.42	1.46
1	A	66	CRO	C1-N3	2.38	1.41	1.37
1	D	66	CRO	CG2-CB2	-2.23	1.42	1.46
1	B	66	CRO	CG2-CB2	-2.06	1.42	1.46
1	A	66	CRO	CA3-N3	-2.02	1.43	1.47
1	C	66	CRO	C2-N3	2.01	1.44	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	66	CRO	C2-N3-C1	-5.52	105.17	107.97
1	B	66	CRO	C2-N3-C1	-5.19	105.34	107.97
1	A	66	CRO	C2-N3-C1	-5.08	105.39	107.97
1	A	66	CRO	N3-C1-N2	4.68	114.70	111.45
1	D	66	CRO	C2-N3-C1	-4.63	105.62	107.97
1	D	66	CRO	N3-C1-N2	4.28	114.42	111.45
1	B	66	CRO	N3-C1-N2	4.23	114.38	111.45
1	C	66	CRO	N3-C1-N2	4.08	114.28	111.45
1	B	66	CRO	CA1-C1-N3	-3.99	119.96	124.75
1	A	66	CRO	CA1-C1-N3	-3.84	120.14	124.75
1	A	66	CRO	CA3-N3-C1	-3.43	123.05	127.16
1	A	66	CRO	CA3-N3-C2	3.38	131.55	123.80
1	C	66	CRO	CA2-C2-N3	3.26	104.91	103.37
1	C	66	CRO	CA1-C1-N3	-3.21	120.89	124.75
1	B	66	CRO	CA3-N3-C2	3.14	131.01	123.80
1	D	66	CRO	CA1-C1-N3	-3.13	120.99	124.75
1	C	66	CRO	O2-C2-CA2	-3.02	129.26	130.96
1	C	66	CRO	CA3-N3-C2	2.99	130.65	123.80
1	C	66	CRO	CE2-CZ-CE1	-2.93	114.82	119.77
1	B	66	CRO	CA3-N3-C1	-2.93	123.65	127.16
1	D	66	CRO	CA3-N3-C2	2.88	130.39	123.80
1	A	66	CRO	CE2-CZ-CE1	-2.82	115.02	119.77
1	D	66	CRO	CE2-CZ-CE1	-2.79	115.06	119.77
1	B	66	CRO	CE2-CZ-CE1	-2.76	115.12	119.77
1	B	66	CRO	CG2-CB2-CA2	2.76	133.32	129.94
1	B	66	CRO	CA2-C2-N3	2.67	104.64	103.37
1	D	66	CRO	CA3-N3-C1	-2.65	123.98	127.16
1	C	66	CRO	CG2-CB2-CA2	2.55	133.07	129.94
1	C	66	CRO	CD2-CE2-CZ	2.54	122.67	119.88
1	C	66	CRO	CA3-N3-C1	-2.49	124.17	127.16
1	D	66	CRO	CD2-CE2-CZ	2.42	122.52	119.88
1	A	66	CRO	CD2-CE2-CZ	2.39	122.49	119.88
1	D	66	CRO	O3-C3-CA3	-2.30	119.44	126.39
1	B	66	CRO	O3-C3-CA3	-2.29	119.46	126.39
1	C	66	CRO	O3-C3-CA3	-2.29	119.47	126.39
1	A	66	CRO	O3-C3-CA3	-2.28	119.50	126.39
1	B	66	CRO	CD2-CE2-CZ	2.25	122.34	119.88
1	A	66	CRO	CA2-C2-N3	2.20	104.41	103.37
1	A	66	CRO	CG2-CB2-CA2	2.18	132.62	129.94
1	B	66	CRO	O2-C2-CA2	-2.15	129.75	130.96
1	A	66	CRO	O2-C2-CA2	-2.12	129.77	130.96
1	D	66	CRO	C1-CA1-N1	-2.10	106.56	109.96
1	A	66	CRO	C1-CA1-N1	-2.05	106.64	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	66	CRO	O2-C2-CA2	-2.01	129.83	130.96

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	C3-CA3-N3-C1
1	A	66	CRO	C3-CA3-N3-C2
1	B	66	CRO	C3-CA3-N3-C1
1	B	66	CRO	C3-CA3-N3-C2
1	C	66	CRO	C3-CA3-N3-C1
1	C	66	CRO	C3-CA3-N3-C2
1	D	66	CRO	C3-CA3-N3-C1
1	D	66	CRO	C3-CA3-N3-C2

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRO	6	0
1	D	66	CRO	8	0
1	C	66	CRO	6	0
1	B	66	CRO	8	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	A	2
1	D	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	66:CRO	C3	68:VAL	N	2.83
1	A	66:CRO	C3	68:VAL	N	2.75
1	C	64:LEU	C	66:CRO	N1	2.55
1	D	66:CRO	C3	68:VAL	N	2.55
1	B	66:CRO	C3	68:VAL	N	2.52
1	B	64:LEU	C	66:CRO	N1	2.49
1	A	64:LEU	C	66:CRO	N1	2.41
1	D	64:LEU	C	66:CRO	N1	2.33

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	226/244 (92%)	-0.39	1 (0%)	92	95	12, 22, 35, 65	0
1	B	226/244 (92%)	-0.02	7 (3%)	49	56	13, 32, 52, 68	0
1	C	226/244 (92%)	0.23	11 (4%)	29	36	20, 36, 56, 75	0
1	D	226/244 (92%)	-0.29	4 (1%)	68	74	13, 24, 39, 58	0
All	All	904/976 (92%)	-0.12	23 (2%)	57	64	12, 28, 50, 75	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	231	HIS	4.2
1	B	231	HIS	4.2
1	C	230	THR	4.2
1	C	6	GLU	3.6
1	B	128	ILE	3.5
1	D	231	HIS	3.4
1	A	231	HIS	3.2
1	C	88	MET	2.9
1	C	68	VAL	2.8
1	C	190	ASP	2.7
1	C	157	GLN	2.6
1	B	172	GLU	2.6
1	C	182	TYR	2.5
1	C	9	THR	2.3
1	D	39	TYR	2.3
1	B	228	GLY	2.3
1	B	182	TYR	2.3
1	B	230	THR	2.2
1	D	230	THR	2.2
1	C	229	ILE	2.1
1	B	229	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	196	PRO	2.1
1	C	86	SER	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	C	66	22/23	0.94	0.20	16,23,29,30	0
1	CRO	B	66	22/23	0.95	0.20	18,22,24,26	0
1	CRO	A	66	22/23	0.96	0.19	13,14,16,23	0
1	CRO	D	66	22/23	0.96	0.17	11,14,16,22	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 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
2	MG	A	701	1/1	0.91	0.13	49,49,49,49	0
2	MG	A	703	1/1	0.91	0.08	45,45,45,45	0
2	MG	A	702	1/1	1.00	0.15	8,8,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.