Full wwPDB X-ray Structure Validation Report (i)

Nov 26, 2024 – 02:13 PM JST

PDB ID	:	8JLL
Title	:	Crystal structure of the Green fluorescent protein SEA227D variant at pH 9.5
Authors	:	Shin, S.C.
Deposited on	:	2023-06-02
Resolution	:	2.69 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:

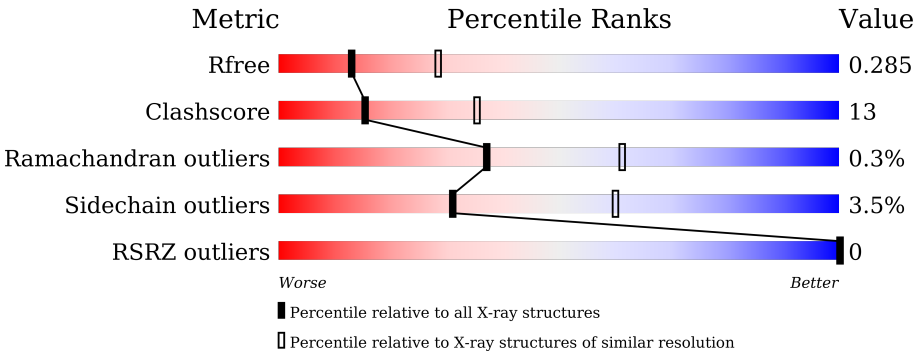
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.69 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	65% 27% • 6%
1	B	236	67% 24% •• 6%
1	C	236	68% 24% • 6%
1	D	236	60% 32% • 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7192 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	223	Total	C	N	O	S	0	0	0
			1798	1146	302	344	6			
1	B	223	Total	C	N	O	S	0	0	0
			1798	1146	302	344	6			
1	C	223	Total	C	N	O	S	0	0	0
			1798	1146	302	344	6			
1	D	223	Total	C	N	O	S	0	0	0
			1798	1146	302	344	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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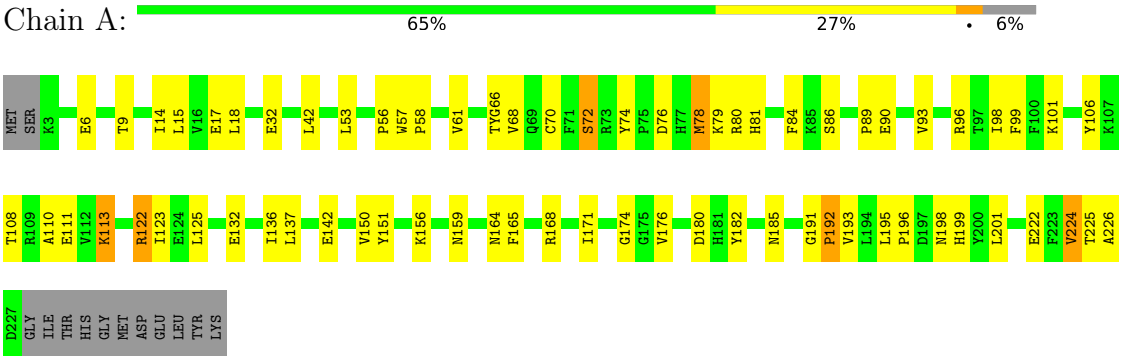
Chain	Residue	Modelled	Actual	Comment	Reference
B	175	GLY	SER	engineered mutation	UNP P42212
B	202	PHE	SER	engineered mutation	UNP P42212
B	204	THR	GLN	engineered mutation	UNP P42212
B	206	THR	ALA	engineered mutation	UNP P42212
B	227	ASP	ALA	engineered mutation	UNP P42212
C	64	LEU	PHE	engineered mutation	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

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.

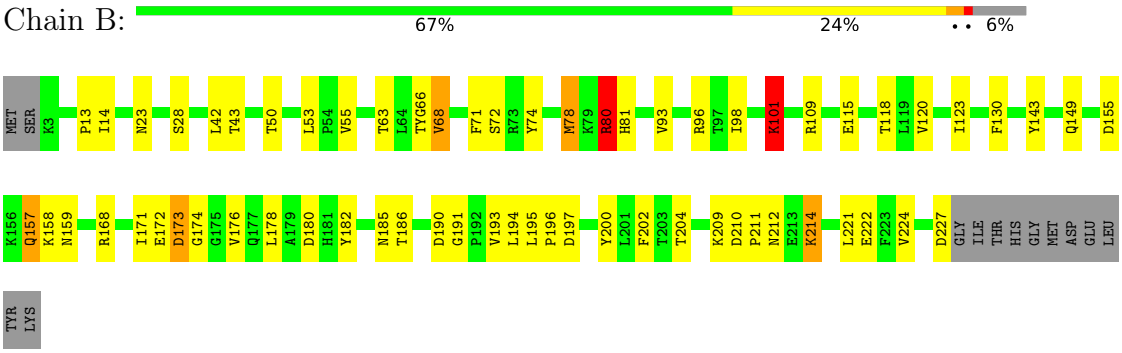
• Molecule 1: Green fluorescent protein

Chain A:



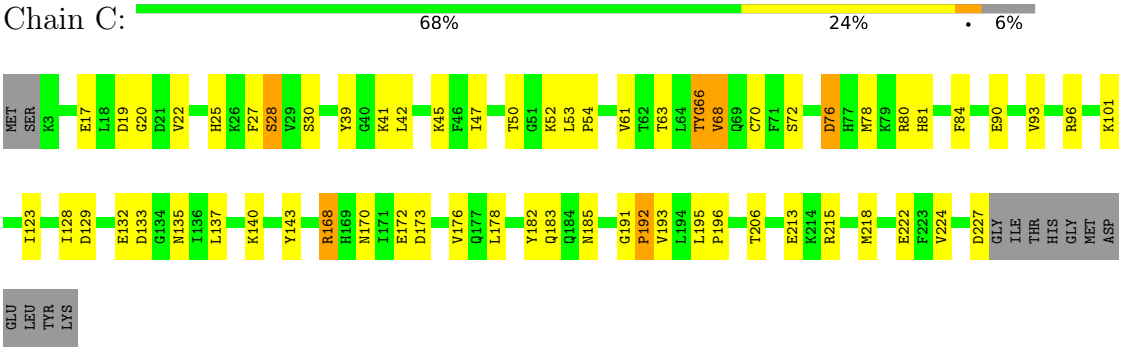
• Molecule 1: Green fluorescent protein

Chain B:



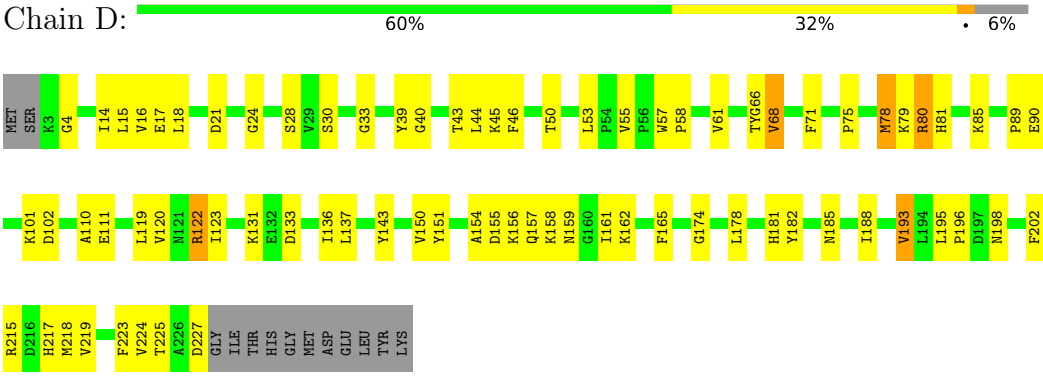
• Molecule 1: Green fluorescent protein

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	76.21Å 80.96Å 179.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.19 – 2.69 48.19 – 2.69	Depositor EDS
% Data completeness (in resolution range)	94.9 (48.19-2.69) 81.0 (48.19-2.69)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.201 , 0.282 0.204 , 0.285	Depositor DCC
R_{free} test set	27925 reflections (6.64%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 16.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7192	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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 (i)

5.1 Standard geometry (i)

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	0.56	3/1817 (0.2%)	0.83	3/2455 (0.1%)
1	B	0.56	1/1817 (0.1%)	0.77	3/2455 (0.1%)
1	C	0.55	1/1817 (0.1%)	0.73	1/2455 (0.0%)
1	D	0.54	1/1817 (0.1%)	0.80	4/2455 (0.2%)
All	All	0.55	6/7268 (0.1%)	0.78	11/9820 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ARG	CG-CD	-7.26	1.33	1.51
1	A	68	VAL	N-CA	-6.74	1.32	1.46
1	D	68	VAL	N-CA	-6.57	1.33	1.46
1	C	68	VAL	N-CA	-6.18	1.33	1.46
1	A	122	ARG	CB-CG	-5.74	1.37	1.52
1	B	68	VAL	N-CA	-5.58	1.35	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	80	ARG	N-CA-CB	-14.56	84.39	110.60
1	D	80	ARG	N-CA-CB	-12.01	88.98	110.60
1	D	193	VAL	N-CA-CB	-11.76	85.63	111.50
1	A	78	MET	CB-CA-C	-11.65	87.09	110.40
1	B	193	VAL	N-CA-CB	-10.04	89.42	111.50
1	C	19	ASP	CB-CG-OD1	-8.59	110.57	118.30
1	B	80	ARG	N-CA-C	-8.01	89.39	111.00
1	A	80	ARG	N-CA-C	7.12	130.22	111.00
1	D	80	ARG	N-CA-C	7.08	130.12	111.00
1	B	101	LYS	CD-CE-NZ	6.86	127.47	111.70
1	D	78	MET	CB-CA-C	-6.03	98.34	110.40

There are no chirality outliers.

There are no planarity outliers.

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	1798	0	1730	42	0
1	B	1798	0	1730	46	0
1	C	1798	0	1730	50	0
1	D	1798	0	1730	58	0
All	All	7192	0	6920	187	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 13.

All (187) 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:174:GLY:HA2	1:B:173:ASP:HA	1.42	0.98
1:B:168:ARG:HG2	1:B:176:VAL:HG11	1.48	0.96
1:A:72:SER:HB2	1:A:224:VAL:HG22	1.51	0.90
1:C:173:ASP:HA	1:D:174:GLY:HA2	1.56	0.87
1:B:72:SER:HA	1:B:224:VAL:HG13	1.63	0.81
1:C:45:LYS:HE2	1:C:47:ILE:HD11	1.64	0.80
1:D:18:LEU:HD12	1:D:123:ILE:HB	1.65	0.78
1:D:78:MET:HG2	1:D:81:HIS:HD2	1.46	0.78
1:B:159:ASN:ND2	1:B:195:LEU:HD11	2.00	0.75
1:B:158:LYS:O	1:B:186:THR:HG22	1.88	0.74
1:C:101:LYS:HE3	1:C:178:LEU:HD12	1.69	0.73
1:B:168:ARG:HG2	1:B:176:VAL:CG1	2.18	0.73
1:D:45:LYS:NZ	1:D:213:GLU:OE1	2.21	0.72
1:B:214:LYS:HD3	1:B:214:LYS:H	1.56	0.71
1:C:213:GLU:OE2	1:C:215:ARG:HG3	1.90	0.70
1:D:213:GLU:OE2	1:D:215:ARG:HD3	1.90	0.70
1:D:28:SER:OG	1:D:50:THR:HG23	1.91	0.70
1:C:173:ASP:HA	1:D:174:GLY:CA	2.22	0.69
1:B:214:LYS:H	1:B:214:LYS:CD	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:THR:HG22	1:B:221:LEU:HD12	1.75	0.67
1:A:174:GLY:CA	1:B:173:ASP:HA	2.22	0.66
1:C:191:GLY:C	1:C:192:PRO:O	2.30	0.66
1:A:81:HIS:O	1:A:196:PRO:HB3	1.95	0.66
1:C:42:LEU:HB2	1:C:222:GLU:HB3	1.79	0.65
1:D:159:ASN:O	1:D:195:LEU:HD11	1.97	0.64
1:C:72:SER:HA	1:C:224:VAL:HG13	1.79	0.63
1:B:42:LEU:HD12	1:B:222:GLU:HB3	1.81	0.62
1:B:202:PHE:HE2	1:B:227:ASP:HB3	1.63	0.61
1:A:6:GLU:O	1:A:9:THR:HG23	2.01	0.61
1:D:89:PRO:HD2	1:D:90:GLU:OE1	1.99	0.61
1:C:72:SER:HB3	1:C:224:VAL:HG22	1.82	0.61
1:C:96:ARG:HG2	1:C:183:GLN:HB2	1.83	0.61
1:C:101:LYS:HE3	1:C:178:LEU:CD1	2.31	0.61
1:A:191:GLY:O	1:A:192:PRO:C	2.37	0.60
1:A:110:ALA:HA	1:A:122:ARG:O	2.00	0.60
1:D:15:LEU:HB3	1:D:120:VAL:HG22	1.84	0.59
1:B:190:ASP:C	1:B:191:GLY:O	2.37	0.59
1:C:20:GLY:HA3	1:C:27:PHE:CZ	2.38	0.58
1:C:172:GLU:O	1:C:173:ASP:HB2	2.02	0.58
1:C:41:LYS:NZ	1:D:227:ASP:OD2	2.35	0.58
1:C:227:ASP:HB2	1:D:39:TYR:CD2	2.37	0.58
1:A:99:PHE:HB2	1:A:180:ASP:HB3	1.86	0.58
1:A:201:LEU:HD23	1:A:226:ALA:HB2	1.86	0.58
1:C:135:ASN:HA	1:C:140:LYS:HB2	1.85	0.58
1:D:14:ILE:HD11	1:D:71:PHE:CE2	2.38	0.58
1:B:81:HIS:CE1	1:B:197:ASP:HB2	2.40	0.56
1:A:74:TYR:OH	1:A:199:HIS:NE2	2.27	0.56
1:C:72:SER:HB3	1:C:224:VAL:CG2	2.35	0.56
1:C:168:ARG:HG2	1:C:176:VAL:HG11	1.87	0.56
1:B:43:THR:HG22	1:B:221:LEU:CD1	2.36	0.56
1:D:46:PHE:O	1:D:217:HIS:HB2	2.05	0.56
1:A:171:ILE:HB	1:A:174:GLY:O	2.06	0.55
1:D:150:VAL:HG22	1:D:165:PHE:CD2	2.41	0.55
1:C:192:PRO:O	1:C:193:VAL:HG23	2.07	0.55
1:A:76:ASP:HA	1:A:79:LYS:CD	2.36	0.55
1:A:151:TYR:CZ	1:A:198:ASN:HB3	2.42	0.55
1:C:128:ILE:O	1:C:129:ASP:HB2	2.07	0.55
1:C:227:ASP:HB2	1:D:39:TYR:CE2	2.41	0.54
1:A:53:LEU:HD22	1:A:57:TRP:CD2	2.42	0.54
1:C:101:LYS:CE	1:C:178:LEU:HD12	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:OE1	1:A:113:LYS:HE2	2.08	0.54
1:C:28:SER:HB2	1:C:50:THR:HG23	1.89	0.54
1:A:56:PRO:HD3	1:A:136:ILE:O	2.07	0.54
1:C:170:ASN:HD22	1:C:170:ASN:N	2.05	0.54
1:C:63:THR:CG2	1:C:123:ILE:HG21	2.38	0.53
1:C:81:HIS:HB3	1:C:196:PRO:CB	2.38	0.53
1:D:155:ASP:OD1	1:D:162:LYS:HD3	2.10	0.52
1:B:158:LYS:N	1:B:158:LYS:HD3	2.25	0.52
1:A:89:PRO:HD2	1:A:90:GLU:OE1	2.10	0.51
1:B:210:ASP:OD1	1:B:211:PRO:HD2	2.10	0.51
1:C:72:SER:CB	1:C:224:VAL:HG22	2.41	0.51
1:A:191:GLY:O	1:A:193:VAL:HG23	2.10	0.51
1:B:190:ASP:O	1:B:191:GLY:O	2.29	0.51
1:A:168:ARG:HB3	1:A:176:VAL:CG1	2.41	0.50
1:B:80:ARG:O	1:B:194:LEU:HD13	2.12	0.50
1:A:191:GLY:O	1:A:192:PRO:O	2.30	0.50
1:B:155:ASP:OD1	1:B:157:GLN:HG2	2.12	0.50
1:D:75:PRO:HG2	1:D:78:MET:HB2	1.93	0.50
1:B:53:LEU:HD23	1:B:55:VAL:O	2.12	0.50
1:D:202:PHE:O	1:D:224:VAL:HA	2.12	0.50
1:D:43:THR:O	1:D:44:LEU:HG	2.13	0.49
1:A:96:ARG:HA	1:A:182:TYR:O	2.12	0.49
1:D:111:GLU:HG2	1:D:188:ILE:HD11	1.94	0.49
1:D:165:PHE:O	1:D:181:HIS:HB2	2.13	0.49
1:C:96:ARG:HA	1:C:182:TYR:O	2.12	0.49
1:C:96:ARG:CG	1:C:183:GLN:HB2	2.42	0.48
1:C:173:ASP:CA	1:D:174:GLY:HA2	2.38	0.48
1:D:18:LEU:HD12	1:D:123:ILE:CB	2.39	0.48
1:D:40:GLY:O	1:D:223:PHE:HA	2.13	0.48
1:A:14:ILE:O	1:A:32:GLU:HA	2.13	0.48
1:B:190:ASP:O	1:B:191:GLY:C	2.52	0.48
1:D:53:LEU:HD23	1:D:55:VAL:O	2.14	0.47
1:A:42:LEU:HD12	1:A:222:GLU:HB3	1.96	0.47
1:A:76:ASP:HA	1:A:79:LYS:HD2	1.95	0.47
1:A:159:ASN:OD1	1:A:195:LEU:HD21	2.15	0.47
1:A:142:GLU:OE2	1:B:174:GLY:HA2	2.14	0.47
1:C:68:VAL:HG23	1:C:68:VAL:O	2.14	0.47
1:C:93:VAL:O	1:C:185:ASN:HA	2.15	0.47
1:D:143:TYR:OH	1:D:218:MET:HG3	2.15	0.47
1:A:168:ARG:HB3	1:A:176:VAL:HG11	1.97	0.47
1:B:98:ILE:HA	1:B:180:ASP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:PHE:O	1:B:224:VAL:HA	2.15	0.47
1:C:132:GLU:HA	1:C:137:LEU:HD12	1.96	0.47
1:A:76:ASP:HA	1:A:79:LYS:HD3	1.97	0.47
1:B:101:LYS:HE2	1:B:178:LEU:HD12	1.96	0.47
1:D:81:HIS:HB3	1:D:196:PRO:HB2	1.97	0.47
1:C:133:ASP:O	1:C:140:LYS:NZ	2.37	0.46
1:D:15:LEU:HD11	1:D:17:GLU:OE2	2.14	0.46
1:C:70:CYS:HB3	1:C:84:PHE:HB3	1.98	0.46
1:D:45:LYS:HG3	1:D:219:VAL:HG22	1.96	0.46
1:B:74:TYR:HD2	1:B:78:MET:O	1.99	0.46
1:D:58:PRO:HA	1:D:61:VAL:HG23	1.97	0.46
1:D:155:ASP:OD1	1:D:158:LYS:NZ	2.47	0.46
1:B:72:SER:HB2	1:B:224:VAL:HG22	1.97	0.46
1:B:101:LYS:HB3	1:B:101:LYS:HE3	1.37	0.46
1:B:171:ILE:HG22	1:B:172:GLU:O	2.16	0.45
1:A:98:ILE:HB	1:A:106:TYR:HB2	1.97	0.45
1:A:101:LYS:HB3	1:A:101:LYS:HE2	1.27	0.45
1:B:13:PRO:O	1:B:118:THR:HG23	2.15	0.45
1:C:96:ARG:HG2	1:C:183:GLN:HA	1.98	0.45
1:D:78:MET:HG2	1:D:81:HIS:CD2	2.38	0.45
1:D:122:ARG:C	1:D:123:ILE:HG13	2.36	0.45
1:D:151:TYR:CZ	1:D:198:ASN:HB3	2.51	0.45
1:D:157:GLN:H	1:D:157:GLN:HG3	1.56	0.45
1:B:14:ILE:HD11	1:B:71:PHE:CE2	2.51	0.45
1:B:81:HIS:O	1:B:196:PRO:HB3	2.16	0.45
1:D:68:VAL:HG11	1:D:119:LEU:HD12	1.99	0.45
1:B:168:ARG:CG	1:B:176:VAL:HG11	2.32	0.45
1:C:96:ARG:HG2	1:C:183:GLN:CB	2.47	0.45
1:A:58:PRO:HA	1:A:61:VAL:HG23	1.99	0.44
1:B:158:LYS:HB3	1:B:186:THR:CG2	2.48	0.44
1:D:154:ALA:HB2	1:D:196:PRO:O	2.17	0.44
1:D:110:ALA:HB2	1:D:123:ILE:HG12	1.97	0.44
1:C:52:LYS:HE2	1:C:52:LYS:HB3	1.86	0.44
1:B:68:VAL:O	1:B:68:VAL:HG23	2.17	0.44
1:B:96:ARG:HA	1:B:182:TYR:O	2.18	0.44
1:D:4:GLY:HA3	1:D:85:LYS:O	2.17	0.44
1:D:203:THR:HA	1:D:223:PHE:O	2.17	0.44
1:D:81:HIS:HB3	1:D:196:PRO:CB	2.48	0.44
1:A:70:CYS:HB3	1:A:84:PHE:HB3	2.00	0.43
1:D:156:LYS:HA	1:D:195:LEU:CD2	2.47	0.43
1:A:150:VAL:HG13	1:A:165:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:THR:CG2	1:B:123:ILE:HG21	2.49	0.43
1:A:18:LEU:HD12	1:A:123:ILE:HG21	2.01	0.43
1:A:74:TYR:HD2	1:A:78:MET:O	2.01	0.43
1:D:96:ARG:HA	1:D:182:TYR:O	2.18	0.43
1:D:178:LEU:HA	1:D:178:LEU:HD23	1.81	0.43
1:B:93:VAL:O	1:B:185:ASN:HA	2.19	0.43
1:D:136:ILE:HG22	1:D:137:LEU:N	2.34	0.43
1:A:76:ASP:OD1	1:A:79:LYS:HD3	2.19	0.43
1:B:143:TYR:CE2	1:B:209:LYS:HE2	2.54	0.43
1:B:23:ASN:ND2	1:B:130:PHE:O	2.51	0.43
1:B:149:GLN:HG3	1:B:200:TYR:CE1	2.54	0.43
1:D:33:GLY:HA3	1:D:44:LEU:HD23	2.01	0.42
1:A:132:GLU:HA	1:A:137:LEU:HD12	2.01	0.42
1:C:76:ASP:C	1:C:78:MET:H	2.23	0.42
1:A:108:THR:CG2	1:A:125:LEU:HD12	2.49	0.42
1:B:28:SER:HB3	1:B:50:THR:HG23	2.02	0.42
1:C:143:TYR:OH	1:C:218:MET:CG	2.68	0.42
1:B:115:GLU:HB2	1:B:120:VAL:HG21	2.02	0.42
1:B:158:LYS:N	1:B:158:LYS:CD	2.83	0.42
1:C:81:HIS:O	1:C:196:PRO:HB3	2.19	0.42
1:D:101:LYS:HE2	1:D:101:LYS:HB3	1.81	0.42
1:C:61:VAL:O	1:C:66:CRO:N1	2.53	0.42
1:D:119:LEU:HD22	1:D:119:LEU:HA	1.86	0.42
1:C:53:LEU:HD12	1:C:54:PRO:HD2	2.01	0.41
1:C:132:GLU:HA	1:C:137:LEU:CD1	2.49	0.41
1:C:17:GLU:OE1	1:C:30:SER:HB3	2.20	0.41
1:C:168:ARG:HG2	1:C:168:ARG:HH11	1.86	0.41
1:D:16:VAL:O	1:D:30:SER:HA	2.19	0.41
1:D:43:THR:C	1:D:44:LEU:HG	2.40	0.41
1:C:195:LEU:N	1:C:195:LEU:CD2	2.83	0.41
1:D:89:PRO:HD2	1:D:90:GLU:CD	2.40	0.41
1:A:15:LEU:HD11	1:A:17:GLU:OE2	2.21	0.41
1:D:102:ASP:O	1:D:131:LYS:CE	2.69	0.41
1:D:154:ALA:HA	1:D:161:ILE:HG22	2.02	0.41
1:C:191:GLY:O	1:C:192:PRO:O	2.38	0.41
1:A:93:VAL:O	1:A:185:ASN:HA	2.21	0.40
1:C:22:VAL:O	1:C:25:HIS:HB2	2.21	0.40
1:C:90:GLU:H	1:C:90:GLU:CD	2.25	0.40
1:D:57:TRP:N	1:D:58:PRO:CD	2.84	0.40
1:D:93:VAL:O	1:D:185:ASN:HA	2.22	0.40
1:A:81:HIS:HB3	1:A:196:PRO:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD13	1:A:195:LEU:HA	1.79	0.40
1:D:21:ASP:OD1	1:D:24:GLY:HA2	2.21	0.40
1:B:78:MET:HB2	1:B:78:MET:HE2	1.75	0.40
1:D:53:LEU:HD22	1:D:57:TRP:CD2	2.57	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	218/236 (92%)	209 (96%)	8 (4%)	1 (0%)	25	49
1	B	218/236 (92%)	210 (96%)	8 (4%)	0	100	100
1	C	218/236 (92%)	206 (94%)	11 (5%)	1 (0%)	25	49
1	D	218/236 (92%)	208 (95%)	9 (4%)	1 (0%)	25	49
All	All	872/944 (92%)	833 (96%)	36 (4%)	3 (0%)	37	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	PRO
1	D	80	ARG
1	C	192	PRO

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%)	186 (96%)	7 (4%)	30	59
1	B	193/206 (94%)	184 (95%)	9 (5%)	22	49
1	C	193/206 (94%)	187 (97%)	6 (3%)	35	64
1	D	193/206 (94%)	188 (97%)	5 (3%)	41	70
All	All	772/824 (94%)	745 (96%)	27 (4%)	31	60

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	A	86	SER
1	A	113	LYS
1	A	156	LYS
1	A	164	ASN
1	A	224	VAL
1	A	225	THR
1	B	78	MET
1	B	80	ARG
1	B	101	LYS
1	B	109	ARG
1	B	157	GLN
1	B	173	ASP
1	B	204	THR
1	B	212	ASN
1	B	214	LYS
1	C	28	SER
1	C	39	TYR
1	C	76	ASP
1	C	80	ARG
1	C	168	ARG
1	C	206	THR
1	D	79	LYS
1	D	122	ARG
1	D	133	ASP
1	D	193	VAL
1	D	225	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	159	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	B	66	1	23,23,24	6.05	10 (43%)	30,32,34	3.30	10 (33%)
1	CRO	C	66	1	23,23,24	6.05	10 (43%)	30,32,34	3.19	9 (30%)
1	CRO	A	66	1	23,23,24	6.06	10 (43%)	30,32,34	3.28	10 (33%)
1	CRO	D	66	1	23,23,24	6.07	10 (43%)	30,32,34	3.19	9 (30%)

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

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	CRO	CB2-CA2	20.81	1.52	1.35
1	A	66	CRO	CB2-CA2	20.80	1.52	1.35
1	B	66	CRO	CB2-CA2	20.73	1.52	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CRO	CB2-CA2	20.70	1.52	1.35
1	B	66	CRO	CA2-C2	-12.83	1.36	1.48
1	D	66	CRO	CA2-C2	-12.82	1.36	1.48
1	C	66	CRO	CA2-C2	-12.81	1.36	1.48
1	A	66	CRO	CA2-C2	-12.79	1.36	1.48
1	C	66	CRO	OG1-CB1	-10.75	1.13	1.43
1	A	66	CRO	OG1-CB1	-10.75	1.13	1.43
1	D	66	CRO	OG1-CB1	-10.74	1.13	1.43
1	B	66	CRO	OG1-CB1	-10.73	1.13	1.43
1	D	66	CRO	O2-C2	6.36	1.36	1.23
1	A	66	CRO	O2-C2	6.32	1.36	1.23
1	C	66	CRO	O2-C2	6.32	1.36	1.23
1	B	66	CRO	O2-C2	6.32	1.36	1.23
1	D	66	CRO	CA2-N2	-4.81	1.28	1.38
1	A	66	CRO	CA2-N2	-4.81	1.28	1.38
1	B	66	CRO	CA2-N2	-4.80	1.28	1.38
1	C	66	CRO	CA2-N2	-4.80	1.28	1.38
1	A	66	CRO	C2-N3	-4.63	1.29	1.39
1	D	66	CRO	C2-N3	-4.62	1.29	1.39
1	C	66	CRO	C2-N3	-4.61	1.29	1.39
1	B	66	CRO	C2-N3	-4.59	1.29	1.39
1	D	66	CRO	C1-N3	-4.48	1.29	1.37
1	B	66	CRO	C1-N3	-4.48	1.29	1.37
1	C	66	CRO	C1-N3	-4.47	1.29	1.37
1	A	66	CRO	C1-N3	-4.43	1.29	1.37
1	C	66	CRO	CG2-CB2	2.59	1.51	1.46
1	A	66	CRO	CG2-CB2	2.57	1.51	1.46
1	D	66	CRO	CG2-CB2	2.56	1.51	1.46
1	B	66	CRO	CG2-CB2	2.53	1.51	1.46
1	A	66	CRO	C1-N2	-2.42	1.28	1.32
1	C	66	CRO	C1-N2	-2.42	1.28	1.32
1	B	66	CRO	C1-N2	-2.42	1.28	1.32
1	D	66	CRO	C1-N2	-2.38	1.28	1.32
1	B	66	CRO	CA3-N3	-2.36	1.42	1.47
1	A	66	CRO	CA3-N3	-2.36	1.42	1.47
1	C	66	CRO	CA3-N3	-2.35	1.42	1.47
1	D	66	CRO	CA3-N3	-2.34	1.42	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	CRO	CA2-C2-N3	9.46	107.84	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	66	CRO	CA2-C2-N3	9.43	107.83	103.37
1	A	66	CRO	CA2-C2-N3	9.36	107.80	103.37
1	D	66	CRO	CA2-C2-N3	9.36	107.80	103.37
1	D	66	CRO	O2-C2-CA2	-7.70	126.64	130.96
1	A	66	CRO	O2-C2-CA2	-7.68	126.65	130.96
1	C	66	CRO	O2-C2-CA2	-7.66	126.66	130.96
1	B	66	CRO	O2-C2-CA2	-7.65	126.67	130.96
1	C	66	CRO	CA2-N2-C1	5.83	110.07	105.77
1	B	66	CRO	CA2-N2-C1	5.83	110.07	105.77
1	A	66	CRO	CA2-N2-C1	5.79	110.04	105.77
1	D	66	CRO	CA2-N2-C1	5.79	110.04	105.77
1	D	66	CRO	CG2-CB2-CA2	-5.48	123.22	129.94
1	A	66	CRO	CG2-CB2-CA2	-5.48	123.23	129.94
1	C	66	CRO	CG2-CB2-CA2	-5.48	123.23	129.94
1	B	66	CRO	CG2-CB2-CA2	-5.46	123.25	129.94
1	B	66	CRO	C1-CA1-N1	5.17	118.35	109.96
1	A	66	CRO	C1-CA1-N1	4.98	118.05	109.96
1	B	66	CRO	C2-CA2-N2	-4.94	105.47	108.93
1	C	66	CRO	C2-CA2-N2	-4.94	105.47	108.93
1	D	66	CRO	C2-CA2-N2	-4.88	105.52	108.93
1	A	66	CRO	C2-CA2-N2	-4.86	105.53	108.93
1	D	66	CRO	N3-C1-N2	-3.99	108.69	111.45
1	C	66	CRO	N3-C1-N2	-3.97	108.71	111.45
1	A	66	CRO	N3-C1-N2	-3.96	108.71	111.45
1	B	66	CRO	N3-C1-N2	-3.93	108.74	111.45
1	C	66	CRO	O3-C3-CA3	-3.69	115.24	126.39
1	B	66	CRO	O3-C3-CA3	-3.69	115.25	126.39
1	D	66	CRO	O3-C3-CA3	-3.69	115.26	126.39
1	A	66	CRO	O3-C3-CA3	-3.67	115.30	126.39
1	D	66	CRO	OG1-CB1-CA1	3.15	115.79	109.04
1	A	66	CRO	OG1-CB1-CA1	3.14	115.77	109.04
1	B	66	CRO	OG1-CB1-CA1	3.13	115.74	109.04
1	C	66	CRO	OG1-CB1-CA1	3.12	115.73	109.04
1	D	66	CRO	CA1-C1-N3	2.58	127.84	124.75
1	C	66	CRO	CA1-C1-N3	2.57	127.83	124.75
1	B	66	CRO	CA1-C1-N3	2.56	127.81	124.75
1	A	66	CRO	CA1-C1-N3	2.56	127.81	124.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	C1-CA1-CB1-CG1
1	B	66	CRO	C1-CA1-CB1-CG1
1	C	66	CRO	C1-CA1-CB1-CG1
1	D	66	CRO	C1-CA1-CB1-CG1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	66	CRO	1	0

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	222/236 (94%)	-1.71	0	100	100	18, 28, 61, 88	0
1	B	222/236 (94%)	-1.73	0	100	100	18, 27, 55, 72	0
1	C	222/236 (94%)	-1.70	0	100	100	20, 30, 57, 76	0
1	D	222/236 (94%)	-1.71	0	100	100	18, 26, 63, 81	0
All	All	888/944 (94%)	-1.71	0	100	100	18, 28, 58, 88	0

There are no RSRZ outliers to report.

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, 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	0.99	0.03	17,22,24,25	0
1	CRO	B	66	22/23	0.99	0.03	17,22,24,25	0
1	CRO	C	66	22/23	0.99	0.03	17,22,24,25	0
1	CRO	D	66	22/23	0.99	0.03	17,22,24,25	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.