Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 04:05 PM EDT

PDB ID	:	2G6X
Title	:	Crystal structure of a novel green fluorescent protein from marine copepod Pontellina plumata
Authors	:	Evdokimov, A.G.; Pokross, M.E.; Chudakov, D.M.
Deposited on	:	2006-02-26
Resolution	:	2.00 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 following versions of software and data (see references (i)) were used in the production of this report:

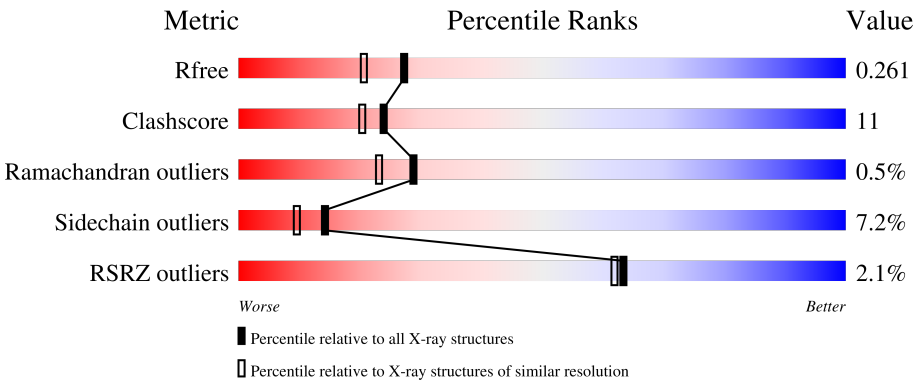
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	217	2% 73% 21% • ••
1	B	217	3% 73% 21% 5%
1	C	217	2% 76% 19% •
1	D	217	% 66% 26% 6% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7109 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1700	1077	289	324	10	0	1	0
1	B	216	1718	1090	291	327	10	0	2	0
1	C	216	1718	1087	294	328	9	0	1	0
1	D	215	1703	1077	290	327	9	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	-	cloning artifact	GB 33243028
A	5	GLU	LYS	engineered mutation	GB 33243028
A	58	CR2	GLY	chromophore	GB 33243028
A	58	CR2	TYR	chromophore	GB 33243028
A	58	CR2	GLY	chromophore	GB 33243028
A	117	MET	VAL	engineered mutation	GB 33243028
A	149	ASP	VAL	engineered mutation	GB 33243028
A	151	ASP	VAL	engineered mutation	GB 33243028
A	155	THR	ALA	engineered mutation	GB 33243028
A	168	SER	PHE	engineered mutation	GB 33243028
A	200	ASP	LEU	engineered mutation	GB 33243028
A	219	ASP	ILE	engineered mutation	GB 33243028
B	1	LEU	-	cloning artifact	GB 33243028
B	5	GLU	LYS	engineered mutation	GB 33243028
B	58	CR2	GLY	chromophore	GB 33243028
B	58	CR2	TYR	chromophore	GB 33243028
B	58	CR2	GLY	chromophore	GB 33243028
B	117	MET	VAL	engineered mutation	GB 33243028
B	149	ASP	VAL	engineered mutation	GB 33243028
B	151	ASP	VAL	engineered mutation	GB 33243028
B	155	THR	ALA	engineered mutation	GB 33243028

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Chain	Residue	Modelled	Actual	Comment	Reference
B	168	SER	PHE	engineered mutation	GB 33243028
B	200	ASP	LEU	engineered mutation	GB 33243028
B	219	ASP	ILE	engineered mutation	GB 33243028
C	1	LEU	-	cloning artifact	GB 33243028
C	5	GLU	LYS	engineered mutation	GB 33243028
C	58	CR2	GLY	chromophore	GB 33243028
C	58	CR2	TYR	chromophore	GB 33243028
C	58	CR2	GLY	chromophore	GB 33243028
C	117	MET	VAL	engineered mutation	GB 33243028
C	149	ASP	VAL	engineered mutation	GB 33243028
C	151	ASP	VAL	engineered mutation	GB 33243028
C	155	THR	ALA	engineered mutation	GB 33243028
C	168	SER	PHE	engineered mutation	GB 33243028
C	200	ASP	LEU	engineered mutation	GB 33243028
C	219	ASP	ILE	engineered mutation	GB 33243028
D	1	LEU	-	cloning artifact	GB 33243028
D	5	GLU	LYS	engineered mutation	GB 33243028
D	58	CR2	GLY	chromophore	GB 33243028
D	58	CR2	TYR	chromophore	GB 33243028
D	58	CR2	GLY	chromophore	GB 33243028
D	117	MET	VAL	engineered mutation	GB 33243028
D	149	ASP	VAL	engineered mutation	GB 33243028
D	151	ASP	VAL	engineered mutation	GB 33243028
D	155	THR	ALA	engineered mutation	GB 33243028
D	168	SER	PHE	engineered mutation	GB 33243028
D	200	ASP	LEU	engineered mutation	GB 33243028
D	219	ASP	ILE	engineered mutation	GB 33243028

- Molecule 2 is water.

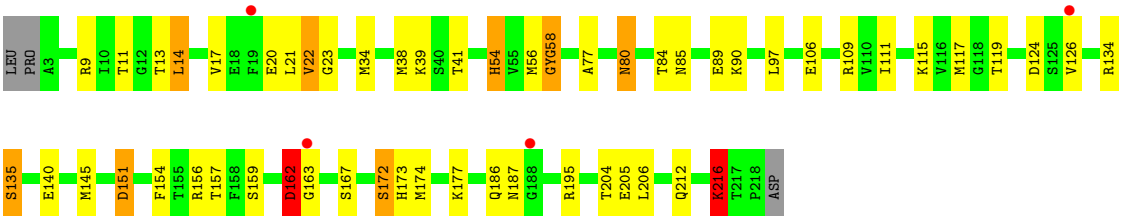
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	66	66	66	0	0
			Total	O		
2	B	78	78	78	0	0
			Total	O		
2	C	58	58	58	0	0
			Total	O		
2	D	68	68	68	0	0

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.

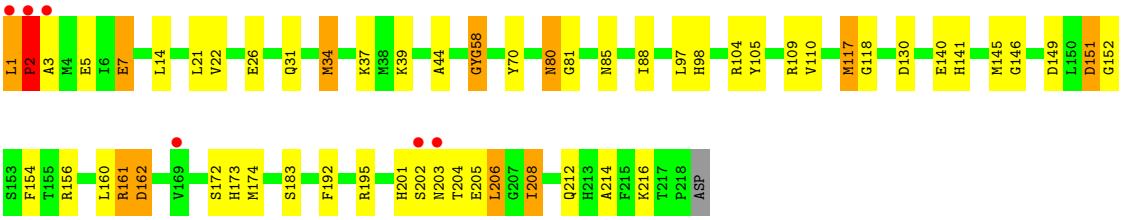
• Molecule 1: green fluorescent protein 2

Chain A:



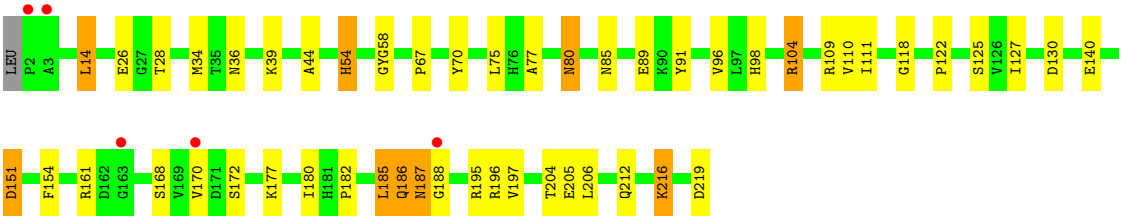
• Molecule 1: green fluorescent protein 2

Chain B:



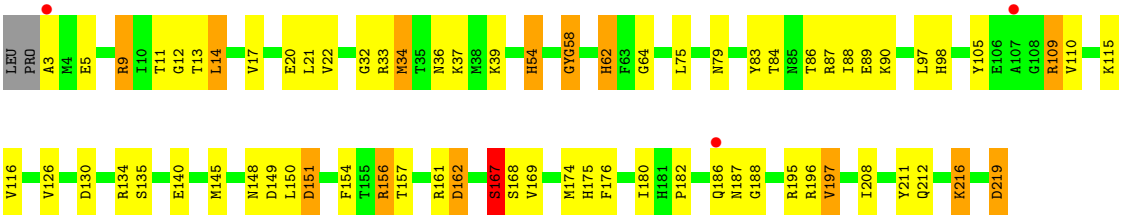
• Molecule 1: green fluorescent protein 2

Chain C:



• Molecule 1: green fluorescent protein 2

Chain D:


LEU
PRO
A3
M4
E5
R9
I10
T11
G12
T13
L14
V17
E20
L21
V22
G32
R33
M34
T35
N36
K37
M38
K39
H54
GYG58
H62
F63
G64
L75
N79
Y83
T84
N85
T86
R87
I88
E89
K90
L97
H98
Y105
E106
A107
G108
R109
V110
K115
V116
V126
D130
R134
S135
E140
M145
N148
D149
L150
D151
F154
T155
R156
T157
R161
D162
S167
S168
V169
M174
H175
F176
I180
H181
P182
Q186
N187
G188
R195
R196
V197
I208
Y211
Q212
K216
D219

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.75Å 97.91Å 172.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.00 43.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (100.00-2.00) 98.1 (43.08-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.246 0.213 , 0.261	Depositor DCC
R_{free} test set	2807 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7109	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: CR2

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	0.60	0/1728	1.40	13/2331 (0.6%)
1	B	0.63	0/1750	1.43	16/2362 (0.7%)
1	C	0.55	0/1747	1.30	8/2357 (0.3%)
1	D	0.61	0/1728	1.42	21/2332 (0.9%)
All	All	0.60	0/6953	1.39	58/9382 (0.6%)

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	1
1	B	0	3
1	D	0	2
All	All	0	6

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	ASP	CB-CG-OD1	-16.51	103.44	118.30
1	A	151	ASP	CB-CG-OD2	-15.18	104.64	118.30
1	D	134	ARG	NE-CZ-NH1	11.33	125.96	120.30
1	D	34	MET	CG-SD-CE	11.02	117.83	100.20
1	B	156	ARG	NE-CZ-NH1	-10.50	115.05	120.30
1	C	75	LEU	CB-CG-CD2	-9.73	94.45	111.00
1	D	162	ASP	CB-CG-OD1	8.84	126.25	118.30
1	B	160	LEU	CB-CG-CD1	-8.60	96.37	111.00
1	A	151	ASP	OD1-CG-OD2	8.31	139.09	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	135	SER	CB-CA-C	-8.23	94.46	110.10
1	A	14	LEU	CA-CB-CG	-8.14	96.57	115.30
1	B	161	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	C	151	ASP	CB-CG-OD1	-7.81	111.27	118.30
1	B	162	ASP	CB-CG-OD2	7.74	125.27	118.30
1	B	130	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	D	75	LEU	CA-CB-CG	7.39	132.29	115.30
1	D	9	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	D	216	LYS	CD-CE-NZ	6.92	127.61	111.70
1	B	130	ASP	CB-CG-OD1	6.55	124.19	118.30
1	D	156	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	A	163	GLY	N-CA-C	-6.53	96.78	113.10
1	C	14	LEU	CA-CB-CG	-6.36	100.67	115.30
1	D	87	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	206	LEU	CB-CG-CD2	6.25	121.62	111.00
1	D	21	LEU	CB-CG-CD1	6.15	121.45	111.00
1	D	151	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	156	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	C	196	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	C	206	LEU	CB-CG-CD1	5.91	121.05	111.00
1	D	134	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	21	LEU	CA-CB-CG	-5.78	102.00	115.30
1	B	146	GLY	N-CA-C	-5.78	98.66	113.10
1	B	151	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	D	14	LEU	CA-CB-CG	-5.73	102.12	115.30
1	A	151	ASP	N-CA-CB	-5.65	100.43	110.60
1	A	216	LYS	CD-CE-NZ	5.63	124.64	111.70
1	C	104	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	C	151	ASP	N-CA-CB	-5.62	100.48	110.60
1	C	104	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	34	MET	CG-SD-CE	-5.61	91.23	100.20
1	A	162	ASP	N-CA-C	5.60	126.11	111.00
1	D	9	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	D	197	VAL	CG1-CB-CG2	5.56	119.79	110.90
1	D	167	SER	N-CA-CB	5.50	118.75	110.50
1	D	109	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	14	LEU	CB-CG-CD2	5.45	120.26	111.00
1	A	56	MET	CA-CB-CG	5.41	122.50	113.30
1	D	195	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	9	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	B	161	ARG	CB-CG-CD	5.30	125.39	111.60
1	B	208	ILE	CG1-CB-CG2	-5.22	99.92	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	33	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	169	VAL	CG1-CB-CG2	-5.10	102.74	110.90
1	B	22	VAL	C-N-CA	-5.07	111.66	122.30
1	B	14	LEU	CA-CB-CG	-5.05	103.69	115.30
1	A	97	LEU	CB-CG-CD2	5.03	119.55	111.00
1	D	135	SER	CB-CA-C	-5.02	100.57	110.10
1	D	196	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	ASP	Peptide
1	B	2	PRO	Peptide
1	B	201	HIS	Peptide
1	B	208	ILE	Peptide
1	D	208	ILE	Peptide
1	D	3	ALA	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	1700	0	1599	35	0
1	B	1718	0	1624	43	0
1	C	1718	0	1615	36	0
1	D	1703	0	1594	39	0
2	A	66	0	0	5	0
2	B	78	0	0	7	0
2	C	58	0	0	0	0
2	D	68	0	0	1	1
All	All	7109	0	6432	147	1

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 11.

All (147) 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:C:187:ASN:HD21	1:C:216:LYS:HE3	1.19	1.05
1:C:182:PRO:O	1:C:186:GLN:HG2	1.55	1.04
1:C:187:ASN:ND2	1:C:216:LYS:HE3	1.74	1.01
1:B:1:LEU:HB2	1:B:2:PRO:HD3	1.53	0.91
1:B:1:LEU:HB2	1:B:2:PRO:CD	2.03	0.87
1:A:54:HIS:HE1	1:A:89:GLU:OE1	1.58	0.86
1:C:187:ASN:HD21	1:C:216:LYS:CE	1.90	0.83
1:A:145[A]:MET:SD	2:A:273:HOH:O	2.37	0.81
1:C:54:HIS:HE1	1:C:89:GLU:OE1	1.67	0.78
1:A:156:ARG:NH1	2:A:266:HOH:O	2.17	0.76
1:C:109:ARG:CB	1:C:109:ARG:HH11	2.00	0.74
1:A:23:GLY:HA3	1:A:38:MET:HG2	1.70	0.72
1:B:88:ILE:HD11	1:B:98:HIS:HD2	1.55	0.72
1:D:88:ILE:HD11	1:D:98:HIS:HD2	1.55	0.72
1:A:54:HIS:CE1	1:A:89:GLU:OE1	2.42	0.70
1:B:202[B]:SER:OG	1:B:205:GLU:HB2	1.92	0.70
1:B:1:LEU:CB	1:B:2:PRO:HD3	2.20	0.70
1:D:54:HIS:HE1	1:D:89:GLU:OE1	1.73	0.70
1:D:187:ASN:HD21	1:D:216:LYS:HE3	1.55	0.69
1:B:81:GLY:CA	2:B:272:HOH:O	2.40	0.69
1:C:187:ASN:CG	1:C:216:LYS:HE3	2.12	0.69
1:A:173:HIS:HB3	2:A:236:HOH:O	1.92	0.69
1:B:81:GLY:N	2:B:272:HOH:O	2.17	0.69
1:D:157:THR:HG22	1:D:167:SER:HB3	1.75	0.68
1:B:104:ARG:HD3	2:B:280:HOH:O	1.95	0.66
1:B:80:ASN:HD22	1:B:80:ASN:C	1.99	0.66
1:C:216:LYS:HZ3	1:C:216:LYS:HB3	1.59	0.66
1:A:54:HIS:CD2	2:A:266:HOH:O	2.48	0.66
1:C:130:ASP:CG	1:C:161[A]:ARG:HH12	2.00	0.64
1:B:34:MET:CE	2:B:230:HOH:O	2.45	0.64
1:B:34:MET:HE1	2:B:230:HOH:O	1.98	0.63
1:B:7:GLU:OE2	1:B:109:ARG:HD3	1.98	0.63
1:C:109:ARG:HB2	1:C:109:ARG:NH1	2.13	0.63
1:D:62:HIS:CD2	1:D:62:HIS:H	2.15	0.63
1:D:88:ILE:HD11	1:D:98:HIS:CD2	2.34	0.63
1:B:204:THR:HG21	2:B:239:HOH:O	1.98	0.63
1:D:187:ASN:ND2	1:D:216:LYS:HE3	2.14	0.62
1:D:11:THR:HG22	1:D:20:GLU:HG3	1.82	0.62
1:B:88:ILE:CD1	1:B:98:HIS:HD2	2.14	0.61
1:A:80:ASN:C	1:A:80:ASN:HD22	2.04	0.61
1:B:195:ARG:HG2	1:B:212:GLN:HG2	1.81	0.61
1:C:39:LYS:HE2	1:C:205:GLU:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:THR:HA	1:D:17:VAL:O	2.02	0.59
1:B:204:THR:CG2	2:B:239:HOH:O	2.49	0.58
1:C:54:HIS:CE1	1:C:89:GLU:OE1	2.55	0.58
1:C:109:ARG:CB	1:C:109:ARG:NH1	2.68	0.57
1:A:39:LYS:HG2	1:A:205:GLU:HG2	1.86	0.57
1:C:109:ARG:HH11	1:C:109:ARG:HB3	1.68	0.57
1:A:22:VAL:HG22	1:A:41:THR:CG2	2.36	0.55
1:C:130:ASP:OD2	1:C:161[A]:ARG:NH1	2.39	0.55
1:D:58:CR2:N2	1:D:58:CR2:HD1	2.22	0.55
1:D:9:ARG:HG3	1:D:22:VAL:HG12	1.88	0.55
1:A:11:THR:HG22	1:A:20:GLU:HG3	1.87	0.55
1:D:5:GLU:HG3	1:D:109:ARG:HG3	1.88	0.55
1:C:187:ASN:OD1	1:C:216:LYS:HE3	2.07	0.55
1:A:140:GLU:HA	1:A:154:PHE:HB3	1.89	0.54
1:C:85:ASN:HD21	1:C:172:SER:HB3	1.72	0.54
1:D:54:HIS:H	1:D:54:HIS:CD2	2.26	0.53
1:A:187:ASN:HD21	1:A:216:LYS:HD2	1.73	0.53
1:D:54:HIS:CE1	1:D:89:GLU:OE1	2.58	0.52
1:C:195:ARG:HG2	1:C:212:GLN:HG2	1.91	0.52
1:B:97:LEU:HD23	1:B:118:GLY:CA	2.39	0.52
1:B:202[B]:SER:HG	1:B:205:GLU:HB2	1.75	0.52
1:D:34:MET:HE2	1:D:36:ASN:HB2	1.92	0.51
1:B:85:ASN:ND2	1:B:174:MET:HG3	2.25	0.51
1:A:90:LYS:HE2	1:D:90:LYS:HE3	1.91	0.51
1:A:85:ASN:HD21	1:A:172:SER:HB3	1.76	0.51
1:A:195:ARG:HG2	1:A:212:GLN:HG2	1.92	0.51
1:C:109:ARG:HH11	1:C:109:ARG:HB2	1.68	0.51
1:B:34:MET:HE3	1:B:58:CR2:HA11	1.93	0.51
1:C:67:PRO:HG2	1:C:70:TYR:CD1	2.47	0.50
1:B:44:ALA:HB1	1:B:203:ASN:ND2	2.26	0.50
1:D:148:ASN:HB3	1:D:176:PHE:O	2.11	0.49
1:A:77:ALA:HA	1:A:80:ASN:ND2	2.27	0.49
1:A:135:SER:OG	1:A:156:ARG:NH1	2.45	0.49
1:B:97:LEU:HD23	1:B:118:GLY:HA2	1.94	0.49
1:A:21:LEU:CD2	1:A:206:LEU:HD13	2.43	0.49
1:B:34:MET:HE1	1:B:58:CR2:HA12	1.94	0.49
1:A:124:ASP:OD1	1:A:124:ASP:C	2.52	0.48
1:D:145:MET:HB2	1:D:149:ASP:HB2	1.96	0.48
1:C:44:ALA:HA	1:C:204:THR:HG22	1.95	0.48
1:D:150:LEU:HG	1:D:180:ILE:HD13	1.95	0.48
1:D:130:ASP:O	1:D:161:ARG:NH1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:GLY:N	2:D:286:HOH:O	2.46	0.47
1:C:89:GLU:HG2	1:C:170:VAL:HG13	1.97	0.47
1:B:34:MET:CE	1:B:58:CR2:HA12	2.44	0.47
1:B:34:MET:HE3	1:B:58:CR2:CA1	2.45	0.47
1:A:109:ARG:HD3	1:A:111:ILE:HD11	1.97	0.47
1:A:80:ASN:C	1:A:80:ASN:ND2	2.68	0.46
1:B:140:GLU:HA	1:B:154:PHE:HB3	1.96	0.46
1:C:39:LYS:HE3	1:C:39:LYS:HB2	1.74	0.46
1:D:88:ILE:HD13	1:D:88:ILE:HA	1.81	0.46
1:A:84:THR:O	1:A:174:MET:HA	2.16	0.46
1:A:23:GLY:HA3	1:A:38:MET:CG	2.44	0.45
1:C:54:HIS:CD2	1:C:54:HIS:H	2.34	0.45
1:A:77:ALA:HA	1:A:80:ASN:HD21	1.81	0.45
1:C:77:ALA:HA	1:C:80:ASN:ND2	2.31	0.45
1:C:104:ARG:HB3	1:C:111:ILE:HB	1.98	0.45
1:C:187:ASN:OD1	1:C:216:LYS:CE	2.65	0.45
1:C:96:VAL:O	1:C:118:GLY:HA2	2.17	0.45
1:D:34:MET:CE	1:D:36:ASN:HB2	2.46	0.45
1:B:70:TYR:HA	1:B:183:SER:HB2	1.98	0.45
1:B:149:ASP:HB3	1:B:173:HIS:CE1	2.52	0.45
1:B:141:HIS:O	1:B:152:GLY:HA2	2.17	0.45
1:C:180:ILE:O	1:C:185:LEU:HD22	2.17	0.45
1:D:154:PHE:HE1	1:D:156:ARG:HD2	1.82	0.44
1:B:2:PRO:HB2	1:B:3:ALA:H	1.54	0.44
1:D:62:HIS:HE1	1:D:105:TYR:OH	2.00	0.44
1:B:145[A]:MET:HE3	1:C:122:PRO:HA	1.99	0.44
1:D:54:HIS:H	1:D:54:HIS:HD2	1.63	0.44
1:D:64:GLY:HA2	1:D:212:GLN:HB2	2.00	0.44
1:B:80:ASN:C	1:B:80:ASN:ND2	2.64	0.44
1:B:192:PHE:O	1:B:214:ALA:HA	2.17	0.44
1:A:134:ARG:HD2	2:A:271:HOH:O	2.19	0.43
1:B:5:GLU:HG3	1:B:109:ARG:NH2	2.33	0.43
1:B:39:LYS:HA	1:B:204:THR:O	2.18	0.43
1:D:97:LEU:HA	1:D:97:LEU:HD12	1.80	0.43
1:A:22:VAL:CG2	1:A:41:THR:CG2	2.96	0.43
1:A:90:LYS:HE3	1:D:90:LYS:NZ	2.33	0.43
1:A:157:THR:HG22	1:A:167:SER:HB3	1.99	0.43
1:D:90:LYS:O	1:D:168:SER:HA	2.19	0.43
1:D:140:GLU:HA	1:D:154:PHE:HB3	2.00	0.43
1:C:140:GLU:HG3	1:C:154:PHE:HD2	1.83	0.43
1:A:13:THR:HA	1:A:17:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:GLN:HE21	1:C:186:GLN:HA	1.84	0.43
1:C:219:ASP:OD2	1:D:219:ASP:C	2.57	0.42
1:D:11:THR:O	1:D:115:LYS:HA	2.20	0.42
1:D:32:GLY:O	1:D:211:TYR:HA	2.19	0.42
1:B:58:CR2:N2	1:B:58:CR2:HD1	2.34	0.42
1:A:115:LYS:HE2	1:A:115:LYS:HB2	1.87	0.42
1:B:80:ASN:ND2	1:B:80:ASN:O	2.52	0.42
1:A:39:LYS:HG2	1:A:205:GLU:CG	2.49	0.42
1:A:58:CR2:N2	1:A:58:CR2:HD1	2.34	0.42
1:B:34:MET:CE	1:B:58:CR2:CA1	2.97	0.42
1:B:37:LYS:HA	1:B:206:LEU:O	2.19	0.42
1:B:85:ASN:HD21	1:B:172:SER:HB3	1.85	0.42
1:A:134:ARG:HG2	1:A:159:SER:HB2	2.01	0.42
1:C:125:SER:OG	1:C:127:ILE:HG12	2.20	0.41
1:B:88:ILE:CD1	1:B:98:HIS:CD2	3.01	0.41
1:C:91:TYR:CD2	1:C:168:SER:HB3	2.56	0.41
1:A:119:THR:HG21	1:D:86:THR:OG1	2.20	0.41
1:B:105:TYR:CE2	1:B:110:VAL:HG23	2.56	0.40
1:D:12:GLY:HA3	1:D:116:VAL:O	2.22	0.40
1:D:182:PRO:O	1:D:186:GLN:HB2	2.21	0.40
1:B:117:MET:HG2	1:C:98:HIS:CE1	2.57	0.40
1:D:84:THR:O	1:D:174:MET:HA	2.22	0.40
1:D:83:TYR:HA	1:D:175:HIS:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:224:HOH:O	2:D:224:HOH:O[4_565]	2.18	0.02

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	210/217 (97%)	197 (94%)	12 (6%)	1 (0%)	29	23
1	B	213/217 (98%)	205 (96%)	7 (3%)	1 (0%)	29	23
1	C	212/217 (98%)	206 (97%)	4 (2%)	2 (1%)	17	11
1	D	210/217 (97%)	207 (99%)	3 (1%)	0	100	100
All	All	845/868 (97%)	815 (96%)	26 (3%)	4 (0%)	29	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	B	2	PRO
1	C	187	ASN
1	C	188	GLY

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	181/183 (99%)	167 (92%)	14 (8%)	13	8
1	B	184/183 (100%)	173 (94%)	11 (6%)	19	14
1	C	183/183 (100%)	169 (92%)	14 (8%)	13	8
1	D	181/183 (99%)	168 (93%)	13 (7%)	14	9
All	All	729/732 (100%)	677 (93%)	52 (7%)	14	10

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	22	VAL
1	A	54	HIS
1	A	80	ASN
1	A	106	GLU
1	A	117	MET
1	A	126	VAL

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Mol	Chain	Res	Type
1	A	151	ASP
1	A	162	ASP
1	A	172	SER
1	A	177	LYS
1	A	186	GLN
1	A	204	THR
1	A	216	LYS
1	B	1	LEU
1	B	7	GLU
1	B	26	GLU
1	B	31	GLN
1	B	34	MET
1	B	80	ASN
1	B	117	MET
1	B	151	ASP
1	B	161	ARG
1	B	162	ASP
1	B	216	LYS
1	C	14	LEU
1	C	26	GLU
1	C	28	THR
1	C	34	MET
1	C	36	ASN
1	C	54	HIS
1	C	80	ASN
1	C	110	VAL
1	C	151	ASP
1	C	177	LYS
1	C	185	LEU
1	C	186	GLN
1	C	197	VAL
1	C	216	LYS
1	D	14	LEU
1	D	37	LYS
1	D	39	LYS
1	D	54	HIS
1	D	62	HIS
1	D	79	ASN
1	D	110	VAL
1	D	126	VAL
1	D	151	ASP
1	D	162	ASP

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Mol	Chain	Res	Type
1	D	167	SER
1	D	197	VAL
1	D	219	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	76	HIS
1	A	80	ASN
1	A	85	ASN
1	A	187	ASN
1	B	76	HIS
1	B	80	ASN
1	B	85	ASN
1	B	98	HIS
1	B	143	HIS
1	C	36	ASN
1	C	54	HIS
1	C	76	HIS
1	C	80	ASN
1	C	85	ASN
1	C	173	HIS
1	C	186	GLN
1	C	187	ASN
1	D	31	GLN
1	D	54	HIS
1	D	62	HIS
1	D	98	HIS
1	D	187	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	CR2	C	58	1	20,20,21	3.84	4 (20%)	25,27,29	3.00	6 (24%)
1	CR2	A	58	1	20,20,21	3.57	5 (25%)	25,27,29	3.54	13 (52%)
1	CR2	B	58	1	20,20,21	3.82	5 (25%)	25,27,29	4.42	10 (40%)
1	CR2	D	58	1	20,20,21	3.64	7 (35%)	25,27,29	3.73	7 (28%)

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	CR2	C	58	1	-	0/6/25/26	0/2/2/2
1	CR2	A	58	1	-	0/6/25/26	0/2/2/2
1	CR2	B	58	1	-	0/6/25/26	0/2/2/2
1	CR2	D	58	1	-	1/6/25/26	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	58	CR2	CB2-CA2	12.75	1.45	1.35
1	C	58	CR2	CB2-CA2	12.18	1.45	1.35
1	D	58	CR2	CB2-CA2	11.37	1.44	1.35
1	A	58	CR2	CB2-CA2	10.11	1.43	1.35
1	A	58	CR2	CA2-C2	-9.62	1.39	1.48
1	C	58	CR2	CA2-C2	-9.44	1.39	1.48
1	B	58	CR2	CA2-C2	-9.05	1.39	1.48
1	D	58	CR2	CA2-C2	-8.94	1.39	1.48
1	C	58	CR2	CA3-N3	-5.57	1.36	1.47
1	A	58	CR2	CA3-N3	-4.52	1.38	1.47
1	B	58	CR2	CA3-N3	-3.99	1.39	1.47
1	D	58	CR2	CA3-N3	-3.90	1.39	1.47
1	A	58	CR2	CG2-CB2	-3.47	1.40	1.46
1	D	58	CR2	O2-C2	3.13	1.29	1.23
1	B	58	CR2	O2-C2	3.10	1.29	1.23
1	A	58	CR2	O2-C2	2.98	1.29	1.23
1	C	58	CR2	O2-C2	2.83	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	58	CR2	CG2-CB2	-2.57	1.41	1.46
1	D	58	CR2	CA1-C1	2.28	1.52	1.49
1	D	58	CR2	C1-N2	2.20	1.36	1.32
1	D	58	CR2	CG2-CB2	-2.16	1.42	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	58	CR2	CA2-C2-N3	14.51	110.23	103.37
1	D	58	CR2	CA2-C2-N3	11.06	108.60	103.37
1	D	58	CR2	O2-C2-CA2	-10.31	125.17	130.96
1	C	58	CR2	CA2-C2-N3	10.28	108.23	103.37
1	A	58	CR2	O2-C2-CA2	8.99	136.01	130.96
1	B	58	CR2	C2-N3-C1	-8.70	103.74	107.99
1	B	58	CR2	O2-C2-CA2	-7.12	126.96	130.96
1	A	58	CR2	CE2-CD2-CG2	-6.50	112.78	121.25
1	B	58	CR2	C1-CA1-N1	-6.33	98.86	112.85
1	C	58	CR2	O3-C3-CA3	-6.32	107.31	126.39
1	D	58	CR2	C2-N3-C1	-6.19	104.97	107.99
1	A	58	CR2	C2-CA2-N2	6.10	113.21	108.93
1	A	58	CR2	CD1-CE1-CZ	-5.48	113.87	119.88
1	D	58	CR2	CG2-CB2-CA2	-5.36	123.37	129.94
1	B	58	CR2	CD1-CE1-CZ	-5.32	114.03	119.88
1	A	58	CR2	C1-CA1-N1	-5.12	101.52	112.85
1	A	58	CR2	CD2-CG2-CD1	5.10	125.19	117.64
1	C	58	CR2	C1-CA1-N1	-4.94	101.92	112.85
1	A	58	CR2	O3-C3-CA3	-4.41	113.08	126.39
1	C	58	CR2	O2-C2-CA2	-4.40	128.49	130.96
1	B	58	CR2	CE2-CZ-CE1	4.11	126.70	119.77
1	B	58	CR2	CD2-CG2-CD1	4.07	123.66	117.64
1	D	58	CR2	C1-CA1-N1	-3.61	104.86	112.85
1	C	58	CR2	C2-N3-C1	-3.57	106.24	107.99
1	B	58	CR2	CE2-CD2-CG2	-3.36	116.86	121.25
1	A	58	CR2	CD2-CG2-CB2	-2.85	111.53	121.22
1	A	58	CR2	CB2-CA2-N2	-2.73	125.05	128.83
1	B	58	CR2	CA3-N3-C1	2.70	131.58	127.86
1	B	58	CR2	C2-CA2-N2	-2.59	107.12	108.93
1	A	58	CR2	CE2-CZ-CE1	2.52	124.01	119.77
1	A	58	CR2	CD2-CE2-CZ	2.42	122.53	119.88
1	D	58	CR2	CD1-CE1-CZ	2.41	122.52	119.88
1	A	58	CR2	O2-C2-N3	-2.39	119.60	124.35
1	C	58	CR2	CG2-CB2-CA2	-2.30	127.12	129.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	58	CR2	CE1-CD1-CG2	-2.23	118.34	121.25
1	A	58	CR2	OH-CZ-CE2	-2.12	113.97	120.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	58	CR2	C3-CA3-N3-C2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	58	CR2	1	0
1	B	58	CR2	6	0
1	D	58	CR2	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	213/217 (98%)	0.07	4 (1%)	66	65	21, 34, 46, 53	0
1	B	215/217 (99%)	-0.02	6 (2%)	53	51	21, 32, 48, 62	0
1	C	215/217 (99%)	0.03	5 (2%)	60	59	23, 35, 48, 62	0
1	D	214/217 (98%)	-0.02	3 (1%)	75	74	23, 33, 47, 60	0
All	All	857/868 (98%)	0.02	18 (2%)	63	62	21, 33, 48, 62	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	PRO	5.8
1	B	1	LEU	5.4
1	B	3	ALA	4.3
1	A	188	GLY	4.2
1	B	203	ASN	3.6
1	C	2	PRO	2.9
1	C	163	GLY	2.9
1	A	163	GLY	2.8
1	D	3	ALA	2.7
1	D	107	ALA	2.5
1	B	202[A]	SER	2.5
1	D	186	GLN	2.2
1	C	3	ALA	2.2
1	C	188	GLY	2.2
1	A	126	VAL	2.1
1	B	169	VAL	2.1
1	C	170	VAL	2.0
1	A	19	PHE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CR2	D	58	19/20	0.93	0.10	26,29,31,31	0
1	CR2	A	58	19/20	0.94	0.12	25,28,29,29	0
1	CR2	C	58	19/20	0.95	0.10	25,28,31,31	0
1	CR2	B	58	19/20	0.97	0.10	21,24,26,27	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.