Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2024 – 10:23 PM EDT

PDB ID	:	2G3O
Title	:	The 2.1A crystal structure of copGFP
Authors	:	Wilmann, P.G.
Deposited on	:	2006-02-20
Resolution	:	2.10 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:

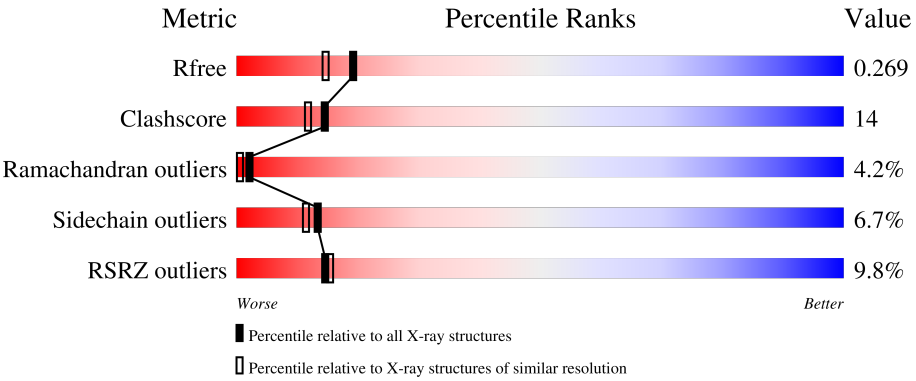
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.10 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	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	220	73% 18% 5%
1	B	220	3% 75% 16% 5%
1	C	220	5% 73% 20%
1	D	220	17% 76% 18%
1	E	220	2% 75% 17% 5%

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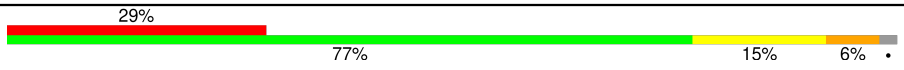
Mol	Chain	Length	Quality of chain
1	F	220	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9837 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
1	A	212	Total	C	N	O	S	0	0	0
			1621	1043	278	292	8			
1	B	213	Total	C	N	O	S	0	0	0
			1609	1034	278	289	8			
1	C	216	Total	C	N	O	S	0	0	0
			1605	1031	269	298	7			
1	D	216	Total	C	N	O	S	0	0	0
			1590	1023	265	295	7			
1	E	216	Total	C	N	O	S	0	0	0
			1603	1031	271	294	7			
1	F	216	Total	C	N	O	S	0	0	0
			1595	1026	267	295	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	CR2	GLY	chromophore	UNP Q6WV12
A	57	CR2	TYR	chromophore	UNP Q6WV12
A	57	CR2	GLY	chromophore	UNP Q6WV12
B	57	CR2	GLY	chromophore	UNP Q6WV12
B	57	CR2	TYR	chromophore	UNP Q6WV12
B	57	CR2	GLY	chromophore	UNP Q6WV12
C	57	CR2	GLY	chromophore	UNP Q6WV12
C	57	CR2	TYR	chromophore	UNP Q6WV12
C	57	CR2	GLY	chromophore	UNP Q6WV12
D	57	CR2	GLY	chromophore	UNP Q6WV12
D	57	CR2	TYR	chromophore	UNP Q6WV12
D	57	CR2	GLY	chromophore	UNP Q6WV12
E	57	CR2	GLY	chromophore	UNP Q6WV12
E	57	CR2	TYR	chromophore	UNP Q6WV12
E	57	CR2	GLY	chromophore	UNP Q6WV12
F	57	CR2	GLY	chromophore	UNP Q6WV12
F	57	CR2	TYR	chromophore	UNP Q6WV12

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Chain	Residue	Modelled	Actual	Comment	Reference
F	57	CR2	GLY	chromophore	UNP Q6WV12

- Molecule 2 is water.

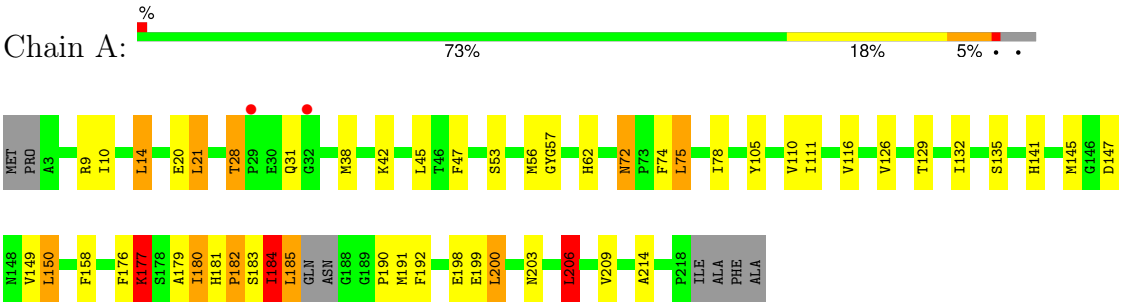
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	47	Total O 47 47	0	0
2	B	47	Total O 47 47	0	0
2	C	29	Total O 29 29	0	0
2	D	40	Total O 40 40	0	0
2	E	16	Total O 16 16	0	0
2	F	35	Total O 35 35	0	0

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.

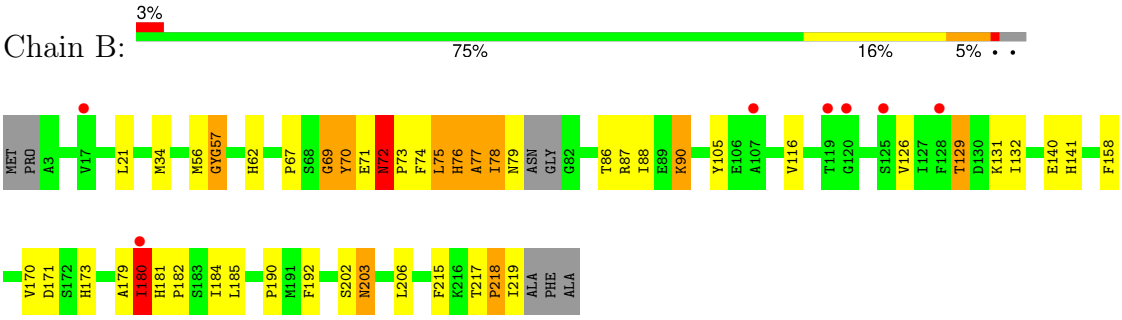
• Molecule 1: green fluorescent protein 2

Chain A:



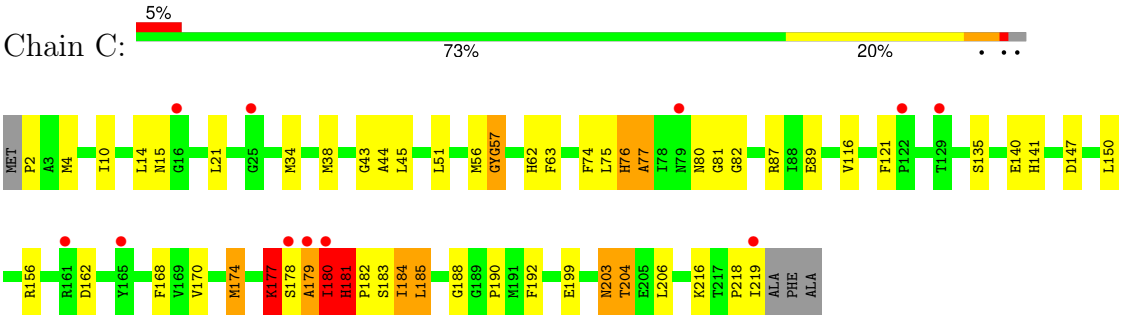
• Molecule 1: green fluorescent protein 2

Chain B:



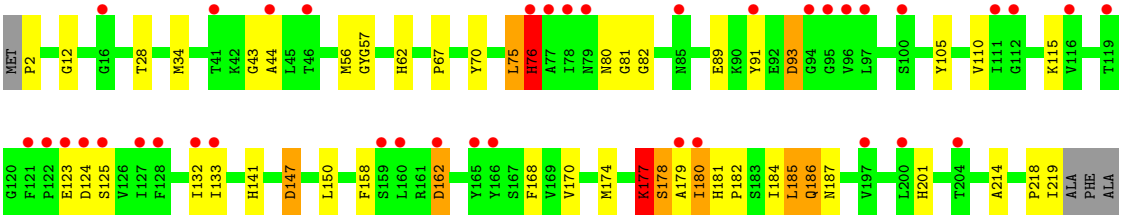
• Molecule 1: green fluorescent protein 2

Chain C:



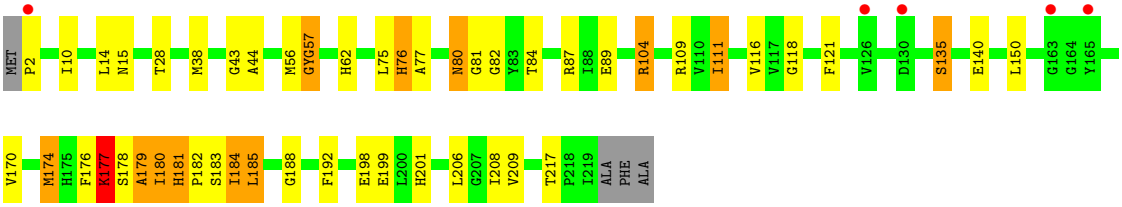
• Molecule 1: green fluorescent protein 2

Chain D:



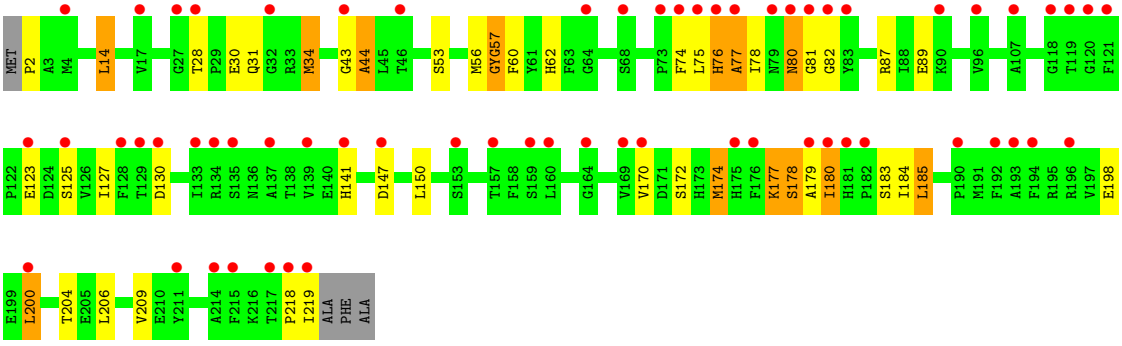
• Molecule 1: green fluorescent protein 2

Chain E:



• Molecule 1: green fluorescent protein 2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	145.95Å 145.95Å 53.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.71 – 2.10 35.71 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.71-2.10) 99.5 (35.71-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.272 0.229 , 0.269	Depositor DCC
R_{free} test set	3752 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 82.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.136 for -h,-k,l 0.179 for h,-h-k,-l 0.096 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9837	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: 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	0.54	2/1645 (0.1%)	0.69	3/2225 (0.1%)
1	B	0.48	0/1632	0.69	1/2210 (0.0%)
1	C	0.41	0/1630	0.68	3/2215 (0.1%)
1	D	0.55	3/1614 (0.2%)	0.71	4/2195 (0.2%)
1	E	0.41	0/1627	0.65	2/2210 (0.1%)
1	F	0.49	0/1619	0.65	1/2200 (0.0%)
All	All	0.48	5/9767 (0.1%)	0.68	14/13255 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	LYS	CE-NZ	8.92	1.71	1.49
1	D	93	ASP	CG-OD2	7.02	1.41	1.25
1	A	185	LEU	C-O	6.09	1.34	1.23
1	D	93	ASP	CG-OD1	5.53	1.38	1.25
1	D	115	LYS	CE-NZ	5.03	1.61	1.49

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	21	LEU	CA-CB-CG	7.86	133.38	115.30
1	D	93	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	D	2	PRO	N-CA-CB	6.02	110.52	103.30
1	A	200	LEU	CA-CB-CG	5.94	128.96	115.30
1	C	2	PRO	N-CA-CB	5.92	110.40	103.30
1	F	2	PRO	N-CA-CB	5.92	110.40	103.30
1	E	2	PRO	N-CA-CB	5.91	110.39	103.30
1	B	21	LEU	CA-CB-CG	5.68	128.35	115.30
1	D	186	GLN	N-CA-C	5.55	125.99	111.00
1	C	203	ASN	C-N-CA	5.53	135.53	121.70
1	A	206	LEU	CA-CB-CG	5.50	127.94	115.30
1	C	203	ASN	N-CA-C	5.43	125.66	111.00
1	D	75	LEU	CA-CB-CG	5.20	127.25	115.30
1	E	181	HIS	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	180	ILE	Peptide
1	E	180	ILE	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	1621	0	1512	34	0
1	B	1609	0	1480	49	0
1	C	1605	0	1420	48	0
1	D	1590	0	1401	41	0
1	E	1603	0	1430	41	0
1	F	1595	0	1411	41	0
2	A	47	0	0	2	0
2	B	47	0	0	2	0
2	C	29	0	0	1	0
2	D	40	0	0	6	0
2	E	16	0	0	1	0
2	F	35	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9837	0	8654	253	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 14.

All (253) 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:177:LYS:NZ	1:A:177:LYS:CE	1.71	1.54
1:B:78:ILE:CB	1:B:79:ASN:HA	1.70	1.19
1:B:181:HIS:HB2	1:B:185:LEU:HG	1.28	1.16
1:F:80:ASN:HB3	1:F:81:GLY:HA2	1.21	1.12
1:D:185:LEU:HA	1:D:187:ASN:H	1.17	1.10
1:B:218:PRO:HB2	1:B:219:ILE:HA	1.13	1.08
1:E:75:LEU:HA	1:E:76:HIS:O	1.57	1.04
1:B:217:THR:HG22	1:B:218:PRO:HA	1.43	1.00
1:B:76:HIS:HA	1:B:78:ILE:HA	1.43	0.99
1:D:75:LEU:HA	1:D:76:HIS:O	1.62	0.97
1:D:185:LEU:HA	1:D:187:ASN:N	1.79	0.96
1:E:180:ILE:HG22	1:E:181:HIS:H	1.34	0.92
1:B:218:PRO:CB	1:B:219:ILE:HA	1.97	0.92
1:C:75:LEU:HA	1:C:76:HIS:O	1.71	0.91
1:E:80:ASN:HA	1:E:179:ALA:HB3	1.52	0.91
1:C:80:ASN:HA	1:C:179:ALA:HB3	1.51	0.89
1:C:180:ILE:HG22	1:C:181:HIS:H	1.37	0.88
1:B:218:PRO:HB2	1:B:219:ILE:CA	2.03	0.84
1:B:76:HIS:HA	1:B:77:ALA:HB3	1.58	0.84
1:C:10:ILE:HD12	1:C:38:MET:HE1	1.59	0.84
1:B:78:ILE:CB	1:B:79:ASN:CA	2.55	0.83
1:C:218:PRO:HA	1:C:219:ILE:CB	2.09	0.82
1:F:80:ASN:HB3	1:F:81:GLY:CA	2.09	0.82
1:F:80:ASN:CB	1:F:81:GLY:HA2	2.09	0.81
1:B:69:GLY:HA2	1:B:70:TYR:O	1.79	0.81
1:A:10:ILE:HD12	1:A:38:MET:HE1	1.62	0.80
1:E:77:ALA:HA	1:E:80:ASN:HB2	1.64	0.79
1:B:56:MET:HE1	1:B:206:LEU:HD23	1.65	0.79
1:E:75:LEU:HA	1:E:76:HIS:C	2.05	0.77
1:F:87:ARG:HD2	1:F:89:GLU:OE2	1.84	0.77
1:E:80:ASN:CB	1:E:81:GLY:HA2	2.16	0.76
1:D:180:ILE:HG22	1:D:181:HIS:H	1.50	0.76
1:D:218:PRO:HA	1:D:219:ILE:CB	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:HA	1:C:76:HIS:C	2.06	0.75
1:A:75:LEU:O	1:A:78:ILE:HG12	1.85	0.75
1:C:180:ILE:HG22	1:C:181:HIS:N	2.02	0.73
1:E:57:CR2:O2	1:E:87:ARG:NH2	2.22	0.73
1:B:73:PRO:HG3	1:B:184:ILE:HD11	1.71	0.71
1:B:76:HIS:CA	1:B:77:ALA:HB3	2.20	0.71
1:B:57:CR2:O2	1:B:87:ARG:NH2	2.24	0.70
1:D:80:ASN:HA	1:D:179:ALA:HB3	1.71	0.70
1:C:77:ALA:HA	1:C:80:ASN:HB2	1.72	0.70
1:B:217:THR:HG22	1:B:218:PRO:CA	2.21	0.70
1:A:181:HIS:O	1:A:183:SER:N	2.25	0.69
1:D:75:LEU:HD12	1:D:75:LEU:O	1.93	0.69
1:B:76:HIS:CA	1:B:78:ILE:HA	2.22	0.69
1:C:180:ILE:CG2	1:C:181:HIS:N	2.55	0.69
1:B:180:ILE:O	1:B:181:HIS:CD2	2.46	0.69
1:D:56:MET:HE3	1:D:201:HIS:HE1	1.58	0.68
1:C:56:MET:HE1	1:C:206:LEU:HD23	1.77	0.67
1:F:177:LYS:N	1:F:178:SER:O	2.28	0.67
1:A:182:PRO:C	1:A:184:ILE:O	2.34	0.66
1:A:126:VAL:O	1:A:129:THR:HG22	1.95	0.66
1:D:185:LEU:CA	1:D:187:ASN:H	2.02	0.66
1:E:56:MET:HE1	1:E:201:HIS:CE1	2.31	0.66
1:D:80:ASN:HB2	1:D:81:GLY:HA2	1.78	0.66
1:F:177:LYS:HB3	1:F:178:SER:CB	2.26	0.65
1:D:177:LYS:N	2:D:234:HOH:O	2.24	0.65
1:E:80:ASN:HB3	1:E:81:GLY:HA2	1.78	0.65
1:E:180:ILE:CG2	1:E:181:HIS:H	2.10	0.65
1:F:75:LEU:HA	1:F:76:HIS:C	2.17	0.65
1:E:10:ILE:HD12	1:E:38:MET:HE1	1.77	0.64
1:E:180:ILE:HG22	1:E:181:HIS:N	2.11	0.64
1:D:93:ASP:OD2	1:D:125:SER:HB2	1.96	0.64
1:A:180:ILE:HG13	1:A:184:ILE:HG13	1.80	0.63
1:E:87:ARG:HD3	1:E:170:VAL:HG11	1.79	0.63
1:B:218:PRO:HD2	1:B:219:ILE:CB	2.29	0.63
1:D:180:ILE:CG2	1:D:181:HIS:H	2.13	0.62
1:D:177:LYS:HB3	1:D:178:SER:CB	2.31	0.61
1:F:130:ASP:HA	2:F:253:HOH:O	2.00	0.61
1:D:80:ASN:HA	1:D:179:ALA:CB	2.31	0.61
1:B:56:MET:CE	1:B:206:LEU:HD23	2.30	0.60
1:C:147:ASP:HB2	1:C:180:ILE:HD11	1.82	0.60
1:B:87:ARG:HD3	1:B:170:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LEU:HA	1:D:76:HIS:C	2.21	0.59
1:E:135:SER:OG	1:E:199:GLU:OE2	2.19	0.59
1:B:202:SER:O	1:B:203:ASN:CB	2.51	0.59
1:B:217:THR:CG2	1:B:218:PRO:HA	2.26	0.59
1:C:56:MET:HE1	1:C:206:LEU:HB3	1.84	0.59
1:A:56:MET:CE	1:A:206:LEU:HD12	2.33	0.59
1:A:62:HIS:H	1:A:62:HIS:CD2	2.21	0.59
1:B:76:HIS:CA	1:B:77:ALA:CB	2.80	0.59
1:E:109:ARG:NH1	1:E:111:ILE:HD12	2.18	0.59
1:D:147:ASP:OD1	1:D:147:ASP:N	2.32	0.58
1:F:74:PHE:O	1:F:77:ALA:HB2	2.04	0.58
1:E:56:MET:HE1	1:E:206:LEU:HB3	1.86	0.58
1:A:183:SER:HA	1:A:184:ILE:C	2.24	0.57
1:D:56:MET:HE3	1:D:201:HIS:CE1	2.38	0.57
1:B:72:ASN:C	1:B:72:ASN:HD22	2.08	0.57
1:B:73:PRO:HG3	1:B:184:ILE:CD1	2.34	0.57
1:B:181:HIS:HB3	1:B:184:ILE:HG13	1.84	0.57
1:E:183:SER:O	1:E:185:LEU:N	2.38	0.57
1:A:56:MET:HE2	1:A:206:LEU:HD12	1.85	0.57
1:A:72:ASN:C	1:A:72:ASN:HD22	2.07	0.57
1:B:62:HIS:CD2	1:B:62:HIS:H	2.23	0.56
1:C:21:LEU:HD11	1:C:45:LEU:HD21	1.87	0.56
1:C:89:GLU:HG2	1:C:170:VAL:HG22	1.87	0.56
1:D:56:MET:CE	1:D:201:HIS:CE1	2.88	0.56
1:F:80:ASN:ND2	1:F:82:GLY:O	2.39	0.56
1:F:62:HIS:H	1:F:62:HIS:CD2	2.22	0.56
1:F:62:HIS:HB3	1:F:75:LEU:HD23	1.86	0.56
1:F:34:MET:HE1	1:F:60:PHE:HB2	1.86	0.56
1:C:80:ASN:CB	1:C:81:GLY:HA2	2.36	0.56
1:C:62:HIS:H	1:C:62:HIS:CD2	2.23	0.56
1:D:180:ILE:HG22	1:D:181:HIS:N	2.18	0.55
1:C:181:HIS:HB3	1:C:182:PRO:O	2.07	0.54
1:A:14:LEU:HD22	1:A:47:PHE:CD2	2.43	0.54
1:E:109:ARG:HH11	1:E:111:ILE:HD12	1.73	0.54
1:D:70:TYR:HA	2:D:251:HOH:O	2.07	0.54
1:A:145:MET:HG2	1:A:149:VAL:HB	1.91	0.53
1:C:183:SER:O	1:C:185:LEU:N	2.41	0.53
1:F:80:ASN:HB3	1:F:82:GLY:HA2	1.91	0.53
1:F:183:SER:C	1:F:185:LEU:H	2.11	0.53
1:D:62:HIS:CD2	1:D:62:HIS:H	2.26	0.52
1:E:56:MET:HE3	1:E:208:ILE:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:PHE:HA	2:B:254:HOH:O	2.10	0.52
1:C:141:HIS:CE1	1:C:190:PRO:HB3	2.44	0.52
1:B:180:ILE:O	1:B:181:HIS:CG	2.62	0.52
2:D:235:HOH:O	1:F:141:HIS:HE1	1.91	0.52
1:D:150:LEU:HD13	1:D:181:HIS:CD2	2.46	0.51
1:C:203:ASN:N	1:C:204:THR:OG1	2.42	0.51
1:F:44:ALA:H	1:F:204:THR:HG22	1.74	0.51
1:F:218:PRO:HA	1:F:219:ILE:CB	2.39	0.51
1:C:80:ASN:HD22	1:C:177:LYS:H	1.59	0.51
1:C:141:HIS:HD2	2:C:229:HOH:O	1.94	0.51
1:D:56:MET:CE	1:D:201:HIS:HE1	2.22	0.50
1:C:203:ASN:H	1:C:204:THR:HG1	1.58	0.50
1:F:150:LEU:HB3	1:F:174:MET:HG3	1.93	0.50
1:B:126:VAL:O	1:B:129:THR:HG22	2.11	0.50
1:E:62:HIS:H	1:E:62:HIS:CD2	2.30	0.50
1:F:76:HIS:O	1:F:78:ILE:N	2.45	0.50
1:E:14:LEU:HD12	1:E:118:GLY:HA3	1.93	0.50
1:E:80:ASN:HD21	1:E:176:PHE:HB3	1.76	0.50
1:A:147:ASP:O	1:A:180:ILE:HG12	2.12	0.49
1:A:150:LEU:HD13	1:A:180:ILE:HD12	1.93	0.49
1:F:147:ASP:HB2	1:F:180:ILE:HD12	1.94	0.49
1:E:56:MET:CE	1:E:201:HIS:CE1	2.95	0.49
1:C:21:LEU:HD21	1:C:206:LEU:HD13	1.94	0.49
1:C:177:LYS:HB3	1:C:178:SER:CB	2.43	0.49
1:D:162:ASP:OD2	1:D:162:ASP:N	2.44	0.49
1:D:80:ASN:CB	1:D:81:GLY:HA2	2.41	0.49
1:E:150:LEU:HB3	1:E:174:MET:HG3	1.94	0.49
1:A:181:HIS:C	1:A:183:SER:H	2.14	0.49
1:C:87:ARG:HD2	1:C:89:GLU:OE2	2.12	0.49
1:F:80:ASN:HA	1:F:179:ALA:HB3	1.94	0.48
1:D:132:ILE:HG23	1:D:158:PHE:HB3	1.96	0.48
1:A:141:HIS:CE1	1:A:190:PRO:HB3	2.48	0.47
1:A:132:ILE:HG23	1:A:158:PHE:HB3	1.95	0.47
1:B:69:GLY:HA2	1:B:70:TYR:C	2.34	0.47
1:E:184:ILE:O	1:E:185:LEU:CB	2.62	0.47
1:D:218:PRO:HB3	1:F:218:PRO:HB3	1.97	0.47
1:E:89:GLU:HG2	1:E:170:VAL:HG13	1.96	0.47
1:A:192:PHE:O	1:A:214:ALA:HA	2.14	0.47
1:B:56:MET:HE1	1:B:206:LEU:HB3	1.96	0.47
1:B:76:HIS:N	1:B:77:ALA:CB	2.77	0.47
1:C:180:ILE:HD13	1:C:180:ILE:HA	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ASN:HB3	2:D:234:HOH:O	2.15	0.47
1:D:81:GLY:HA2	1:D:82:GLY:HA2	1.66	0.47
1:A:135:SER:OG	1:A:199:GLU:OE2	2.32	0.47
1:F:150:LEU:O	1:F:174:MET:HG2	2.15	0.47
1:C:190:PRO:O	1:C:216:LYS:HD3	2.15	0.47
1:F:81:GLY:HA2	1:F:82:GLY:HA2	1.63	0.47
1:C:15:ASN:HD21	1:C:121:PHE:HB2	1.79	0.46
1:E:104:ARG:HG3	1:E:111:ILE:HB	1.97	0.46
1:F:14:LEU:HD21	1:F:127:ILE:CD1	2.45	0.46
1:D:180:ILE:CG2	1:D:181:HIS:N	2.78	0.46
1:A:176:PHE:CD2	1:A:180:ILE:HG22	2.51	0.46
1:B:88:ILE:HG22	1:B:90:LYS:HE2	1.96	0.46
2:A:226:HOH:O	1:B:141:HIS:HE1	1.97	0.46
1:F:200:LEU:HD12	1:F:200:LEU:N	2.31	0.46
1:B:179:ALA:HA	1:B:180:ILE:CB	2.45	0.46
1:C:74:PHE:O	1:C:77:ALA:HB3	2.15	0.46
1:C:56:MET:CE	1:C:206:LEU:HD23	2.46	0.46
1:F:34:MET:CE	1:F:60:PHE:HB2	2.45	0.46
1:D:123:GLU:OE2	1:D:123:GLU:HA	2.16	0.45
1:B:202:SER:O	1:B:203:ASN:HB3	2.15	0.45
1:A:203:ASN:HB2	2:A:247:HOH:O	2.15	0.45
1:B:62:HIS:HE1	1:B:105:TYR:OH	1.99	0.45
1:B:181:HIS:CB	1:B:185:LEU:HG	2.20	0.45
1:C:218:PRO:CA	1:C:219:ILE:CB	2.90	0.45
1:A:198:GLU:HB2	1:A:209:VAL:HB	1.99	0.44
1:B:76:HIS:N	1:B:77:ALA:HB3	2.32	0.44
1:E:76:HIS:HB3	1:E:77:ALA:H	1.49	0.44
1:E:80:ASN:ND2	1:E:178:SER:O	2.50	0.44
1:F:56:MET:HE1	1:F:206:LEU:HD23	1.98	0.44
1:B:141:HIS:CE1	1:B:190:PRO:HB3	2.53	0.44
1:C:38:MET:HE1	1:C:56:MET:HB3	2.00	0.44
1:A:20:GLU:HB3	1:A:42:LYS:HD2	1.99	0.44
1:D:67:PRO:HD3	1:D:214:ALA:O	2.17	0.44
1:C:184:ILE:O	1:C:185:LEU:CB	2.65	0.44
1:F:80:ASN:ND2	1:F:177:LYS:H	2.15	0.44
1:F:75:LEU:HD12	1:F:75:LEU:O	2.18	0.44
1:B:71:GLU:O	1:B:72:ASN:CB	2.65	0.44
1:C:80:ASN:CB	1:C:82:GLY:HA2	2.48	0.44
1:E:84:THR:O	1:E:174:MET:HA	2.17	0.43
1:B:132:ILE:HG23	1:B:158:PHE:HB3	2.00	0.43
1:C:177:LYS:HB3	1:C:178:SER:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:TYR:CD2	1:D:110:VAL:HG12	2.52	0.43
1:B:67:PRO:O	1:B:70:TYR:HB2	2.17	0.43
1:C:81:GLY:HA2	1:C:82:GLY:HA2	1.64	0.43
1:C:135:SER:OG	1:C:199:GLU:OE2	2.28	0.43
1:E:75:LEU:O	1:E:75:LEU:HD12	2.18	0.43
1:B:87:ARG:HD3	1:B:170:VAL:CG1	2.47	0.43
1:F:198:GLU:HB2	1:F:209:VAL:HB	2.00	0.43
1:B:215:PHE:HB2	1:B:217:THR:O	2.19	0.43
1:D:105:TYR:HD2	1:D:110:VAL:HG12	1.84	0.43
1:A:78:ILE:HG22	1:A:105:TYR:CE2	2.54	0.43
1:A:141:HIS:HE1	2:B:223:HOH:O	2.01	0.43
1:A:72:ASN:ND2	1:A:75:LEU:H	2.17	0.43
1:C:147:ASP:HB2	1:C:180:ILE:CD1	2.48	0.43
1:E:140:GLU:O	1:E:192:PHE:HA	2.19	0.43
1:E:81:GLY:HA2	1:E:82:GLY:HA2	1.66	0.42
1:A:10:ILE:CD1	1:A:38:MET:HE1	2.40	0.42
1:A:28:THR:HG23	1:A:31:GLN:HG2	2.01	0.42
1:D:141:HIS:HE1	2:F:227:HOH:O	2.03	0.42
1:F:80:ASN:O	1:F:179:ALA:HB2	2.19	0.42
1:C:150:LEU:HB3	1:C:174:MET:CG	2.49	0.42
1:E:76:HIS:CD2	1:E:182:PRO:HG3	2.54	0.42
1:E:15:ASN:HD21	1:E:121:PHE:HB2	1.84	0.42
1:F:80:ASN:ND2	1:F:178:SER:O	2.53	0.42
1:C:76:HIS:HB3	1:C:77:ALA:H	1.54	0.41
1:D:141:HIS:HD2	2:D:228:HOH:O	2.03	0.41
1:E:109:ARG:HH11	1:E:111:ILE:CD1	2.33	0.41
1:F:125:SER:OG	1:F:127:ILE:HG12	2.20	0.41
1:A:53:SER:HA	1:A:56:MET:HE3	2.01	0.41
1:B:140:GLU:O	1:B:192:PHE:HA	2.20	0.41
1:C:57:CR2:O2	1:C:87:ARG:NH2	2.50	0.41
1:C:140:GLU:O	1:C:192:PHE:HA	2.20	0.41
1:A:72:ASN:HD22	1:A:74:PHE:H	1.67	0.41
1:E:176:PHE:HB3	2:E:228:HOH:O	2.20	0.41
1:E:177:LYS:HB3	1:E:178:SER:CB	2.51	0.41
1:D:177:LYS:HE2	1:D:177:LYS:HA	2.03	0.41
1:F:76:HIS:HB3	1:F:77:ALA:H	1.62	0.41
1:C:156:ARG:HD3	1:C:168:PHE:CZ	2.56	0.41
1:A:105:TYR:CD2	1:A:110:VAL:HG12	2.55	0.41
1:D:91:TYR:CD2	1:D:168:PHE:HB3	2.56	0.41
1:E:180:ILE:CG2	1:E:181:HIS:N	2.76	0.41
1:B:129:THR:HG23	1:B:131:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:HD12	1:C:75:LEU:O	2.20	0.41
1:C:80:ASN:CA	1:C:179:ALA:HB3	2.36	0.41
1:E:177:LYS:CG	1:E:178:SER:CB	2.99	0.41
1:F:141:HIS:HD2	2:F:249:HOH:O	2.03	0.41
1:F:80:ASN:HD21	1:F:177:LYS:H	1.69	0.40
1:F:89:GLU:HG2	1:F:170:VAL:HG22	2.04	0.40
1:A:184:ILE:HA	1:A:185:LEU:CB	2.50	0.40
1:C:80:ASN:HB2	1:C:82:GLY:HA2	2.04	0.40
1:E:198:GLU:HB2	1:E:209:VAL:HB	2.03	0.40
1:B:90:LYS:NZ	1:B:171:ASP:OD2	2.55	0.40
1:C:4:MET:HB3	1:C:63:PHE:HE2	1.87	0.40
1:D:89:GLU:HG2	1:D:170:VAL:HG22	2.03	0.40
1:F:57:CR2:O2	1:F:87:ARG:NH2	2.55	0.40
1:D:12:GLY:HA2	2:D:241:HOH:O	2.20	0.40
1:F:53:SER:HA	1:F:56:MET:CE	2.51	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	205/220 (93%)	193 (94%)	9 (4%)	3 (2%)	8	5
1	B	206/220 (94%)	186 (90%)	9 (4%)	11 (5%)	1	0
1	C	211/220 (96%)	189 (90%)	10 (5%)	12 (6%)	1	0
1	D	211/220 (96%)	192 (91%)	9 (4%)	10 (5%)	2	0
1	E	211/220 (96%)	191 (90%)	12 (6%)	8 (4%)	2	1
1	F	211/220 (96%)	192 (91%)	10 (5%)	9 (4%)	2	0
All	All	1255/1320 (95%)	1143 (91%)	59 (5%)	53 (4%)	2	0

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ILE
1	B	70	TYR
1	B	76	HIS
1	B	77	ALA
1	B	182	PRO
1	B	218	PRO
1	C	76	HIS
1	C	177	LYS
1	C	180	ILE
1	C	184	ILE
1	C	185	LEU
1	C	204	THR
1	D	76	HIS
1	D	177	LYS
1	D	180	ILE
1	D	186	GLN
1	E	76	HIS
1	E	177	LYS
1	E	179	ALA
1	E	184	ILE
1	E	185	LEU
1	F	77	ALA
1	F	80	ASN
1	A	179	ALA
1	A	182	PRO
1	B	75	LEU
1	B	180	ILE
1	C	44	ALA
1	C	77	ALA
1	C	179	ALA
1	D	43	GLY
1	E	43	GLY
1	F	43	GLY
1	F	180	ILE
1	F	184	ILE
1	B	72	ASN
1	C	43	GLY
1	C	188	GLY
1	D	44	ALA
1	D	184	ILE
1	D	185	LEU
1	F	185	LEU
1	B	78	ILE

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Mol	Chain	Res	Type
1	C	181	HIS
1	F	44	ALA
1	E	44	ALA
1	F	178	SER
1	B	69	GLY
1	B	203	ASN
1	D	178	SER
1	F	177	LYS
1	E	188	GLY
1	D	182	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	161/183 (88%)	145 (90%)	16 (10%)	6 4
1	B	156/183 (85%)	148 (95%)	8 (5%)	20 19
1	C	150/183 (82%)	141 (94%)	9 (6%)	16 14
1	D	147/183 (80%)	138 (94%)	9 (6%)	15 13
1	E	150/183 (82%)	141 (94%)	9 (6%)	16 14
1	F	148/183 (81%)	138 (93%)	10 (7%)	13 11
All	All	912/1098 (83%)	851 (93%)	61 (7%)	13 11

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	14	LEU
1	A	21	LEU
1	A	28	THR
1	A	45	LEU
1	A	72	ASN
1	A	75	LEU
1	A	111	ILE

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Mol	Chain	Res	Type
1	A	116	VAL
1	A	150	LEU
1	A	177	LYS
1	A	180	ILE
1	A	184	ILE
1	A	191	MET
1	A	200	LEU
1	A	206	LEU
1	B	34	MET
1	B	72	ASN
1	B	75	LEU
1	B	86	THR
1	B	90	LYS
1	B	116	VAL
1	B	129	THR
1	B	173	HIS
1	C	14	LEU
1	C	34	MET
1	C	51	LEU
1	C	116	VAL
1	C	162	ASP
1	C	174	MET
1	C	177	LYS
1	C	180	ILE
1	C	181	HIS
1	D	28	THR
1	D	34	MET
1	D	76	HIS
1	D	124	ASP
1	D	133	ILE
1	D	147	ASP
1	D	162	ASP
1	D	174	MET
1	D	177	LYS
1	E	28	THR
1	E	80	ASN
1	E	104	ARG
1	E	111	ILE
1	E	116	VAL
1	E	135	SER
1	E	174	MET
1	E	177	LYS

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Mol	Chain	Res	Type
1	E	217	THR
1	F	14	LEU
1	F	28	THR
1	F	30	GLU
1	F	31	GLN
1	F	34	MET
1	F	76	HIS
1	F	123	GLU
1	F	172	SER
1	F	174	MET
1	F	200	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	72	ASN
1	A	141	HIS
1	A	148	ASN
1	B	62	HIS
1	B	72	ASN
1	B	141	HIS
1	C	15	ASN
1	C	62	HIS
1	C	80	ASN
1	C	141	HIS
1	D	62	HIS
1	D	141	HIS
1	E	62	HIS
1	E	76	HIS
1	E	80	ASN
1	E	141	HIS
1	F	62	HIS
1	F	141	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

6 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	57	1	20,20,21	2.76	6 (30%)	25,27,29	6.71	11 (44%)
1	CR2	E	57	1	20,20,21	2.64	6 (30%)	25,27,29	6.53	12 (48%)
1	CR2	A	57	1	20,20,21	2.66	5 (25%)	25,27,29	5.97	11 (44%)
1	CR2	B	57	1	20,20,21	2.67	5 (25%)	25,27,29	5.90	12 (48%)
1	CR2	F	57	1	20,20,21	2.73	6 (30%)	25,27,29	6.10	14 (56%)
1	CR2	D	57	1	20,20,21	2.72	6 (30%)	25,27,29	6.09	14 (56%)

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	57	1	-	0/6/25/26	0/2/2/2
1	CR2	E	57	1	-	0/6/25/26	0/2/2/2
1	CR2	A	57	1	-	0/6/25/26	0/2/2/2
1	CR2	B	57	1	-	0/6/25/26	0/2/2/2
1	CR2	F	57	1	-	0/6/25/26	0/2/2/2
1	CR2	D	57	1	-	0/6/25/26	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	57	CR2	CG2-CB2	-9.61	1.29	1.46
1	D	57	CR2	CG2-CB2	-9.58	1.29	1.46
1	F	57	CR2	CG2-CB2	-9.55	1.29	1.46
1	A	57	CR2	CG2-CB2	-9.39	1.29	1.46
1	B	57	CR2	CG2-CB2	-9.20	1.29	1.46
1	E	57	CR2	CG2-CB2	-9.14	1.30	1.46
1	A	57	CR2	OH-CZ	-5.09	1.25	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	57	CR2	OH-CZ	-5.02	1.25	1.37
1	C	57	CR2	OH-CZ	-4.90	1.26	1.37
1	B	57	CR2	OH-CZ	-4.81	1.26	1.37
1	F	57	CR2	OH-CZ	-4.72	1.26	1.37
1	E	57	CR2	OH-CZ	-4.71	1.26	1.37
1	F	57	CR2	O2-C2	3.04	1.29	1.23
1	C	57	CR2	O2-C2	3.01	1.29	1.23
1	E	57	CR2	O2-C2	2.95	1.29	1.23
1	D	57	CR2	O2-C2	2.71	1.28	1.23
1	B	57	CR2	O2-C2	2.70	1.28	1.23
1	C	57	CR2	C2-N3	-2.66	1.33	1.40
1	E	57	CR2	CA2-N2	-2.57	1.33	1.38
1	F	57	CR2	C2-N3	-2.53	1.34	1.40
1	C	57	CR2	CA2-N2	-2.50	1.33	1.38
1	A	57	CR2	O2-C2	2.47	1.28	1.23
1	D	57	CR2	C2-N3	-2.47	1.34	1.40
1	E	57	CR2	C2-N3	-2.46	1.34	1.40
1	B	57	CR2	C2-N3	-2.45	1.34	1.40
1	B	57	CR2	C1-N2	2.41	1.36	1.32
1	A	57	CR2	C2-N3	-2.38	1.34	1.40
1	F	57	CR2	CA2-N2	-2.25	1.33	1.38
1	F	57	CR2	C1-N2	2.21	1.36	1.32
1	D	57	CR2	C1-N2	2.21	1.36	1.32
1	C	57	CR2	C1-N2	2.19	1.36	1.32
1	E	57	CR2	C1-N2	2.14	1.36	1.32
1	D	57	CR2	CA2-N2	-2.13	1.34	1.38
1	A	57	CR2	C1-N2	2.06	1.36	1.32

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	57	CR2	CG2-CB2-CA2	28.97	164.31	129.87
1	E	57	CR2	CG2-CB2-CA2	27.23	162.23	129.87
1	D	57	CR2	CG2-CB2-CA2	24.69	159.22	129.87
1	F	57	CR2	CG2-CB2-CA2	24.59	159.10	129.87
1	A	57	CR2	CG2-CB2-CA2	23.55	157.86	129.87
1	B	57	CR2	CG2-CB2-CA2	23.16	157.39	129.87
1	E	57	CR2	CB2-CA2-C2	11.70	136.53	122.36
1	B	57	CR2	CB2-CA2-C2	11.69	136.53	122.36
1	A	57	CR2	CB2-CA2-C2	11.48	136.28	122.36
1	F	57	CR2	CB2-CA2-C2	10.99	135.67	122.36
1	D	57	CR2	CB2-CA2-C2	10.90	135.57	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	57	CR2	CB2-CA2-C2	10.29	134.83	122.36
1	E	57	CR2	CB2-CA2-N2	-9.13	116.37	128.76
1	B	57	CR2	CB2-CA2-N2	-8.97	116.58	128.76
1	F	57	CR2	CB2-CA2-N2	-8.77	116.85	128.76
1	A	57	CR2	CB2-CA2-N2	-8.71	116.94	128.76
1	D	57	CR2	CB2-CA2-N2	-8.50	117.22	128.76
1	C	57	CR2	CB2-CA2-N2	-7.83	118.13	128.76
1	A	57	CR2	O2-C2-CA2	-6.07	127.15	131.02
1	F	57	CR2	O2-C2-CA2	-5.96	127.22	131.02
1	D	57	CR2	O2-C2-CA2	-5.68	127.40	131.02
1	C	57	CR2	O2-C2-CA2	-5.63	127.43	131.02
1	B	57	CR2	CA2-C2-N3	4.93	107.64	103.50
1	A	57	CR2	CA2-C2-N3	4.87	107.59	103.50
1	B	57	CR2	O2-C2-CA2	-4.77	127.97	131.02
1	C	57	CR2	CA2-C2-N3	4.67	107.42	103.50
1	D	57	CR2	CA2-C2-N3	4.63	107.39	103.50
1	F	57	CR2	CA2-C2-N3	4.43	107.22	103.50
1	E	57	CR2	CA2-C2-N3	4.40	107.19	103.50
1	E	57	CR2	O2-C2-CA2	-4.39	128.22	131.02
1	A	57	CR2	C2-N3-C1	-4.15	106.21	108.08
1	E	57	CR2	C2-N3-C1	-3.96	106.30	108.08
1	D	57	CR2	C2-N3-C1	-3.93	106.31	108.08
1	F	57	CR2	C2-N3-C1	-3.74	106.40	108.08
1	B	57	CR2	C2-N3-C1	-3.72	106.40	108.08
1	C	57	CR2	C2-N3-C1	-3.60	106.46	108.08
1	C	57	CR2	CA1-C1-N3	3.08	126.65	122.52
1	A	57	CR2	C2-CA2-N2	-3.02	106.78	108.95
1	B	57	CR2	C2-CA2-N2	-3.01	106.79	108.95
1	E	57	CR2	CA1-C1-N3	2.78	126.24	122.52
1	D	57	CR2	CD2-CG2-CB2	-2.77	111.71	121.22
1	F	57	CR2	CD2-CG2-CB2	-2.73	111.82	121.22
1	F	57	CR2	C1-CA1-N1	-2.73	106.81	112.85
1	F	57	CR2	CA1-C1-N3	2.71	126.14	122.52
1	C	57	CR2	C2-CA2-N2	-2.67	107.04	108.95
1	C	57	CR2	C1-CA1-N1	-2.65	106.98	112.85
1	B	57	CR2	CD1-CG2-CB2	-2.64	112.14	121.22
1	D	57	CR2	CE1-CD1-CG2	-2.62	117.83	121.22
1	F	57	CR2	CE1-CD1-CG2	-2.62	117.83	121.22
1	B	57	CR2	CA1-C1-N3	2.62	126.03	122.52
1	E	57	CR2	C2-CA2-N2	-2.60	107.09	108.95
1	A	57	CR2	CD1-CG2-CB2	-2.59	112.34	121.22
1	B	57	CR2	CE2-CD2-CG2	-2.56	117.91	121.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	CR2	C1-CA1-N1	-2.54	107.23	112.85
1	D	57	CR2	C2-CA2-N2	-2.51	107.15	108.95
1	D	57	CR2	C1-CA1-N1	-2.48	107.37	112.85
1	A	57	CR2	CA1-C1-N3	2.31	125.61	122.52
1	D	57	CR2	O3-C3-CA3	-2.30	115.12	125.47
1	E	57	CR2	CD2-CG2-CB2	-2.27	113.44	121.22
1	D	57	CR2	CA1-C1-N3	2.26	125.55	122.52
1	C	57	CR2	CD2-CG2-CB2	-2.21	113.64	121.22
1	C	57	CR2	CA1-C1-N2	-2.20	121.34	124.28
1	E	57	CR2	CE1-CD1-CG2	-2.19	118.39	121.22
1	A	57	CR2	CD2-CG2-CB2	2.17	128.69	121.22
1	F	57	CR2	CA1-C1-N2	-2.15	121.40	124.28
1	F	57	CR2	C2-CA2-N2	-2.12	107.44	108.95
1	B	57	CR2	C1-CA1-N1	-2.08	108.26	112.85
1	E	57	CR2	CA3-N3-C2	2.07	128.22	123.67
1	E	57	CR2	CA1-C1-N2	-2.06	121.51	124.28
1	F	57	CR2	CD1-CG2-CB2	2.06	128.30	121.22
1	D	57	CR2	CD1-CG2-CB2	2.06	128.29	121.22
1	B	57	CR2	CD2-CG2-CB2	2.06	128.29	121.22
1	D	57	CR2	CA3-N3-C2	2.02	128.11	123.67
1	F	57	CR2	O3-C3-CA3	-2.01	116.42	125.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	57	CR2	1	0
1	E	57	CR2	1	0
1	B	57	CR2	1	0
1	F	57	CR2	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	211/220 (95%)	-0.15	2 (0%) 81 82	35, 39, 43, 48	0
1	B	212/220 (96%)	-0.08	7 (3%) 49 51	34, 39, 45, 57	0
1	C	215/220 (97%)	0.04	11 (5%) 34 36	35, 39, 42, 48	0
1	D	215/220 (97%)	0.90	38 (17%) 4 5	36, 39, 42, 48	0
1	E	215/220 (97%)	0.06	5 (2%) 61 63	35, 39, 41, 48	0
1	F	215/220 (97%)	1.39	63 (29%) 1 1	35, 39, 42, 48	0
All	All	1283/1320 (97%)	0.36	126 (9%) 14 15	34, 39, 42, 57	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	GLY	5.3
1	F	179	ALA	5.0
1	D	96	VAL	4.7
1	F	160	LEU	4.5
1	C	179	ALA	4.5
1	F	217	THR	4.1
1	F	135	SER	4.1
1	F	82	GLY	4.1
1	D	125	SER	4.0
1	F	175	HIS	4.0
1	F	107	ALA	3.8
1	D	180	ILE	3.7
1	D	91	TYR	3.7
1	F	164	GLY	3.5
1	F	81	GLY	3.4
1	B	128	PHE	3.4
1	D	128	PHE	3.3
1	F	74	PHE	3.3
1	F	125	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	182	PRO	3.3
1	F	32	GLY	3.3
1	F	181	HIS	3.3
1	D	160	LEU	3.2
1	F	192	PHE	3.2
1	D	44	ALA	3.2
1	F	169	VAL	3.1
1	F	194	PHE	3.1
1	F	73	PRO	3.0
1	F	27	GLY	3.0
1	F	75	LEU	3.0
1	C	178	SER	3.0
1	D	166	TYR	3.0
1	F	80	ASN	3.0
1	D	159	SER	3.0
1	E	163	GLY	3.0
1	F	130	ASP	2.9
1	F	121	PHE	2.9
1	F	219	ILE	2.9
1	F	211	TYR	2.9
1	D	112	GLY	2.9
1	D	79	ASN	2.8
1	E	126	VAL	2.8
1	F	147	ASP	2.8
1	D	76	HIS	2.8
1	F	193	ALA	2.7
1	D	94	GLY	2.7
1	F	218	PRO	2.7
1	F	43	GLY	2.7
1	D	127	ILE	2.7
1	F	79	ASN	2.6
1	F	137	ALA	2.6
1	D	179	ALA	2.6
1	F	134	ARG	2.6
1	F	153	SER	2.6
1	D	200	LEU	2.6
1	D	124	ASP	2.5
1	F	180	ILE	2.5
1	B	17	VAL	2.5
1	F	139	VAL	2.5
1	F	176	PHE	2.5
1	F	215	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	123	GLU	2.5
1	B	180	ILE	2.5
1	D	78	ILE	2.5
1	F	133	ILE	2.5
1	F	96	VAL	2.5
1	F	76	HIS	2.4
1	F	141	HIS	2.4
1	D	16	GLY	2.4
1	F	119	THR	2.4
1	F	83	TYR	2.4
1	D	111	ILE	2.4
1	D	133	ILE	2.4
1	F	196	ARG	2.4
1	F	214	ALA	2.4
1	D	46	THR	2.4
1	D	122	PRO	2.4
1	F	128	PHE	2.4
1	E	130	ASP	2.4
1	F	123	GLU	2.4
1	C	219	ILE	2.4
1	D	100	SER	2.3
1	F	68	SER	2.3
1	C	25	GLY	2.3
1	D	132	ILE	2.3
1	B	119	THR	2.3
1	D	116	VAL	2.3
1	C	180	ILE	2.3
1	C	79	ASN	2.3
1	A	29	PRO	2.3
1	F	64	GLY	2.3
1	F	120	GLY	2.3
1	D	97	LEU	2.3
1	F	159	SER	2.3
1	D	95	GLY	2.2
1	D	41	THR	2.2
1	F	157	THR	2.2
1	E	2	PRO	2.2
1	F	200	LEU	2.2
1	F	129	THR	2.2
1	C	16	GLY	2.2
1	F	4	MET	2.2
1	D	121	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	165	TYR	2.2
1	D	204	THR	2.2
1	F	190	PRO	2.2
1	D	197	VAL	2.2
1	F	17	VAL	2.2
1	C	129	THR	2.1
1	E	165	TYR	2.1
1	F	118	GLY	2.1
1	C	161	ARG	2.1
1	F	46	THR	2.1
1	F	170	VAL	2.1
1	F	90	LYS	2.1
1	F	28	THR	2.1
1	B	107	ALA	2.1
1	C	122	PRO	2.1
1	D	119	THR	2.1
1	B	120	GLY	2.0
1	F	77	ALA	2.0
1	B	125	SER	2.0
1	D	85	ASN	2.0
1	D	77	ALA	2.0
1	D	165	TYR	2.0
1	D	162	ASP	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	CR2	E	57	19/20	0.95	0.08	32,35,38,39	0
1	CR2	C	57	19/20	0.97	0.07	32,35,38,38	0
1	CR2	D	57	19/20	0.97	0.08	30,33,37,37	0
1	CR2	B	57	19/20	0.97	0.07	21,26,34,34	0
1	CR2	F	57	19/20	0.97	0.07	30,34,37,39	0
1	CR2	A	57	19/20	0.98	0.06	22,25,33,33	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.