Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 03:36 AM EDT

PDB ID	:	5K19
Title	:	Crystal structure of WD repeat-containing protein 20
Authors	:	Li, H.; D'Andrea, A.D.; Zheng, N.
Deposited on	:	2016-05-17
Resolution	:	2.60 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 (i)) were used in the production of this report:

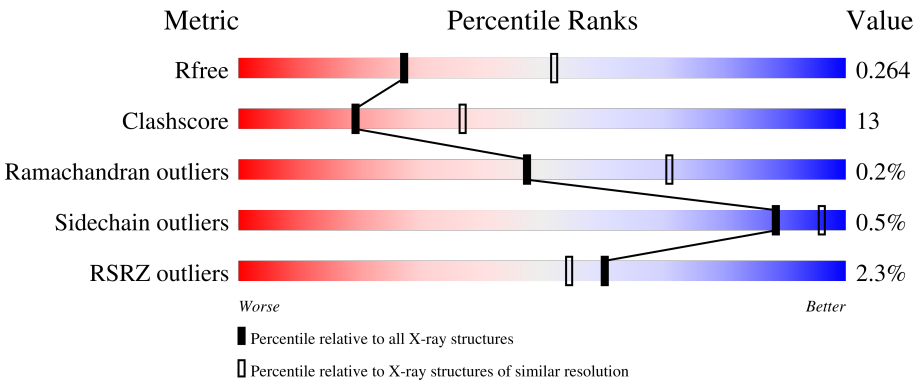
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	569	% 51% 14% 34%
1	B	569	51% 13% • 34%
1	C	569	4% 45% 17% • 37%

2 Entry composition (i)

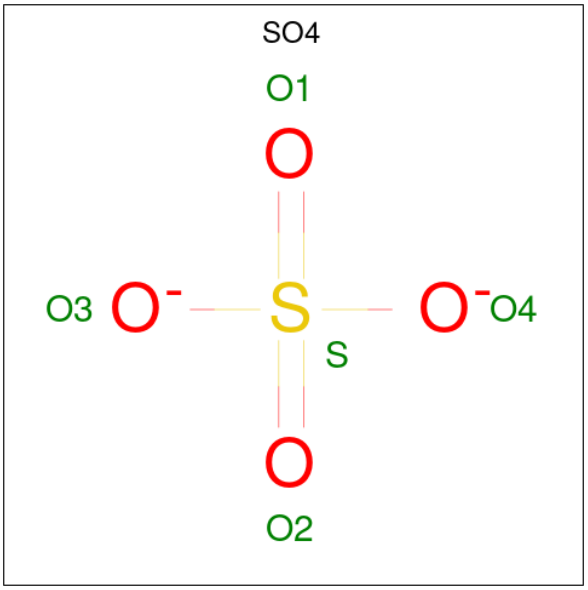
There are 4 unique types of molecules in this entry. The entry contains 8526 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 WD repeat-containing protein 20.

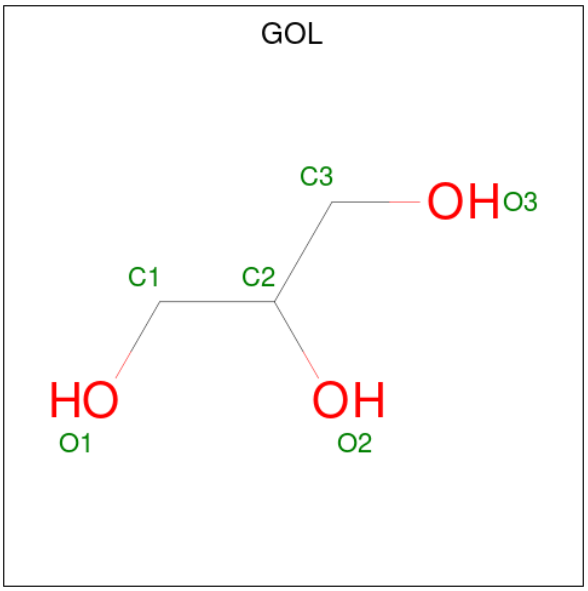
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	376	2899	1871	483	529	16	0	0	0
1	B	373	2867	1847	483	521	16	0	0	0
1	C	359	2663	1722	440	486	15	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0

- Molecule 4 is water.

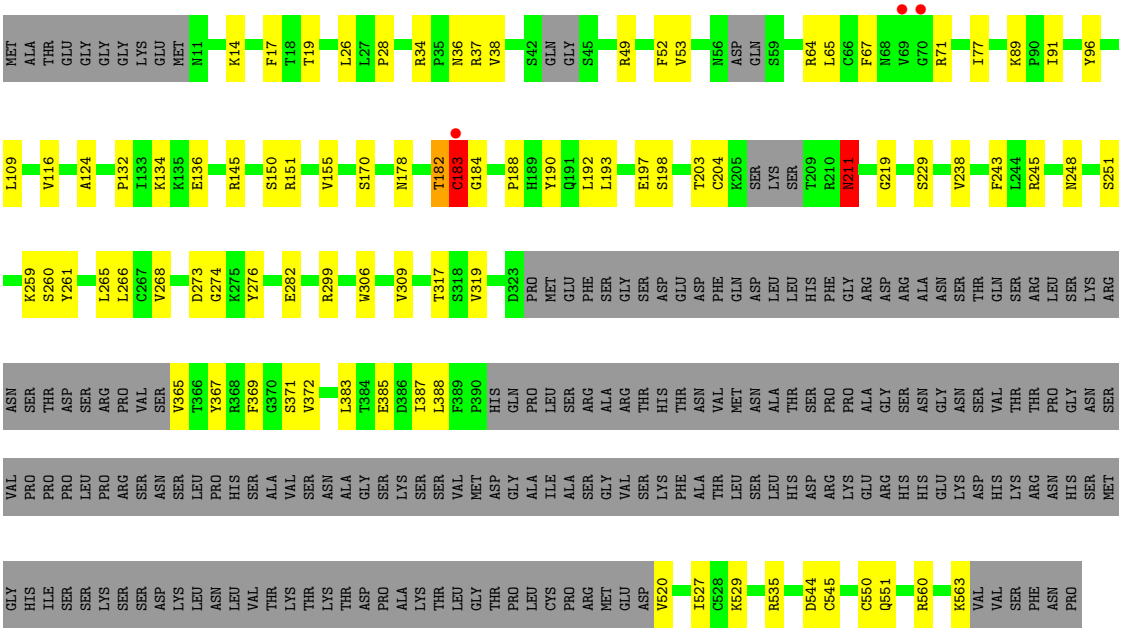
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	29	29	29	0	0
			Total	O		
4	B	25	25	25	0	0
			Total	O		
4	C	3	3	3	0	0

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.

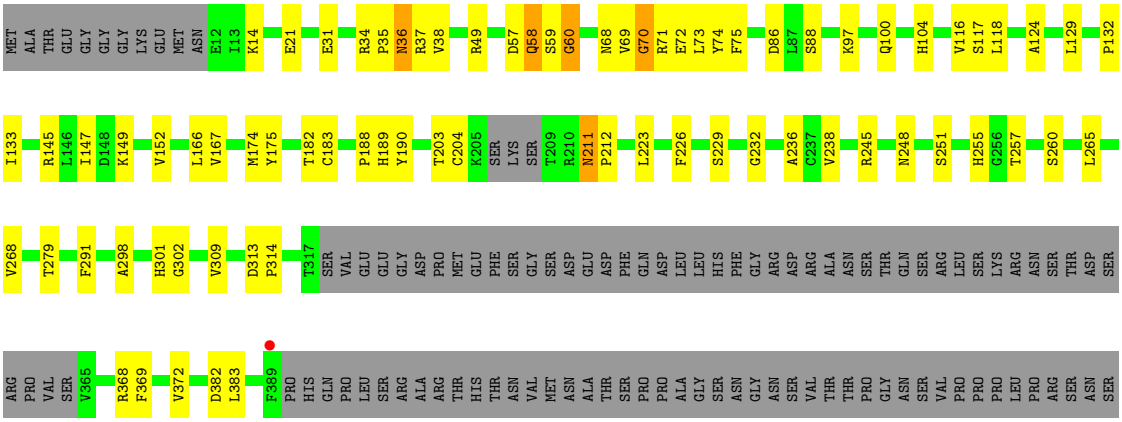
• Molecule 1: WD repeat-containing protein 20

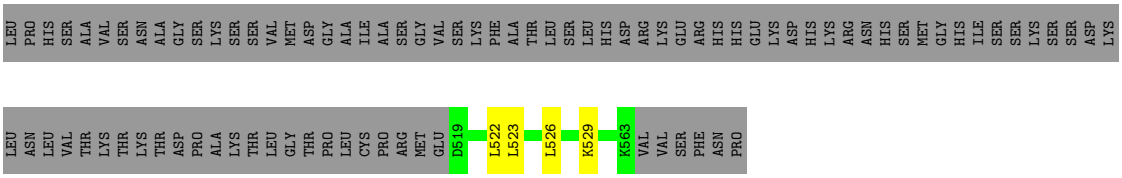
Chain A:



• Molecule 1: WD repeat-containing protein 20

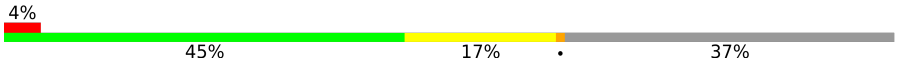
Chain B:

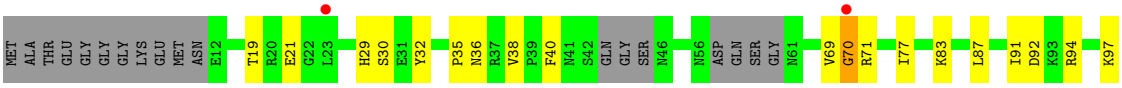


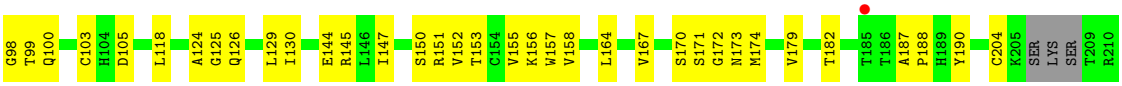


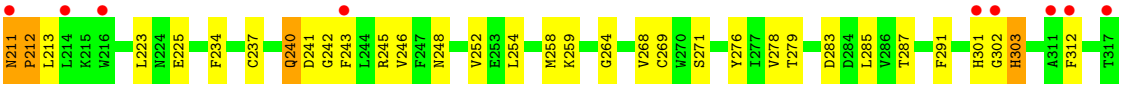
- Molecule 1: WD repeat-containing protein 20

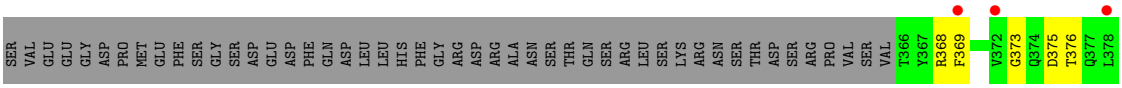
Chain C:

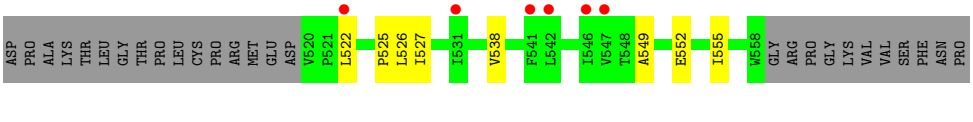












4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	120.01Å 120.01Å 95.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.63 – 2.60 45.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.63-2.60) 91.8 (45.63-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.61Å)	Xtriage
Refinement program	PHENIX dev_1760	Depositor
R, R_{free}	0.191 , 0.257 0.208 , 0.264	Depositor DCC
R_{free} test set	2241 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.216 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8526	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: GOL, SO4

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	0/2971	0.72	2/4035 (0.0%)
1	B	0.62	5/2940 (0.2%)	0.78	8/3998 (0.2%)
1	C	0.48	1/2732 (0.0%)	0.61	3/3736 (0.1%)
All	All	0.55	6/8643 (0.1%)	0.71	13/11769 (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	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	70	GLY	N-CA	-11.60	1.28	1.46
1	B	70	GLY	N-CA	-8.94	1.32	1.46
1	B	60	GLY	N-CA	-6.04	1.36	1.46
1	B	69	VAL	C-N	5.90	1.43	1.33
1	B	58	GLN	C-N	5.65	1.47	1.34
1	B	60	GLY	CA-C	-5.01	1.43	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	36	ASN	O-C-N	9.27	137.53	122.70
1	B	69	VAL	CB-CA-C	8.96	128.42	111.40
1	B	60	GLY	O-C-N	7.79	135.17	122.70
1	B	36	ASN	CA-C-N	-7.48	100.74	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	70	GLY	O-C-N	6.65	133.35	122.70
1	A	211	ASN	C-N-CD	6.13	141.28	128.40
1	B	211	ASN	C-N-CD	6.03	141.07	128.40
1	A	211	ASN	N-CA-C	6.02	127.25	111.00
1	C	211	ASN	C-N-CD	5.99	140.97	128.40
1	C	69	VAL	CB-CA-C	-5.97	100.05	111.40
1	B	59	SER	CA-C-N	-5.96	104.27	116.20
1	C	70	GLY	CA-C-O	5.30	130.15	120.60
1	B	36	ASN	C-N-CA	-5.21	108.68	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	THR	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	2899	0	2794	74	0
1	B	2867	0	2745	65	0
1	C	2663	0	2425	74	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	6	0	8	2	0
3	B	18	0	24	7	0
3	C	6	0	8	0	0
4	A	29	0	0	5	0
4	B	25	0	0	2	0
4	C	3	0	0	1	0
All	All	8526	0	8004	213	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 (213) 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:266:LEU:HD11	1:A:282:GLU:HG3	1.46	0.98
1:A:211:ASN:O	1:A:211:ASN:ND2	1.97	0.96
1:C:268:VAL:HG12	1:C:269:CYS:N	1.82	0.92
1:B:145:ARG:HH22	3:B:603:GOL:H2	1.33	0.91
1:A:178:ASN:H	1:A:211:ASN:HD21	1.17	0.90
1:A:183:CYS:HB3	1:A:184:GLY:HA2	1.52	0.89
1:C:182:THR:O	1:C:211:ASN:HB2	1.73	0.89
1:C:171:SER:OG	1:C:173:ASN:ND2	2.05	0.88
1:A:544:ASP:HA	1:A:563:LYS:HD3	1.57	0.85
1:A:36:ASN:ND2	4:A:701:HOH:O	1.89	0.85
1:A:52:PHE:CE1	1:A:65:LEU:HD12	2.14	0.82
1:C:151:ARG:HG2	1:C:170:SER:HB2	1.61	0.81
1:A:183:CYS:CB	1:A:184:GLY:HA2	2.12	0.80
1:C:268:VAL:CG1	1:C:269:CYS:N	2.45	0.80
1:C:150:SER:HB2	1:C:170:SER:HB3	1.67	0.76
1:B:182:THR:O	1:B:211:ASN:HB2	1.87	0.75
1:A:365:VAL:N	1:A:385:GLU:OE2	2.20	0.74
1:B:302:GLY:N	4:B:701:HOH:O	2.06	0.73
1:A:178:ASN:H	1:A:211:ASN:ND2	1.85	0.73
1:A:274:GLY:HA3	3:A:602:GOL:H12	1.68	0.73
1:B:58:GLN:C	1:B:60:GLY:N	2.43	0.72
1:C:70:GLY:O	1:C:100:GLN:HB3	1.89	0.72
1:A:178:ASN:N	1:A:211:ASN:HD21	1.89	0.70
1:B:145:ARG:NH2	3:B:603:GOL:H2	2.05	0.69
1:A:182:THR:OG1	1:A:183:CYS:HB2	1.91	0.69
1:A:550:CYS:SG	4:A:708:HOH:O	2.52	0.68
1:C:125:GLY:HA2	1:C:152:VAL:HG23	1.76	0.68
1:A:151:ARG:HG2	1:A:170:SER:HB2	1.76	0.68
1:C:105:ASP:OD1	1:C:156:LYS:NZ	2.26	0.68
1:C:124:ALA:HB1	1:C:145:ARG:HD3	1.79	0.65
1:C:268:VAL:CG1	1:C:269:CYS:H	2.09	0.64
1:A:182:THR:O	1:A:211:ASN:HB2	1.97	0.64
1:B:70:GLY:O	1:B:100:GLN:OE1	2.16	0.64
1:A:150:SER:HB2	1:A:170:SER:HB3	1.79	0.63
1:A:365:VAL:HG12	1:A:385:GLU:HG3	1.79	0.63
1:C:70:GLY:O	1:C:100:GLN:CD	2.36	0.63
1:B:34:ARG:HH21	1:B:38:VAL:HG22	1.64	0.63
1:B:21:GLU:CD	1:B:368:ARG:HH22	2.03	0.62
1:A:520:VAL:N	4:A:703:HOH:O	2.32	0.62
1:C:77:ILE:HG23	4:C:703:HOH:O	1.98	0.62
1:C:70:GLY:O	1:C:100:GLN:OE1	2.17	0.62
1:B:248:ASN:HB3	1:B:251:SER:OG	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASN:O	1:C:213:LEU:N	2.34	0.61
1:C:71:ARG:NH2	1:C:97:LYS:C	2.55	0.61
1:B:382:ASP:HB2	1:B:526:LEU:HD21	1.83	0.60
1:A:238:VAL:HG13	1:A:268:VAL:CG1	2.32	0.60
1:B:369:PHE:HE2	1:B:383:LEU:HD23	1.66	0.59
1:B:245:ARG:HG2	1:B:257:THR:HG22	1.84	0.59
1:B:49:ARG:HH11	3:B:604:GOL:H12	1.67	0.58
1:A:124:ALA:HB1	1:A:145:ARG:HD3	1.86	0.58
1:A:34:ARG:NH2	1:A:38:VAL:O	2.36	0.58
1:C:240:GLN:HA	1:C:264:GLY:HA3	1.85	0.57
1:B:260:SER:HB3	1:B:265:LEU:HD21	1.85	0.57
1:A:183:CYS:SG	1:A:184:GLY:HA2	2.45	0.57
1:B:248:ASN:CG	1:B:251:SER:OG	2.42	0.57
1:A:219:GLY:HA3	1:A:245:ARG:NH2	2.19	0.57
1:B:21:GLU:OE1	1:B:368:ARG:NH2	2.37	0.57
1:A:369:PHE:HE1	1:A:383:LEU:HD23	1.70	0.56
1:C:243:PHE:CZ	1:C:259:LYS:HD2	2.40	0.56
1:C:538:VAL:HB	1:C:549:ALA:HB3	1.88	0.56
1:C:312:PHE:CD1	1:C:369:PHE:HB3	2.41	0.56
1:B:71:ARG:NH1	1:B:97:LYS:O	2.37	0.56
1:C:302:GLY:O	1:C:379:CYS:SG	2.64	0.56
1:C:285:LEU:HD11	1:C:301:HIS:CD2	2.42	0.55
1:A:317:THR:HG22	1:A:319:VAL:H	1.70	0.55
1:A:383:LEU:HA	1:A:387:ILE:HD12	1.89	0.55
1:C:32:TYR:HB2	1:C:555:ILE:HB	1.88	0.55
1:A:183:CYS:CB	1:A:184:GLY:CA	2.83	0.55
1:C:36:ASN:OD1	1:C:38:VAL:HG13	2.08	0.54
1:B:36:ASN:O	1:B:37:ARG:HB2	2.08	0.54
1:C:71:ARG:HH21	1:C:97:LYS:C	2.10	0.54
1:B:166:LEU:HD21	1:B:174:MET:HE1	1.90	0.54
1:A:282:GLU:HG2	1:A:306:TRP:CE2	2.43	0.53
1:B:248:ASN:CG	1:B:251:SER:HG	2.09	0.53
1:A:183:CYS:HB3	1:A:184:GLY:CA	2.35	0.53
1:B:301:HIS:HA	4:B:701:HOH:O	2.07	0.53
1:A:17:PHE:CD2	1:A:527:ILE:HD13	2.42	0.53
1:A:188:PRO:HG2	1:A:190:TYR:CZ	2.44	0.53
1:B:58:GLN:C	1:B:60:GLY:H	2.11	0.53
1:A:65:LEU:CD2	1:A:67:PHE:HD1	2.21	0.52
1:C:71:ARG:NH2	1:C:97:LYS:O	2.42	0.52
1:B:301:HIS:NE2	1:B:522:LEU:HD11	2.23	0.52
1:A:535:ARG:HG3	1:A:551:GLN:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:HB2	3:A:602:GOL:H11	1.91	0.52
1:A:248:ASN:OD1	1:A:251:SER:HB3	2.10	0.52
1:B:68:ASN:HB3	1:B:73:LEU:HD12	1.92	0.52
1:A:34:ARG:HG2	4:A:701:HOH:O	2.10	0.51
1:A:26:LEU:O	1:A:28:PRO:HD3	2.11	0.51
1:A:192:LEU:HD23	1:A:193:LEU:N	2.26	0.51
1:B:174:MET:HG3	1:B:223:LEU:HD13	1.92	0.51
1:C:283:ASP:O	1:C:285:LEU:HD13	2.10	0.51
1:B:166:LEU:HD12	1:B:175:TYR:O	2.11	0.51
1:B:188:PRO:HG2	1:B:190:TYR:CZ	2.46	0.51
1:B:124:ALA:O	1:B:145:ARG:HD2	2.10	0.50
1:A:52:PHE:HE1	1:A:65:LEU:HD12	1.73	0.50
1:A:273:ASP:OD2	1:A:367:TYR:OH	2.19	0.50
1:B:226:PHE:HA	1:B:236:ALA:O	2.12	0.50
1:A:52:PHE:CZ	1:A:65:LEU:HD12	2.45	0.50
1:B:248:ASN:CB	1:B:251:SER:OG	2.60	0.49
1:B:70:GLY:O	1:B:100:GLN:HB3	2.12	0.49
1:A:309:VAL:HB	1:A:372:VAL:HG22	1.95	0.49
1:B:117:SER:HB3	1:B:129:LEU:HD11	1.94	0.49
1:C:188:PRO:HB2	1:C:190:TYR:CE1	2.47	0.49
1:A:238:VAL:CG1	1:A:268:VAL:CG1	2.90	0.49
1:B:189:HIS:O	1:B:204:CYS:HA	2.13	0.49
1:C:103:CYS:SG	1:C:155:VAL:HG22	2.53	0.49
1:A:53:VAL:HG12	1:A:64:ARG:HB2	1.94	0.49
1:A:369:PHE:CE1	1:A:383:LEU:HD23	2.47	0.49
1:C:382:ASP:OD1	1:C:526:LEU:HD11	2.13	0.49
1:A:19:THR:CG2	1:A:527:ILE:HD12	2.43	0.48
1:A:116:VAL:HG23	1:A:132:PRO:HD2	1.95	0.48
1:C:152:VAL:HG13	1:C:167:VAL:HG23	1.96	0.48
1:A:155:VAL:HG23	1:A:155:VAL:O	2.12	0.48
1:C:303:HIS:CE1	1:C:373:GLY:HA3	2.49	0.47
1:B:238:VAL:HG13	1:B:268:VAL:CG1	2.44	0.47
1:B:116:VAL:HG23	1:B:133:ILE:HD12	1.96	0.47
1:C:77:ILE:HG12	1:C:91:ILE:HD11	1.97	0.47
1:C:70:GLY:O	1:C:100:GLN:CB	2.60	0.47
1:C:303:HIS:HD1	1:C:375:ASP:CG	2.17	0.47
1:B:368:ARG:HD3	1:B:382:ASP:OD1	2.15	0.47
1:B:248:ASN:OD1	1:B:251:SER:OG	2.33	0.47
1:A:14:LYS:HG3	1:A:529:LYS:HD2	1.97	0.46
1:A:259:LYS:NZ	4:A:706:HOH:O	2.48	0.46
1:A:260:SER:HB3	1:A:265:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ASP:OD1	1:B:88:SER:HB3	2.15	0.46
1:C:19:THR:OG1	1:C:21:GLU:OE1	2.26	0.46
1:C:278:VAL:HA	1:C:287:THR:O	2.16	0.46
1:C:525:PRO:HB2	1:C:527:ILE:O	2.16	0.46
1:A:71:ARG:HB3	1:A:96:TYR:O	2.14	0.46
1:C:29:HIS:CD2	1:C:30:SER:OG	2.68	0.46
1:C:147:ILE:HD11	1:C:212:PRO:HD3	1.98	0.46
1:C:276:TYR:CZ	1:C:388:LEU:HD22	2.51	0.46
1:A:134:LYS:HE3	1:A:136:GLU:OE1	2.16	0.45
1:A:183:CYS:SG	1:A:184:GLY:C	2.94	0.45
1:A:183:CYS:SG	1:A:184:GLY:CA	3.04	0.45
1:A:197:GLU:O	1:A:198:SER:HB2	2.15	0.45
1:B:268:VAL:HG12	1:B:279:THR:HG22	1.96	0.45
1:C:99:THR:HG21	1:C:126:GLN:OE1	2.16	0.45
1:B:368:ARG:HG3	1:B:369:PHE:N	2.32	0.45
1:C:268:VAL:HG22	1:C:279:THR:HG22	1.99	0.45
1:A:367:TYR:HB2	1:A:383:LEU:HG	1.99	0.45
1:B:57:ASP:OD1	1:B:57:ASP:N	2.50	0.45
1:C:40:PHE:H	1:C:552:GLU:HA	1.82	0.45
1:A:545:CYS:HA	1:A:560:ARG:HG3	1.99	0.44
1:A:64:ARG:CZ	1:A:77:ILE:HG12	2.48	0.44
1:B:190:TYR:HA	1:B:203:THR:O	2.16	0.44
1:A:276:TYR:CZ	1:A:388:LEU:HD22	2.53	0.44
1:C:70:GLY:O	1:C:100:GLN:CG	2.66	0.44
1:B:31:GLU:OE1	1:B:37:ARG:NH1	2.51	0.44
1:A:203:THR:HG22	1:A:204:CYS:H	1.80	0.44
1:B:149:LYS:HD3	3:B:603:GOL:O2	2.18	0.44
1:C:375:ASP:O	1:C:376:THR:OG1	2.25	0.44
1:C:144:GLU:OE1	1:C:144:GLU:N	2.51	0.44
1:A:49:ARG:HA	1:A:49:ARG:HD3	1.84	0.44
1:C:118:LEU:O	1:C:129:LEU:HD12	2.16	0.44
1:C:94:ARG:HD2	1:C:130:ILE:CD1	2.48	0.44
1:C:144:GLU:CD	1:C:144:GLU:H	2.20	0.44
1:C:190:TYR:CE2	1:C:204:CYS:SG	3.11	0.44
1:C:225:GLU:OE1	1:C:268:VAL:N	2.37	0.44
1:B:35:PRO:C	1:B:37:ARG:N	2.71	0.43
1:B:72:GLU:OE2	1:B:74:TYR:OH	2.28	0.43
1:C:234:PHE:CZ	1:C:291:PHE:HZ	2.36	0.43
1:B:255:HIS:CD2	1:B:291:PHE:CE1	3.07	0.43
1:C:158:VAL:HG12	1:C:164:LEU:O	2.18	0.43
1:A:266:LEU:N	1:A:266:LEU:HD12	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASN:CG	1:B:38:VAL:HG13	2.38	0.43
1:C:167:VAL:O	1:C:174:MET:HA	2.19	0.43
1:B:14:LYS:HG3	1:B:529:LYS:HD3	2.00	0.43
1:C:151:ARG:NH1	1:C:153:THR:HG22	2.33	0.43
1:B:49:ARG:HD2	3:B:604:GOL:O1	2.19	0.43
1:B:152:VAL:HG13	1:B:167:VAL:HG23	2.01	0.43
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.71	0.42
1:B:183:CYS:HB3	1:B:211:ASN:CB	2.48	0.42
1:A:261:TYR:HE1	1:A:299:ARG:NH2	2.17	0.42
1:C:246:VAL:O	1:C:254:LEU:HD12	2.19	0.42
1:C:29:HIS:CD2	1:C:83:LYS:HA	2.55	0.42
1:C:182:THR:C	1:C:211:ASN:HB2	2.36	0.42
1:B:313:ASP:HA	1:B:314:PRO:HD3	1.90	0.42
1:C:151:ARG:CG	1:C:170:SER:HB2	2.41	0.42
1:C:187:ALA:HA	1:C:188:PRO:HD3	1.91	0.42
1:C:223:LEU:HD11	1:C:237:CYS:HB3	2.01	0.42
1:B:229:SER:O	1:B:232:GLY:N	2.43	0.42
1:C:35:PRO:HB3	1:C:87:LEU:O	2.18	0.42
1:B:298:ALA:HB1	1:B:523:LEU:HG	2.01	0.42
1:C:241:ASP:OD2	1:C:245:ARG:NH2	2.53	0.42
1:A:238:VAL:HB	1:A:265:LEU:HB2	2.01	0.42
1:B:183:CYS:HB3	1:B:211:ASN:HB2	2.01	0.42
1:B:238:VAL:CG1	1:B:268:VAL:CG1	2.98	0.42
1:C:271:SER:OG	1:C:276:TYR:N	2.45	0.42
1:C:301:HIS:ND1	1:C:522:LEU:HD11	2.34	0.41
1:B:49:ARG:NH1	3:B:604:GOL:H12	2.32	0.41
1:B:147:ILE:HD11	1:B:212:PRO:HD3	2.02	0.41
1:C:21:GLU:OE2	1:C:368:ARG:NH2	2.54	0.41
1:A:243:PHE:CE1	1:A:259:LYS:HD2	2.56	0.41
1:B:36:ASN:HB3	1:B:38:VAL:HG13	2.02	0.41
1:A:77:ILE:HG13	1:A:91:ILE:HD11	2.02	0.41
1:A:89:LYS:HB2	1:A:89:LYS:HE3	1.78	0.41
1:B:238:VAL:HB	1:B:265:LEU:HB2	2.02	0.41
1:A:17:PHE:HD2	1:A:527:ILE:HD13	1.85	0.41
1:A:36:ASN:O	1:A:37:ARG:HB2	2.20	0.41
1:C:92:ASP:OD2	1:C:94:ARG:NH1	2.53	0.41
1:A:309:VAL:O	1:A:371:SER:HA	2.21	0.41
1:B:75:PHE:CD2	1:B:132:PRO:HB2	2.56	0.41
1:C:71:ARG:NH2	1:C:98:GLY:O	2.54	0.41
1:C:258:MET:HG2	1:C:259:LYS:N	2.36	0.41
1:C:157:TRP:CH2	1:C:179:VAL:HG21	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLY:HA2	1:C:264:GLY:HA2	2.02	0.40
1:B:369:PHE:CE2	1:B:383:LEU:HD23	2.52	0.40
1:C:172:GLY:O	1:C:173:ASN:OD1	2.40	0.40
1:B:104:HIS:HB2	1:B:118:LEU:HD11	2.04	0.40
1:B:309:VAL:HB	1:B:372:VAL:HG22	2.04	0.40
1:C:248:ASN:O	1:C:252:VAL:N	2.54	0.40
1:A:529:LYS:NZ	3:B:602:GOL:H11	2.37	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	364/569 (64%)	342 (94%)	21 (6%)	1 (0%)	41	64
1	B	365/569 (64%)	342 (94%)	23 (6%)	0	100	100
1	C	347/569 (61%)	319 (92%)	27 (8%)	1 (0%)	41	64
All	All	1076/1707 (63%)	1003 (93%)	71 (7%)	2 (0%)	47	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	CYS
1	C	212	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	310/499 (62%)	308 (99%)	2 (1%)	86 95
1	B	303/499 (61%)	303 (100%)	0	100 100
1	C	266/499 (53%)	264 (99%)	2 (1%)	81 92
All	All	879/1497 (59%)	875 (100%)	4 (0%)	88 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	CYS
1	A	211	ASN
1	C	240	GLN
1	C	303	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	211	ASN
1	C	173	ASN
1	C	240	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands 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	$\#\|Z\| > 2$
2	SO4	B	601	-	4,4,4	0.18	0	6,6,6	0.17	0
3	GOL	B	602	-	5,5,5	0.26	0	5,5,5	0.28	0
3	GOL	A	602	-	5,5,5	0.42	0	5,5,5	0.40	0
3	GOL	C	601	-	5,5,5	0.50	0	5,5,5	0.49	0
2	SO4	A	601	-	4,4,4	0.17	0	6,6,6	0.14	0
3	GOL	B	604	-	5,5,5	0.33	0	5,5,5	0.63	0
3	GOL	B	603	-	5,5,5	0.43	0	5,5,5	0.47	0

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
3	GOL	B	602	-	-	1/4/4/4	-
3	GOL	A	602	-	-	4/4/4/4	-
3	GOL	C	601	-	-	2/4/4/4	-
3	GOL	B	604	-	-	2/4/4/4	-
3	GOL	B	603	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	C1-C2-C3-O3
3	A	602	GOL	O2-C2-C3-O3
3	C	601	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-C3
3	B	604	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	601	GOL	O1-C1-C2-O2
3	B	604	GOL	O1-C1-C2-O2
3	B	602	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GOL	1	0
3	A	602	GOL	2	0
3	B	604	GOL	3	0
3	B	603	GOL	3	0

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	376/569 (66%)	-0.13	3 (0%)	86	84	38, 54, 84, 109	0
1	B	373/569 (65%)	-0.13	1 (0%)	94	93	40, 58, 88, 111	0
1	C	359/569 (63%)	0.31	21 (5%)	23	17	65, 91, 109, 115	0
All	All	1108/1707 (64%)	0.01	25 (2%)	60	54	38, 64, 103, 115	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	185	THR	5.0
1	C	317	THR	3.4
1	C	546	ILE	3.3
1	C	311	ALA	3.2
1	A	183	CYS	3.2
1	C	541	PHE	3.1
1	C	214	LEU	3.1
1	C	216	TRP	3.1
1	C	522	LEU	3.0
1	C	302	GLY	3.0
1	B	389	PHE	2.9
1	C	547	VAL	2.6
1	C	70	GLY	2.6
1	C	372	VAL	2.6
1	C	23	LEU	2.4
1	C	312	PHE	2.4
1	C	378	LEU	2.4
1	C	301	HIS	2.3
1	C	531	ILE	2.3
1	A	69	VAL	2.2
1	C	542	LEU	2.2
1	C	243	PHE	2.1
1	C	369	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	70	GLY	2.1
1	C	211	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	GOL	B	603	6/6	0.80	0.31	74,79,81,84	0
3	GOL	C	601	6/6	0.86	0.22	81,84,87,92	0
2	SO4	A	601	5/5	0.87	0.15	95,101,120,122	0
3	GOL	B	604	6/6	0.88	0.33	59,64,69,70	0
3	GOL	B	602	6/6	0.89	0.14	61,65,68,68	0
3	GOL	A	602	6/6	0.91	0.23	63,68,71,72	0
2	SO4	B	601	5/5	0.92	0.11	88,91,101,106	0

6.5 Other polymers (i)

There are no such residues in this entry.