



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 AM GMT

PDB ID : 2WNV  
Title : COMPLEX BETWEEN C1Q GLOBULAR HEADS AND DEOXYRIBOSE  
Authors : Garlatti, V.; Chouquet, A.; Lunardi, T.; Thielens, N.M.; Arlaud, G.J.; Gaboriaud, C.  
Deposited on : 2009-07-20  
Resolution : 1.25 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

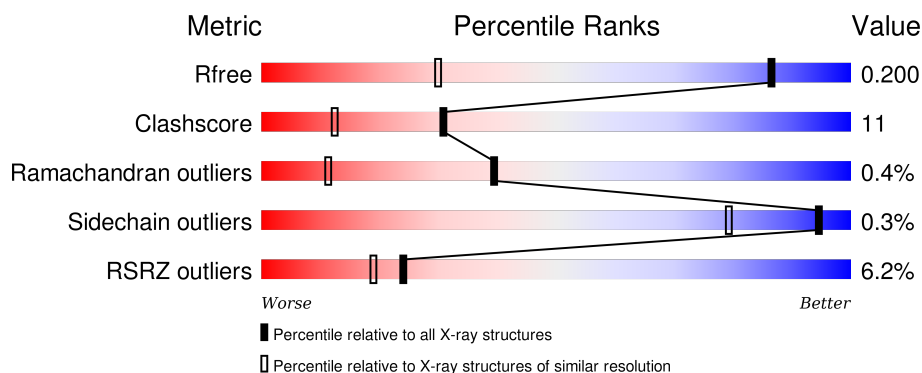
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.25 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))
$R_{free}$	91344	1442 (1.30-1.22)
Clashscore	102246	1530 (1.30-1.22)
Ramachandran outliers	100387	1467 (1.30-1.22)
Sidechain outliers	100360	1465 (1.30-1.22)
RSRZ outliers	91569	1442 (1.30-1.22)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	134	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	134	<div> <div>7%</div> <div>81%</div> <div>19%</div> </div>
2	B	136	<div> <div>11%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
2	E	136	<div> <div>11%</div> <div>87%</div> <div>8%</div> <div>..</div> </div>
3	C	131	<div> <div>2%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	131	<div> <div></div> <div>%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1224	-	-	-	X
4	NAG	D	1224	-	-	-	X
6	2DR	C	1218	-	-	X	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7548 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 COMPLEMENT C1Q SUBCOMPONENT SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	8	1
			1091	699	187	201	4			
1	D	134	Total	C	N	O	S	0	14	1
			1156	733	199	217	7			

- Molecule 2 is a protein called COMPLEMENT C1Q SUBCOMPONENT SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	8	1
			1073	690	185	190	8			
2	E	130	Total	C	N	O	S	0	7	1
			1066	677	186	196	7			

- Molecule 3 is a protein called COMPLEMENT C1Q SUBCOMPONENT SUBUNIT C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	129	Total	C	N	O	S	0	4	0
			1034	661	173	196	4			
3	F	129	Total	C	N	O	S	0	4	0
			1033	663	172	194	4			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

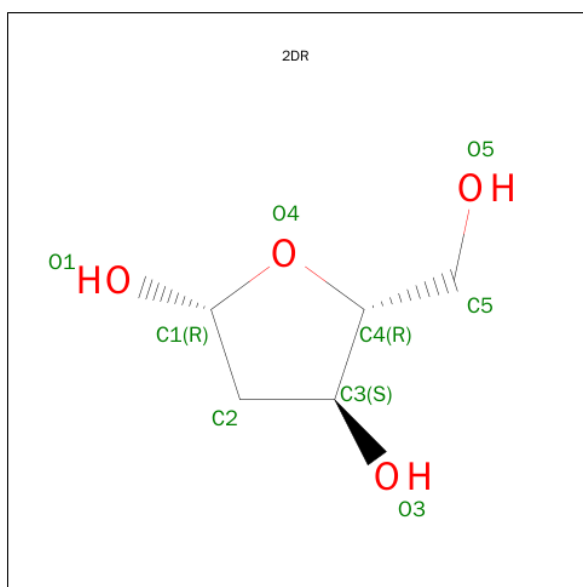


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		

- Molecule 6 is 2-DEOXY-BETA-D-ERYTHRO-PENTOFURANOSE (three-letter code: 2DR) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			9	5	4		

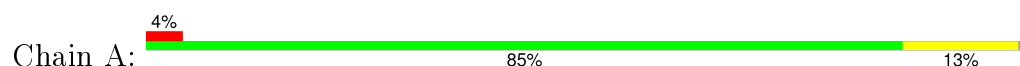
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	197	Total	O	0	0
			197	197		
7	B	157	Total	O	0	0
			157	157		
7	C	196	Total	O	0	0
			196	196		
7	D	193	Total	O	0	0
			193	193		
7	E	139	Total	O	0	0
			139	139		
7	F	172	Total	O	0	0
			172	172		

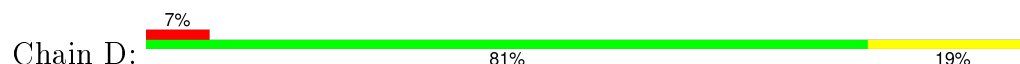
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

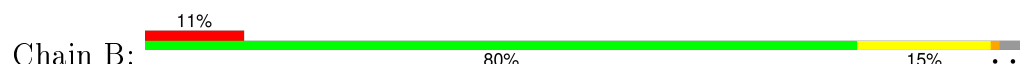
- Molecule 1: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT A



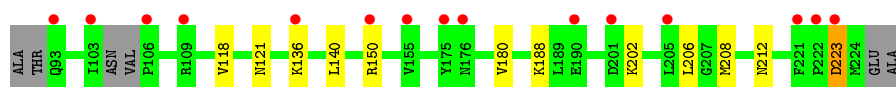
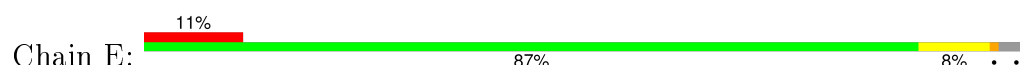
- Molecule 1: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT A



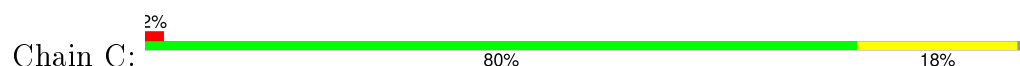
- Molecule 2: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT B



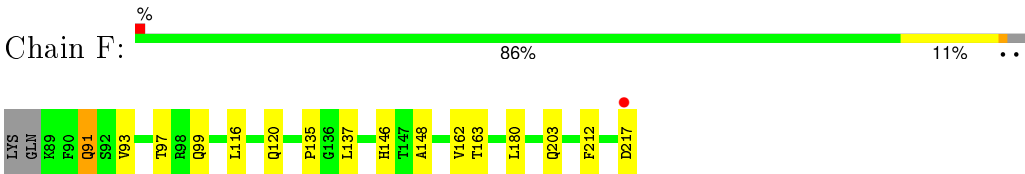
- Molecule 2: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT B



- Molecule 3: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT C



- Molecule 3: COMPLEMENT C1Q SUBCOMPONENT SUBUNIT C





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.35Å 48.33Å 88.06Å 92.39° 92.60° 113.57°	Depositor
Resolution (Å)	19.71 – 1.25 19.71 – 1.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.71-1.25) 81.2 (19.71-1.25)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.24 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.175 , 0.202 0.174 , 0.200	Depositor DCC
$R_{free}$ test set	8368 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	9.1	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 47.9	EDS
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 167346 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, NAG, 2DR

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	0.38	0/1124	0.55	0/1527
1	D	0.38	0/1184	0.57	0/1607
2	B	0.39	0/1117	0.55	0/1506
2	E	0.39	0/1085	0.54	0/1464
3	C	0.36	0/1061	0.56	0/1446
3	F	0.37	0/1060	0.55	0/1446
All	All	0.38	0/6631	0.55	0/8996

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1091	0	1052	16	0
1	D	1156	0	1097	29	0
2	B	1073	0	1072	32	0
2	E	1066	0	1034	12	0
3	C	1034	0	989	43	0
3	F	1033	0	994	18	0
4	A	15	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	15	0	14	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	C	9	0	10	18	0
7	A	197	0	0	8	0
7	B	157	0	0	13	1
7	C	196	0	0	25	0
7	D	193	0	0	9	0
7	E	139	0	0	5	1
7	F	172	0	0	7	0
All	All	7548	0	6277	138	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 (138) 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)
3:C:209:PHE:HA	7:C:2096:HOH:O	1.40	1.17
2:B:103[B]:ILE:HD13	2:B:114[B]:ARG:NE	1.66	1.10
1:A:95:PHE:HB3	7:A:2029:HOH:O	1.51	1.09
3:C:142:TYR:HA	7:C:2096:HOH:O	1.56	1.06
3:C:111:ARG:HD2	7:C:2193:HOH:O	1.56	1.04
1:A:173:LYS:HE2	7:A:2133:HOH:O	1.61	1.01
7:A:2124:HOH:O	3:C:172:ASN:HB3	1.61	0.98
3:C:214:LEU:HB2	7:C:2184:HOH:O	1.69	0.92
2:B:107[B]:LEU:HD12	2:B:203:ASN:HB2	1.56	0.85
6:C:1218:2DR:H51C	1:D:163:ARG:H	1.45	0.82
3:C:141:VAL:O	7:C:2096:HOH:O	1.98	0.82
2:B:103[B]:ILE:HD13	2:B:114[B]:ARG:HE	1.43	0.81
3:C:111:ARG:CB	6:C:1218:2DR:H1	2.13	0.79
3:C:111:ARG:HB3	6:C:1218:2DR:H1	1.64	0.79
1:D:157[B]:SER:OG	7:D:2088:HOH:O	2.03	0.77
2:B:103[B]:ILE:HD12	2:B:114[B]:ARG:HG3	1.67	0.75
2:B:202:LYS:HB3	7:B:2079:HOH:O	1.86	0.74
3:C:137:LEU:HD12	7:C:2184:HOH:O	1.89	0.73
2:B:159:ARG:NH2	7:B:2087:HOH:O	2.21	0.72
3:C:113:ASN:HB3	6:C:1218:2DR:C2	2.20	0.72
3:C:98:ARG:HH21	6:C:1218:2DR:H52C	1.54	0.72
3:C:99:GLN:CD	7:C:2018:HOH:O	2.28	0.71
1:D:184:VAL:HG11	3:F:93[B]:VAL:HG11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103[B]:ILE:CD1	2:B:114[B]:ARG:NE	2.49	0.71
2:B:152:ASN:HB3	7:B:2079:HOH:O	1.91	0.70
3:C:99:GLN:OE1	3:F:97[A]:THR:HG21	1.91	0.70
7:C:2018:HOH:O	3:F:99:GLN:CD	2.30	0.69
3:C:97[A]:THR:HG21	3:F:99:GLN:OE1	1.93	0.69
2:E:212[B]:ASN:HD22	3:F:163:THR:H	1.41	0.69
7:B:2149:HOH:O	3:C:165:CYS:SG	2.50	0.69
2:E:208:MET:O	2:E:212[A]:ASN:ND2	2.27	0.67
3:F:135:PRO:HG2	3:F:217:ASP:OXT	1.94	0.67
3:C:135:PRO:HG2	3:C:217:ASP:OXT	1.95	0.66
2:E:180:VAL:HB	7:E:2099:HOH:O	1.97	0.65
1:A:183:MET:HE3	3:C:116:LEU:HD13	1.79	0.65
1:D:154[B]:VAL:HG23	1:D:162:ARG:O	1.98	0.63
2:B:117:HIS:HE1	7:C:2101:HOH:O	1.81	0.63
7:C:2018:HOH:O	3:F:99:GLN:CG	2.47	0.62
3:F:93[A]:VAL:HG23	3:F:212:PHE:HB3	1.81	0.62
1:D:183[A]:MET:HE3	3:F:116:LEU:HD13	1.82	0.61
1:A:100[B]:ARG:NH2	7:A:2009:HOH:O	2.07	0.61
2:B:103[B]:ILE:CD1	2:B:114[B]:ARG:CD	2.79	0.60
3:C:137:LEU:HB3	7:C:2184:HOH:O	2.00	0.60
2:E:150:ARG:HG3	2:E:206:LEU:HD11	1.84	0.59
3:C:91:GLN:HG3	7:C:2010:HOH:O	2.02	0.59
3:C:113:ASN:HB3	6:C:1218:2DR:H22C	1.84	0.59
3:C:111:ARG:HB2	6:C:1218:2DR:H1	1.83	0.59
1:D:219:ILE:HG22	7:F:2165:HOH:O	2.03	0.59
1:D:199:PRO:HA	7:D:2016:HOH:O	2.03	0.58
6:C:1218:2DR:C5	1:D:163:ARG:H	2.12	0.58
1:D:222:SER:HA	7:D:2186:HOH:O	2.03	0.58
3:C:99:GLN:CG	7:C:2018:HOH:O	2.51	0.57
2:B:150[A]:ARG:NH2	7:B:2066:HOH:O	2.38	0.57
1:D:118:GLN:HG2	2:E:140:LEU:HD11	1.87	0.56
1:A:118:GLN:HG2	2:B:140:LEU:HD11	1.88	0.56
1:D:197:LYS:HG3	7:D:2016:HOH:O	2.05	0.56
2:B:103[B]:ILE:HD12	2:B:114[B]:ARG:CG	2.36	0.56
2:E:223:ASP:HA	7:E:2138:HOH:O	2.06	0.55
2:B:202:LYS:HE2	7:B:2065:HOH:O	2.06	0.55
3:C:98:ARG:HG3	6:C:1218:2DR:O3	2.07	0.54
2:E:136:LYS:HG2	7:E:2058:HOH:O	2.07	0.54
6:C:1218:2DR:H51C	1:D:163:ARG:CB	2.38	0.54
1:D:184:VAL:HG11	3:F:93[B]:VAL:CG1	2.38	0.53
1:D:220:PHE:HB3	7:F:2007:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:PRO:O	2:B:223:ASP:CB	2.57	0.53
3:C:111:ARG:HB2	6:C:1218:2DR:C1	2.38	0.53
3:C:215:PHE:N	7:C:2184:HOH:O	2.40	0.53
3:C:203[A]:GLN:HG2	7:F:2148:HOH:O	2.08	0.53
1:A:106:GLY:N	7:A:2016:HOH:O	2.42	0.53
2:B:107[B]:LEU:CD1	2:B:203:ASN:HB2	2.36	0.53
2:B:161:ARG:O	2:B:161:ARG:HG2	2.09	0.53
3:F:146:HIS:HD2	3:F:148:ALA:O	1.93	0.52
1:A:188[A]:GLN:NE2	7:A:2147:HOH:O	2.43	0.52
1:A:183:MET:CE	3:C:116:LEU:HD13	2.40	0.52
1:A:170:THR:HG23	7:A:2124:HOH:O	2.09	0.52
2:B:202:LYS:HG2	7:B:2079:HOH:O	2.11	0.51
2:B:167:VAL:HG13	7:B:2087:HOH:O	2.10	0.51
6:C:1218:2DR:H51C	1:D:163:ARG:N	2.22	0.50
1:A:98:ILE:HG22	1:A:213[B]:VAL:HG22	1.92	0.50
3:C:217:ASP:HA	7:C:2188:HOH:O	2.12	0.50
7:D:2105:HOH:O	2:E:202:LYS:HE2	2.11	0.50
1:D:183[A]:MET:CE	3:F:116:LEU:HD13	2.42	0.49
3:C:146:HIS:HD2	3:C:148:ALA:O	1.95	0.49
3:C:203[B]:GLN:HG3	3:F:203:GLN:HG3	1.95	0.49
1:D:188[A]:GLN:NE2	7:D:2135:HOH:O	2.45	0.48
3:C:113:ASN:HB3	6:C:1218:2DR:H21C	1.92	0.48
6:C:1218:2DR:H51C	1:D:163:ARG:HB2	1.94	0.48
3:C:111:ARG:NH1	7:C:2071:HOH:O	2.46	0.48
3:C:209:PHE:CA	7:C:2096:HOH:O	2.22	0.47
3:F:146:HIS:HE1	7:F:2124:HOH:O	1.97	0.47
1:A:154[B]:VAL:HG22	7:A:2088:HOH:O	2.14	0.47
2:B:103[B]:ILE:CD1	2:B:114[B]:ARG:CG	2.93	0.47
1:D:100[B]:ARG:NH1	7:D:2008:HOH:O	2.47	0.47
3:C:97[A]:THR:HG23	3:C:114:ALA:HB3	1.95	0.47
2:B:103[B]:ILE:CD1	2:B:114[B]:ARG:HG3	2.40	0.47
1:A:160:GLN:HG3	7:F:2037:HOH:O	2.14	0.47
3:F:137:LEU:HD21	3:F:180:LEU:HD22	1.97	0.47
1:D:194:TRP:NE1	1:D:196[A]:GLU:HG3	2.29	0.46
3:F:91:GLN:NE2	7:F:2007:HOH:O	2.48	0.46
3:F:120:GLN:NE2	7:F:2051:HOH:O	2.42	0.46
1:D:194:TRP:CD1	1:D:196[A]:GLU:HG3	2.51	0.46
1:D:183[A]:MET:HE2	1:D:185:LEU:CD2	2.45	0.46
3:C:102:GLN:HG3	7:C:2060:HOH:O	2.16	0.46
2:B:206:LEU:HD22	2:B:208[A]:MET:HE1	1.96	0.46
1:D:119:GLU:HG2	7:D:2031:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:LYS:N	7:C:2002:HOH:O	2.48	0.45
1:D:92:ARG:N	1:D:93:PRO:HD3	2.32	0.45
2:B:150[B]:ARG:HD2	7:B:2068:HOH:O	2.15	0.45
2:E:118[A]:VAL:HG21	2:E:121:ASN:HB2	1.99	0.45
2:E:188:LYS:NZ	7:E:2108:HOH:O	2.38	0.44
2:B:107[B]:LEU:HD22	2:B:113:ILE:HG12	2.00	0.44
1:D:144:LEU:HD11	1:D:176:PHE:HB3	1.99	0.44
2:B:211:ALA:HA	7:B:2149:HOH:O	2.18	0.44
1:D:104[B]:MET:SD	1:D:206[B]:GLN:NE2	2.88	0.43
6:C:1218:2DR:H4	7:C:2195:HOH:O	2.18	0.43
2:B:107[B]:LEU:HD13	2:B:199:ALA:HB1	2.00	0.43
1:D:194:TRP:HE1	1:D:196[A]:GLU:HG3	1.84	0.43
3:C:146:HIS:HE1	7:C:2142:HOH:O	2.02	0.43
2:E:212[A]:ASN:OD1	3:F:162:VAL:HA	2.18	0.43
2:B:202:LYS:CB	7:B:2079:HOH:O	2.58	0.42
1:D:154[B]:VAL:HG13	1:D:194:TRP:CE2	2.54	0.42
3:C:115:VAL:HG12	7:C:2039:HOH:O	2.19	0.42
4:D:1224:NAG:H2	7:D:2191:HOH:O	2.20	0.42
1:A:144:LEU:HD11	1:A:176:PHE:HB3	2.01	0.41
2:B:109:ARG:HD3	7:B:2013:HOH:O	2.20	0.41
3:C:203[A]:GLN:HB2	7:C:2169:HOH:O	2.20	0.41
3:C:141:VAL:HG11	7:C:2092:HOH:O	2.20	0.41
3:C:111:ARG:HB2	6:C:1218:2DR:H4	2.03	0.41
1:A:175[B]:LEU:HD12	2:B:173:TYR:HB3	2.03	0.41
1:A:154[A]:VAL:CG1	1:A:194:TRP:CE2	3.04	0.40
2:E:118[A]:VAL:HG12	7:E:2025:HOH:O	2.21	0.40
6:C:1218:2DR:C5	7:C:2195:HOH:O	2.70	0.40
1:A:165:LEU:HD21	3:C:97[B]:THR:HG21	2.04	0.40
2:B:111:GLN:NE2	7:B:2017:HOH:O	2.54	0.40
3:C:111:ARG:HB2	6:C:1218:2DR:C4	2.51	0.40
1:D:98:ILE:HG22	1:D:213[A]:VAL:HG22	2.02	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)
7:B:2091:HOH:O	7:E:2110:HOH:O[1_556]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	136/134 (102%)	129 (95%)	6 (4%)	1 (1%)	26	4
1	D	146/134 (109%)	138 (94%)	8 (6%)	0	100	100
2	B	135/136 (99%)	129 (96%)	5 (4%)	1 (1%)	26	4
2	E	132/136 (97%)	127 (96%)	4 (3%)	1 (1%)	24	3
3	C	131/131 (100%)	125 (95%)	6 (5%)	0	100	100
3	F	131/131 (100%)	126 (96%)	5 (4%)	0	100	100
All	All	811/802 (101%)	774 (95%)	34 (4%)	3 (0%)	39	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	223	ASP
2	E	223	ASP
1	A	222	SER

### 5.3.2 Protein sidechains

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	122/117 (104%)	122 (100%)	0	100	100
1	D	129/117 (110%)	129 (100%)	0	100	100
2	B	117/117 (100%)	115 (98%)	2 (2%)	68	29
2	E	115/117 (98%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	116/115 (101%)	116 (100%)	0	100	100
3	F	116/115 (101%)	115 (99%)	1 (1%)	84	56
All	All	715/698 (102%)	712 (100%)	3 (0%)	94	77

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	150[A]	ARG
2	B	150[B]	ARG
3	F	91	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	172	ASN
1	A	186	GLN
2	B	117	HIS
2	B	191	GLN
3	C	102	GLN
3	C	146	HIS
1	D	186	GLN
2	E	117	HIS
2	E	191	GLN
3	F	91	GLN
3	F	146	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z  > 2$
4	NAG	A	1224	-	15,15,15	0.38	0	17,21,21	0.93	1 (5%)
6	2DR	C	1218	-	9,9,9	0.74	0	10,12,12	0.73	0
4	NAG	D	1224	-	15,15,15	0.41	0	17,21,21	0.61	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
4	NAG	A	1224	-	-	0/6/26/26	0/1/1/1
6	2DR	C	1218	-	-	0/2/14/14	0/1/1/1
4	NAG	D	1224	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1224	NAG	O5-C5-C4	2.07	113.56	109.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1218	2DR	18	0
4	D	1224	NAG	1	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	132/134 (98%)	0.37	6 (4%)	37	30	5, 10, 18, 24	4 (3%)
1	D	134/134 (100%)	0.34	9 (6%)	21	16	5, 10, 20, 24	2 (1%)
2	B	132/136 (97%)	0.53	15 (11%)	7	5	6, 12, 20, 24	8 (6%)
2	E	130/136 (95%)	0.54	15 (11%)	6	5	7, 13, 21, 25	6 (4%)
3	C	129/131 (98%)	-0.01	3 (2%)	64	57	5, 8, 14, 20	1 (0%)
3	F	129/131 (98%)	0.03	1 (0%)	87	86	5, 9, 14, 21	2 (1%)
All	All	786/802 (98%)	0.30	49 (6%)	24	19	5, 10, 20, 25	23 (2%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	ALA	15.8
1	D	223	ALA	10.0
2	B	92	THR	8.5
1	A	91	PRO	7.1
1	D	91	PRO	7.0
1	D	104[A]	MET	5.3
2	E	222	PRO	5.1
1	D	90	GLN	4.8
1	D	222	SER	4.6
2	E	103[A]	ILE	4.5
2	B	103[A]	ILE	4.4
2	E	175	TYR	4.3
1	A	90	GLN	4.2
2	B	175	TYR	4.0
1	A	222	SER	3.8
2	B	161	ARG	3.8
2	B	107[A]	LEU	3.6
1	D	105	GLY	3.6
2	E	223	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	129	ARG	3.2
3	F	217	ASP	3.2
2	E	221	PHE	3.1
2	B	105	VAL	3.0
2	E	106	PRO	2.9
2	B	221	PHE	2.9
2	E	205[A]	LEU	2.8
2	B	176	ASN	2.8
2	E	136	LYS	2.8
2	B	150[A]	ARG	2.7
2	E	155[A]	VAL	2.7
1	D	175	LEU	2.6
2	B	102	THR	2.6
3	C	217	ASP	2.4
2	B	136	LYS	2.4
2	E	93	GLN	2.4
2	E	109	ARG	2.4
1	A	175[A]	LEU	2.3
2	E	176	ASN	2.3
2	B	209	GLU	2.3
2	E	150	ARG	2.3
1	D	100[A]	ARG	2.3
2	B	223	ASP	2.3
1	A	101[A]	ASN	2.2
2	E	190	GLU	2.2
2	E	201	ASP	2.2
3	C	203[A]	GLN	2.2
1	D	220	PHE	2.1
3	C	90	PHE	2.1
2	B	208[A]	MET	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	2DR	C	1218	9/9	0.56	0.29	12.89	23,24,24,25	9
4	NAG	D	1224	15/15	0.50	0.40	11.37	52,59,63,63	0
4	NAG	A	1224	15/15	0.47	0.32	3.70	45,52,57,57	0
5	CA	B	1225	1/1	1.00	0.03	-2.82	8,8,8,8	0
5	CA	E	1225	1/1	1.00	0.03	-5.19	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.