Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 09:49 pm GMT

PDB ID	:	2JG8
Title	:	Crystallographic structure of human C1q globular heads complexed to phosphatidyl-serine
Authors	:	Paidassi, H.; Tacnet-Delorme, P.; Garlatti, V.; Darnault, C.; Ghebrehiwet, B.; Gaboriaud, C.; Arlaud, G.J.; Frachet, P.
Deposited on	:	2007-02-09
Resolution	:	2.05 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:

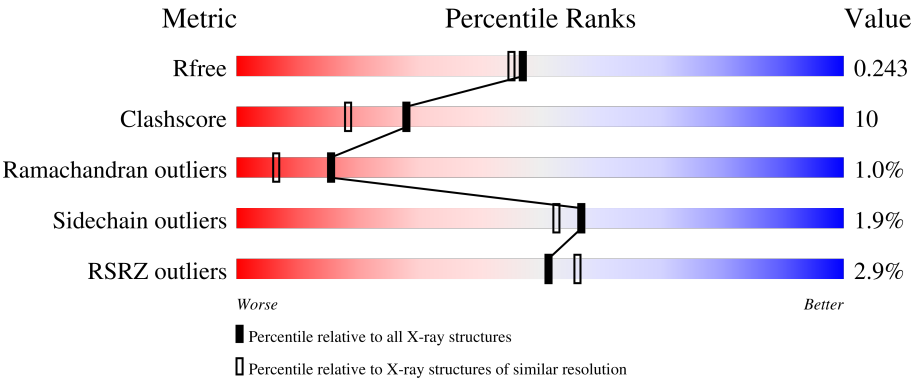
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	134	2% 83% 15%
1	D	134	3% 77% 20%
2	B	136	6% 75% 19%
2	E	136	6% 77% 16%
3	C	131	79% 19%

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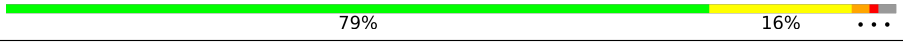
Mol	Chain	Length	Quality of chain
3	F	131	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6724 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	133	Total	C	N	O	S	16	7	0
			1090	695	187	202	6			
1	D	133	Total	C	N	O	S	20	8	0
			1100	702	190	202	6			

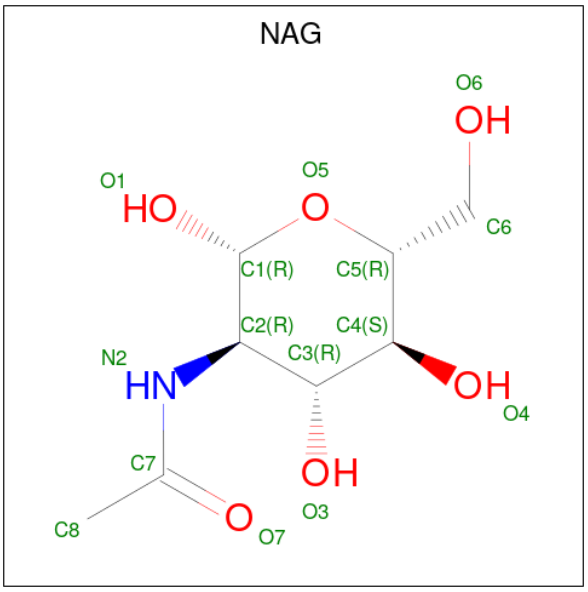
- Molecule 2 is a protein called Complement C1q subcomponent subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	52	5	1
			1093	687	194	205	7			
2	E	133	Total	C	N	O	S	41	1	1
			1051	664	185	195	7			

- Molecule 3 is a protein called Complement C1q subcomponent subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	131	Total	C	N	O	S	12	4	0
			1034	664	173	193	4			
3	F	129	Total	C	N	O	S	25	5	0
			1027	659	173	191	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

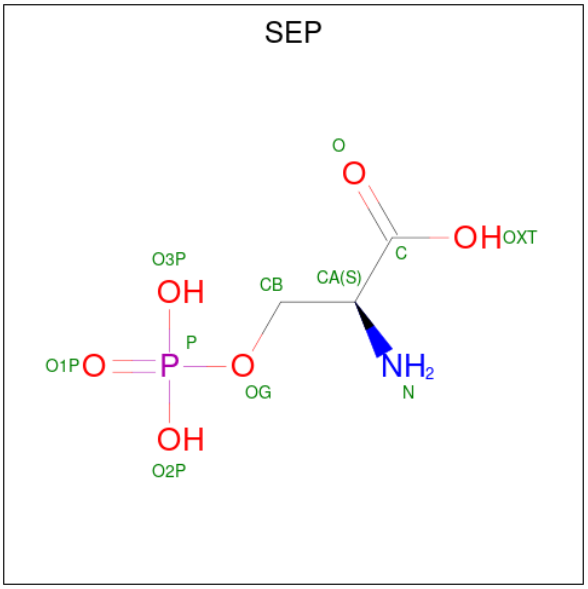


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 15 8 1 6	0	0

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

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

- Molecule 6 is PHOSPHOSERINE (three-letter code: SEP) (formula: $C_3H_8NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

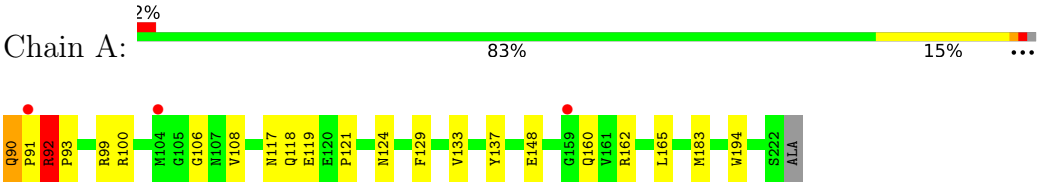
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total	O	0	0
			60	60		
7	B	28	Total	O	0	0
			28	28		
7	C	60	Total	O	0	0
			60	60		
7	D	59	Total	O	0	0
			59	59		
7	E	35	Total	O	0	0
			35	35		
7	F	60	Total	O	0	0
			60	60		

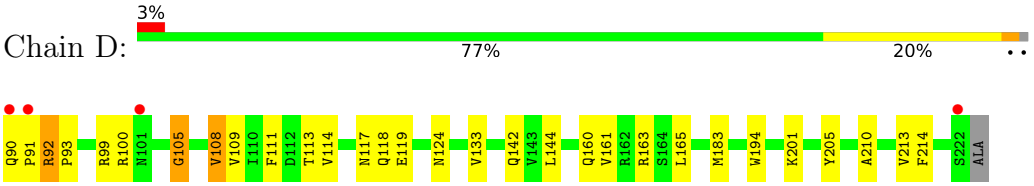
3 Residue-property plots (i)

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.

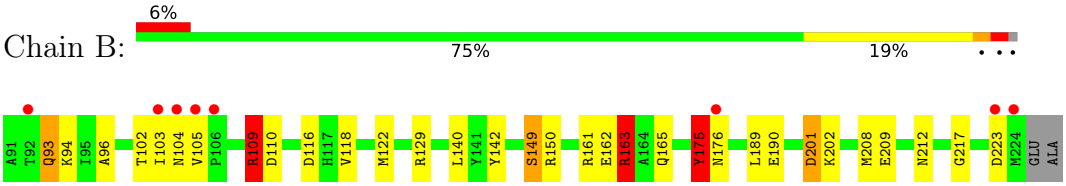
• Molecule 1: Complement C1q subcomponent subunit A



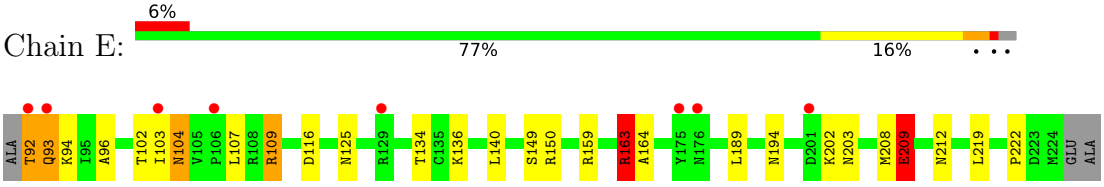
• Molecule 1: Complement C1q subcomponent subunit A



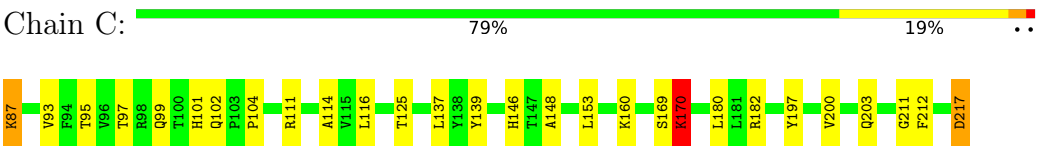
• Molecule 2: Complement C1q subcomponent subunit B



• Molecule 2: Complement C1q subcomponent subunit B

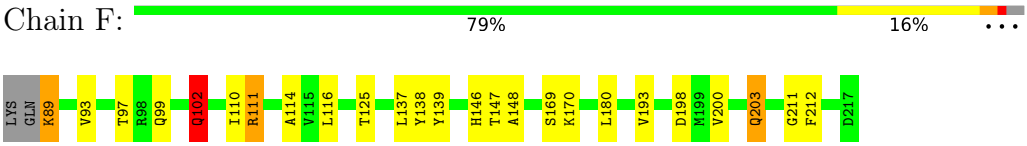


• Molecule 3: Complement C1q subcomponent subunit C



• Molecule 3: Complement C1q subcomponent subunit C

Chain F:


79%
16%
LYS
GLN
K89
V93
T97
R98
Q99
Q102
I110
R111
A114
V115
L116
T125
L137
Y138
Y139
H146
T147
A148
S169
K170
L180
V193
D198
M199
V200
Q203
G211
F212
D217

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.09Å 48.07Å 84.70Å 91.34° 93.34° 113.68°	Depositor
Resolution (Å)	19.94 – 2.05 19.94 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-2.05) 89.7 (19.94-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.80 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.241 0.183 , 0.243	Depositor DCC
R_{free} test set	1948 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 62.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.079 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6724	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: SEP, CA, NAG

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	1.03	2/1136 (0.2%)	0.77	7/1540 (0.5%)
1	D	0.43	1/1146 (0.1%)	0.69	4/1553 (0.3%)
2	B	1.42	12/1118 (1.1%)	1.34	15/1510 (1.0%)
2	E	2.72	8/1076 (0.7%)	1.37	13/1454 (0.9%)
3	C	0.70	2/1081 (0.2%)	0.68	4/1471 (0.3%)
3	F	0.72	3/1074 (0.3%)	0.61	0/1462
All	All	1.39	28/6631 (0.4%)	0.96	43/8990 (0.5%)

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
2	B	0	2
2	E	0	3
3	C	0	1
3	F	0	2
All	All	0	9

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	93	GLN	N-CA	75.95	2.98	1.46
2	B	109	ARG	CB-CG	-27.35	0.78	1.52
1	A	92	ARG	N-CA	25.76	1.97	1.46
2	E	109	ARG	CB-CG	-24.05	0.87	1.52
2	E	93	GLN	C-O	-21.68	0.82	1.23
2	B	149	SER	CB-OG	-20.91	1.15	1.42
2	E	149	SER	CB-OG	-20.74	1.15	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	GLN	CB-CG	18.71	2.03	1.52
2	B	93	GLN	C-O	-17.10	0.90	1.23
3	C	87	LYS	N-CA	16.91	1.80	1.46
2	E	104	ASN	CA-C	14.92	1.91	1.52
3	F	89	LYS	CB-CG	-14.34	1.13	1.52
2	E	93	GLN	C-N	-11.76	1.07	1.34
2	E	163	ARG	CB-CG	11.37	1.83	1.52
2	B	93	GLN	N-CA	10.77	1.67	1.46
2	B	175	TYR	N-CA	10.18	1.66	1.46
2	E	150	ARG	CB-CG	-9.71	1.26	1.52
2	B	150	ARG	CB-CG	-9.55	1.26	1.52
3	F	102	GLN	CA-C	8.85	1.75	1.52
3	F	203	GLN	CA-C	8.15	1.74	1.52
2	B	201	ASP	CA-C	7.45	1.72	1.52
2	B	93	GLN	C-N	7.43	1.51	1.34
2	B	175	TYR	CA-C	7.25	1.71	1.52
1	D	109	VAL	N-CA	-6.78	1.32	1.46
2	B	201	ASP	N-CA	6.30	1.58	1.46
3	C	87	LYS	CA-C	6.25	1.69	1.52
2	B	129	ARG	N-CA	6.07	1.58	1.46
2	B	129	ARG	CA-C	5.10	1.66	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	175	TYR	CA-C-O	-24.15	69.39	120.10
2	E	209	GLU	CA-C-O	-21.40	75.16	120.10
2	E	209	GLU	CA-C-N	19.94	156.09	116.20
2	E	92	THR	C-N-CA	-19.62	72.66	121.70
2	B	175	TYR	CA-C-N	19.46	160.00	117.20
2	E	104	ASN	CA-C-O	-16.21	86.07	120.10
2	E	163	ARG	CB-CG-CD	-15.07	72.41	111.60
2	B	93	GLN	CA-C-O	-14.94	88.74	120.10
2	B	163	ARG	CB-CG-CD	-12.88	78.12	111.60
2	B	93	GLN	C-N-CA	11.98	151.66	121.70
2	B	150	ARG	CA-CB-CG	11.00	137.60	113.40
2	E	150	ARG	CA-CB-CG	10.90	137.39	113.40
2	B	93	GLN	O-C-N	-10.66	105.64	122.70
2	B	201	ASP	CA-C-O	10.19	141.49	120.10
2	B	201	ASP	CA-C-N	-10.11	94.96	117.20
2	E	93	GLN	CA-C-O	-9.89	99.33	120.10
1	A	90	GLN	CA-CB-CG	9.88	135.14	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	ARG	CA-C-O	-9.49	100.18	120.10
2	E	209	GLU	N-CA-C	8.26	133.31	111.00
2	B	93	GLN	CA-C-N	8.16	135.16	117.20
1	A	160	GLN	CB-CG-CD	-7.93	90.97	111.60
3	C	170	LYS	CA-C-O	-7.76	103.81	120.10
1	D	90	GLN	CA-CB-CG	7.69	130.32	113.40
1	A	90	GLN	CB-CG-CD	7.68	131.57	111.60
2	E	104	ASN	CA-C-N	-7.51	100.68	117.20
3	C	87	LYS	CA-C-N	-7.16	101.46	117.20
3	C	87	LYS	CA-C-O	6.92	134.62	120.10
2	B	175	TYR	CB-CA-C	6.87	124.15	110.40
1	D	92	ARG	CA-CB-CG	6.84	128.46	113.40
2	E	93	GLN	CA-C-N	6.83	132.23	117.20
2	B	163	ARG	CA-CB-CG	6.37	127.41	113.40
2	B	150	ARG	CB-CG-CD	5.99	127.17	111.60
1	A	92	ARG	N-CA-C	5.97	127.12	111.00
3	C	170	LYS	CB-CA-C	-5.96	98.49	110.40
2	E	103	ILE	C-N-CA	-5.90	106.95	121.70
1	A	160	GLN	CA-CB-CG	5.77	126.10	113.40
1	D	201	LYS	N-CA-CB	5.76	120.96	110.60
2	B	201	ASP	N-CA-C	5.70	126.39	111.00
2	B	165	GLN	CA-CB-CG	-5.65	100.97	113.40
1	A	92	ARG	CA-CB-CG	5.62	125.75	113.40
2	E	150	ARG	CB-CG-CD	5.61	126.19	111.60
2	E	93	GLN	C-N-CA	5.35	135.07	121.70
1	D	108	VAL	C-N-CA	5.06	134.34	121.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	ARG	Mainchain
2	B	175	TYR	Mainchain
2	B	93	GLN	Mainchain
3	C	170	LYS	Mainchain
2	E	104	ASN	Mainchain
2	E	209	GLU	Mainchain,Peptide
3	F	102	GLN	Mainchain
3	F	203	GLN	Mainchain

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	1090	0	1046	21	6
1	D	1100	0	1062	25	8
2	B	1093	0	1057	20	8
2	E	1051	0	1024	14	1
3	C	1034	0	1012	32	5
3	F	1027	0	1003	28	0
4	A	15	0	15	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	D	10	0	5	3	0
7	A	60	0	0	4	0
7	B	28	0	0	5	0
7	C	60	0	0	9	0
7	D	59	0	0	6	0
7	E	35	0	0	3	0
7	F	60	0	0	4	0
All	All	6724	0	6224	122	14

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 10.

All (122) 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:D:160:GLN:CG	6:D:1223:SEP:H	1.24	1.50
1:D:160:GLN:HG3	6:D:1223:SEP:N	1.13	1.43
2:E:93:GLN:O	2:E:94:LYS:N	1.69	1.22
3:C:111:ARG:NE	3:C:125:THR:O	2.01	0.93
1:D:99:ARG:O	1:D:100[A]:ARG:HG3	1.68	0.93
2:E:92:THR:N	7:E:2001:HOH:O	1.99	0.93
3:C:99:GLN:OE1	3:F:97:THR:HG21	1.75	0.87
3:C:102:GLN:HG3	7:C:2010:HOH:O	1.74	0.86
3:C:102:GLN:HE22	1:D:163:ARG:NH1	1.75	0.84
2:B:104:ASN:HD21	2:B:208:MET:CE	1.94	0.81
1:D:160:GLN:CG	6:D:1223:SEP:N	2.04	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ARG:NH2	2:B:190[A]:GLU:OE1	2.15	0.80
3:C:97:THR:HG21	3:F:99:GLN:OE1	1.82	0.79
2:B:162[B]:GLU:OE2	7:B:2019:HOH:O	2.02	0.78
3:C:93:VAL:HG23	3:C:212:PHE:HB3	1.66	0.75
3:C:102:GLN:NE2	1:D:163:ARG:NH1	2.34	0.74
2:B:104:ASN:HD21	2:B:208:MET:HE1	1.52	0.74
1:A:99:ARG:NH2	7:A:2002:HOH:O	2.22	0.72
2:B:209:GLU:HG3	7:B:2026:HOH:O	1.91	0.70
1:A:118:GLN:O	1:A:119[A]:GLU:HB2	1.90	0.70
1:D:161:VAL:HG22	7:D:2028:HOH:O	1.90	0.69
3:C:182:ARG:NE	7:C:2060:HOH:O	2.19	0.65
1:A:118:GLN:HG2	2:B:140:LEU:HD11	1.78	0.65
1:D:142:GLN:OE1	1:D:213[B]:VAL:CG1	2.45	0.65
3:F:198:ASP:OD2	3:F:200[B]:VAL:HG22	1.97	0.64
1:D:92:ARG:N	1:D:93:PRO:HD3	2.13	0.63
2:B:104:ASN:HD21	2:B:208:MET:HE3	1.66	0.61
1:D:99:ARG:NH2	7:D:2004:HOH:O	2.34	0.61
1:A:165[A]:LEU:CD1	3:C:116:LEU:HD11	2.31	0.61
1:A:183[A]:MET:HE3	3:C:116:LEU:HD13	1.84	0.60
1:D:142:GLN:OE1	1:D:213[B]:VAL:HG11	2.01	0.59
3:F:93:VAL:HG23	3:F:212:PHE:HB3	1.83	0.59
3:C:217:ASP:OD1	7:C:2060:HOH:O	2.17	0.59
1:A:91:PRO:HA	7:A:2001:HOH:O	2.02	0.59
1:A:117:ASN:OD1	1:A:121:PRO:HD2	2.03	0.58
1:D:91:PRO:HB3	1:D:133:VAL:HG21	1.85	0.58
1:A:183[A]:MET:CE	3:C:116:LEU:HD13	2.34	0.58
2:E:107:LEU:O	2:E:203:ASN:ND2	2.34	0.58
3:F:147:THR:OG1	3:F:200[B]:VAL:HG23	2.04	0.57
1:A:165[A]:LEU:HD11	3:C:116:LEU:HD11	1.84	0.57
2:B:162[B]:GLU:CD	2:B:162[B]:GLU:H	2.07	0.56
2:E:219:LEU:HD21	2:E:222:PRO:HG3	1.87	0.56
1:D:99:ARG:HD3	7:D:2051:HOH:O	2.03	0.56
3:F:97:THR:HG23	3:F:114:ALA:HB3	1.88	0.56
3:F:102:GLN:C	3:F:102:GLN:N	2.60	0.56
1:A:106:GLY:HA3	7:A:2005:HOH:O	2.05	0.56
1:A:99:ARG:O	1:A:100:ARG:HG3	2.06	0.55
3:C:203:GLN:HG2	7:C:2055:HOH:O	2.06	0.55
3:C:217:ASP:CG	7:C:2060:HOH:O	2.44	0.55
2:B:104:ASN:ND2	2:B:208:MET:HE1	2.22	0.55
2:E:102:THR:OG1	2:E:116:ASP:OD2	2.25	0.55
2:B:96:ALA:HB1	3:C:180:LEU:HD13	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:110:ILE:HD11	3:F:193:VAL:HG13	1.88	0.54
1:D:183[A]:MET:HE3	3:F:116:LEU:HD13	1.89	0.54
2:B:103:ILE:HG12	7:B:2007:HOH:O	2.08	0.53
2:E:134:THR:OG1	2:E:194:ASN:ND2	2.41	0.53
1:A:124:ASN:CG	4:A:1223:NAG:O1	2.48	0.52
3:F:198:ASP:CG	3:F:200[B]:VAL:HG22	2.30	0.52
3:F:147:THR:HG1	3:F:200[B]:VAL:HG23	1.73	0.51
1:D:144:LEU:CD2	1:D:210:ALA:HB3	2.39	0.51
3:C:200[B]:VAL:CG2	7:C:2053:HOH:O	2.57	0.51
3:C:101:HIS:HB3	7:C:2012:HOH:O	2.10	0.51
2:E:96:ALA:HB1	3:F:180:LEU:HD13	1.93	0.50
1:A:121:PRO:HB2	1:A:129:PHE:CE1	2.46	0.50
3:C:139:TYR:O	3:C:211:GLY:HA2	2.12	0.50
2:B:103:ILE:CG1	7:B:2007:HOH:O	2.59	0.50
3:F:146:HIS:HE1	7:F:2045:HOH:O	1.94	0.50
1:D:118:GLN:O	1:D:119[B]:GLU:HB2	2.11	0.50
1:D:99:ARG:O	1:D:100[A]:ARG:CG	2.53	0.49
3:F:169:SER:O	3:F:170:LYS:HB2	2.13	0.49
3:C:146:HIS:HD2	3:C:148:ALA:O	1.96	0.49
3:C:153:LEU:HD23	3:C:160:LYS:HD3	1.93	0.49
2:B:104:ASN:ND2	2:B:208:MET:CE	2.70	0.49
3:C:146:HIS:HE1	7:C:2045:HOH:O	1.96	0.49
3:C:200[B]:VAL:HG21	7:C:2053:HOH:O	2.12	0.48
3:F:200[B]:VAL:HG21	7:F:2054:HOH:O	2.13	0.48
3:C:99:GLN:OE1	3:F:97:THR:CG2	2.57	0.48
1:D:118:GLN:HG2	2:E:140:LEU:HD11	1.95	0.48
1:D:124:ASN:ND2	7:D:2017:HOH:O	2.46	0.48
3:F:111[A]:ARG:NE	3:F:125:THR:O	2.47	0.47
1:D:165[A]:LEU:HD11	3:F:116:LEU:HD21	1.96	0.47
2:E:202:LYS:N	2:E:202:LYS:HD2	2.29	0.47
1:D:105:GLY:O	7:D:2006:HOH:O	2.20	0.47
1:A:133:VAL:O	1:A:137:TYR:OH	2.26	0.47
2:B:122:MET:SD	3:C:137:LEU:HD13	2.55	0.47
1:A:108:VAL:HG22	1:A:194:TRP:CD1	2.50	0.47
1:D:114:VAL:HG11	1:D:117:ASN:HB2	1.98	0.46
2:B:102:THR:OG1	2:B:116:ASP:OD2	2.34	0.46
2:B:109:ARG:O	2:B:110:ASP:HB2	2.16	0.46
2:E:202:LYS:N	2:E:202:LYS:CD	2.79	0.45
1:A:100:ARG:HG2	7:A:2053:HOH:O	2.16	0.45
2:E:125:ASN:OD1	2:E:136:LYS:HE3	2.17	0.45
2:B:202:LYS:HE2	7:B:2024:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:THR:CG2	3:F:99:GLN:OE1	2.60	0.45
2:E:208:MET:O	2:E:212:ASN:ND2	2.50	0.45
1:A:91:PRO:HB3	1:A:133:VAL:HG11	1.98	0.45
1:D:108:VAL:HG22	1:D:194:TRP:CD1	2.51	0.44
3:F:139:TYR:O	3:F:211:GLY:HA2	2.17	0.44
2:E:164:ALA:HB2	7:E:2018:HOH:O	2.16	0.44
1:A:118:GLN:O	1:A:119[B]:GLU:HB2	2.18	0.44
1:A:162:ARG:HB3	3:F:111[A]:ARG:NH1	2.32	0.43
3:F:89:LYS:N	7:F:2001:HOH:O	2.51	0.43
2:B:208:MET:O	2:B:212:ASN:ND2	2.52	0.43
3:F:200[B]:VAL:CG2	7:F:2054:HOH:O	2.66	0.43
3:F:146:HIS:HD2	3:F:148:ALA:O	2.02	0.42
3:F:137:LEU:HG	3:F:138:TYR:N	2.33	0.42
3:F:198:ASP:OD1	3:F:200[B]:VAL:HG22	2.19	0.42
2:B:142:TYR:O	2:B:217:GLY:HA2	2.20	0.42
1:D:111:PHE:CE1	1:D:214:PHE:HB2	2.54	0.42
3:C:97:THR:HG23	3:C:114:ALA:HB3	2.02	0.41
2:B:103:ILE:HG22	2:B:105:VAL:H	1.85	0.41
1:A:93:PRO:HG3	1:A:119[A]:GLU:OE1	2.20	0.41
3:C:104:PRO:HD2	3:C:197:TYR:O	2.21	0.41
3:F:97:THR:CG2	3:F:114:ALA:HB3	2.49	0.41
1:A:165[A]:LEU:HD13	3:C:116:LEU:HD11	2.00	0.41
1:D:144:LEU:HD23	1:D:205:TYR:CD2	2.56	0.41
2:E:159:ARG:NH2	7:E:2017:HOH:O	2.45	0.40
3:C:95:THR:CG2	3:C:116:LEU:HD12	2.52	0.40

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ARG:NH2	1:D:113:THR:CB[1_554]	0.57	1.63
1:A:148:GLU:OE2	3:C:87:LYS:NZ[1_445]	0.78	1.42
1:A:148:GLU:CD	3:C:87:LYS:NZ[1_445]	0.82	1.38
2:B:163:ARG:CZ	1:D:113:THR:CG2[1_554]	1.20	1.00
2:B:163:ARG:NH2	1:D:113:THR:OG1[1_554]	1.31	0.89
2:B:163:ARG:NH1	1:D:113:THR:CG2[1_554]	1.37	0.83
2:B:163:ARG:NH2	1:D:113:THR:CG2[1_554]	1.61	0.59
2:B:163:ARG:CZ	1:D:113:THR:CB[1_554]	1.61	0.59
1:A:148:GLU:OE1	3:C:87:LYS:NZ[1_445]	1.62	0.58
1:A:148:GLU:OE2	3:C:87:LYS:CE[1_445]	1.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ARG:CZ	1:D:113:THR:OG1[1_554]	1.78	0.42
2:B:163:ARG:NH2	1:D:113:THR:CA[1_554]	2.10	0.10
1:A:117:ASN:N	2:E:163:ARG:NH2[1_554]	2.11	0.09
1:A:148:GLU:CG	3:C:87:LYS:NZ[1_445]	2.13	0.07

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	138/134 (103%)	127 (92%)	10 (7%)	1 (1%)	22 12
1	D	139/134 (104%)	129 (93%)	9 (6%)	1 (1%)	22 12
2	B	137/136 (101%)	125 (91%)	8 (6%)	4 (3%)	4 0
2	E	132/136 (97%)	123 (93%)	8 (6%)	1 (1%)	19 10
3	C	133/131 (102%)	128 (96%)	4 (3%)	1 (1%)	19 10
3	F	132/131 (101%)	124 (94%)	8 (6%)	0	100 100
All	All	811/802 (101%)	756 (93%)	47 (6%)	8 (1%)	15 6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	94	LYS
2	B	175	TYR
2	E	209	GLU
2	B	201	ASP
2	B	176	ASN
3	C	170	LYS
1	D	105	GLY
1	A	92	ARG

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	124/117 (106%)	123 (99%)	1 (1%)	81 82
1	D	125/117 (107%)	125 (100%)	0	100 100
2	B	119/117 (102%)	113 (95%)	6 (5%)	24 16
2	E	115/117 (98%)	112 (97%)	3 (3%)	46 39
3	C	119/115 (104%)	117 (98%)	2 (2%)	60 57
3	F	118/115 (103%)	116 (98%)	2 (2%)	60 57
All	All	720/698 (103%)	706 (98%)	14 (2%)	57 53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
2	B	109	ARG
2	B	118	VAL
2	B	149	SER
2	B	163	ARG
2	B	189	LEU
2	B	223	ASP
3	C	169	SER
3	C	217	ASP
2	E	109	ARG
2	E	163	ARG
2	E	189	LEU
3	F	111[A]	ARG
3	F	111[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	186	GLN
2	B	104	ASN

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Mol	Chain	Res	Type
3	C	102	GLN
3	C	146	HIS
3	C	167	HIS
3	C	203	GLN
1	D	124	ASN
1	D	172	ASN
1	D	186	GLN
2	E	191	GLN
2	E	194	ASN
3	F	146	HIS
3	F	167	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
6	SEP	D	1223	-	8,9,10	1.49	1 (12%)	8,12,14	1.60	2 (25%)
4	NAG	A	1223	-	15,15,15	0.48	0	21,21,21	0.85	1 (4%)

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
6	SEP	D	1223	-	-	0/5/8/10	-
4	NAG	A	1223	-	-	4/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1223	SEP	P-O1P	3.27	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1223	SEP	OG-CB-CA	3.09	111.16	108.14
6	D	1223	SEP	P-OG-CB	-2.58	111.19	118.30
4	A	1223	NAG	O5-C1-C2	2.28	111.80	109.52

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1223	NAG	C8-C7-N2-C2
4	A	1223	NAG	O7-C7-N2-C2
4	A	1223	NAG	O5-C5-C6-O6
4	A	1223	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1223	SEP	3	0
4	A	1223	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	93:GLN	C	94:LYS	N	1.07

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	133/134 (99%)	-0.01	3 (2%) 60 64	8, 15, 28, 50	3 (2%)
1	D	133/134 (99%)	0.05	4 (3%) 50 54	8, 16, 27, 37	4 (3%)
2	B	134/136 (98%)	0.26	8 (5%) 21 23	8, 19, 33, 58	9 (6%)
2	E	133/136 (97%)	0.25	8 (6%) 21 23	10, 19, 33, 54	8 (6%)
3	C	131/131 (100%)	-0.22	0 100 100	4, 12, 21, 30	2 (1%)
3	F	129/131 (98%)	-0.31	0 100 100	6, 12, 21, 25	5 (3%)
All	All	793/802 (98%)	0.01	23 (2%) 51 56	4, 15, 29, 58	31 (3%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	224	MET	5.3
2	E	92	THR	4.7
2	E	175	TYR	4.6
2	B	92	THR	4.1
2	E	106	PRO	4.0
2	B	104	ASN	3.3
1	A	91	PRO	3.1
1	A	159	GLY	3.0
1	D	91	PRO	3.0
2	B	103	ILE	2.8
2	E	201	ASP	2.6
1	D	90	GLN	2.6
2	B	223	ASP	2.5
2	E	176	ASN	2.4
2	B	176	ASN	2.4
1	D	222	SER	2.3
1	A	104[A]	MET	2.3
2	E	129	ARG	2.3
2	E	103	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	101[A]	ASN	2.1
2	B	105	VAL	2.0
2	B	106	PRO	2.0
2	E	93	GLN	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, 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
4	NAG	A	1223	15/15	0.66	0.26	68,69,69,69	0
6	SEP	D	1223	10/11	0.87	0.36	41,41,42,42	10
5	CA	E	1224	1/1	0.98	0.03	22,22,22,22	0
5	CA	B	1224	1/1	0.99	0.04	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.