Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 08:31 PM EDT

PDB ID	:	4F33
Title	:	Crystal Structure of therapeutic antibody MORAb-009
Authors	:	Xia, D.; Ma, J.; Tang, W.K.; Esser, L.
Deposited on	:	2012-05-08
Resolution	:	1.75 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:

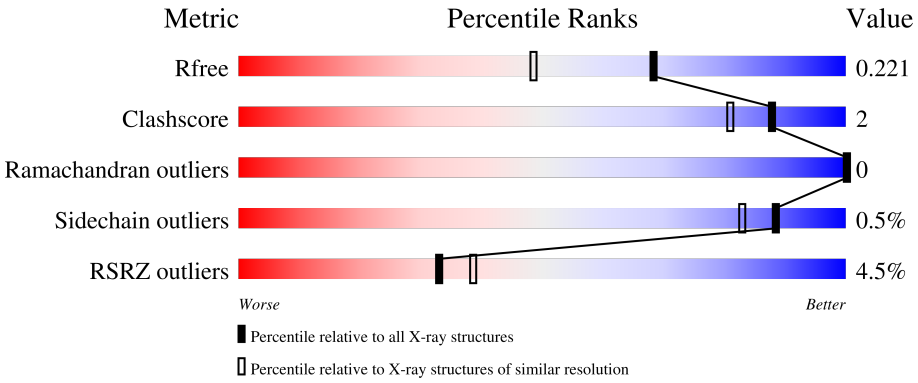
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.75 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	213	95%
1	C	213	94% 5%
1	E	213	94% 5%
1	G	213	92% 7%
2	B	231	7% 91% 5%

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Mol	Chain	Length	Quality of chain
2	D	231	13% 92% 5%
2	F	231	5% 92% 5%
2	H	231	5% 90% 5% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27005 atoms, of which 12809 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.

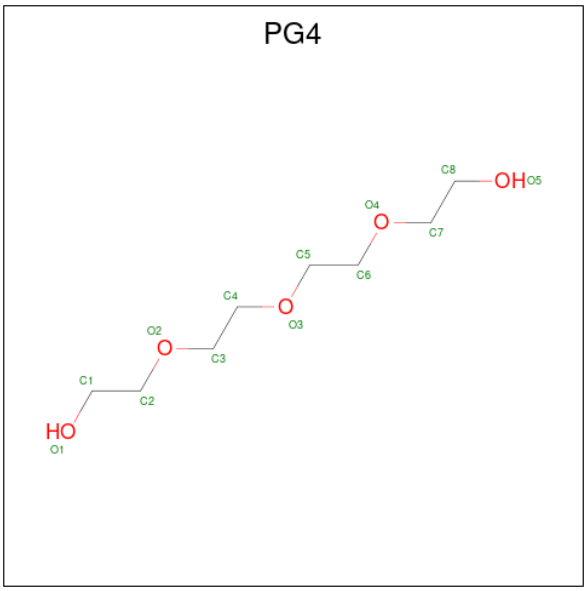
- Molecule 1 is a protein called MORAb-009 FAB light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	211	Total	C	H	N	O	S	0	0	0
			3166	1006	1551	270	332	7			
1	C	211	Total	C	H	N	O	S	0	0	0
			3166	1006	1551	270	332	7			
1	E	211	Total	C	H	N	O	S	0	0	0
			3166	1006	1551	270	332	7			
1	G	211	Total	C	H	N	O	S	0	0	0
			3166	1006	1551	270	332	7			

- Molecule 2 is a protein called MORAb-009 FAB heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	220	Total	C	H	N	O	S	0	2	0
			3249	1037	1608	269	327	8			
2	D	220	Total	C	H	N	O	S	0	1	0
			3240	1035	1602	269	327	7			
2	F	220	Total	C	H	N	O	S	0	2	0
			3249	1037	1608	269	327	8			
2	H	220	Total	C	H	N	O	S	0	2	0
			3248	1037	1607	269	327	8			

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			31	8	18	5		
3	A	1	Total	C	H	O	0	0
			31	8	18	5		
3	C	1	Total	C	H	O	0	0
			31	8	18	5		
3	C	1	Total	C	H	O	0	0
			31	8	18	5		
3	E	1	Total	C	H	O	0	0
			31	8	18	5		
3	E	1	Total	C	H	O	0	0
			31	8	18	5		
3	E	1	Total	C	H	O	0	0
			31	8	18	5		
3	G	1	Total	C	H	O	0	0
			31	8	18	5		
3	G	1	Total	C	H	O	0	0
			31	8	18	5		
3	G	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	125	Total	O	0	0
			125	125		

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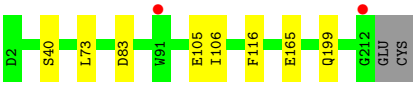
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	130	Total O 130 130	0	0
4	D	86	Total O 86 86	0	0
4	E	140	Total O 140 140	0	0
4	F	151	Total O 151 151	0	0
4	G	140	Total O 140 140	0	0
4	H	119	Total O 119 119	0	0

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.

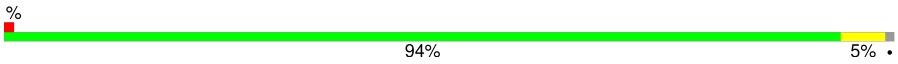
• Molecule 1: MORAb-009 FAB light chain

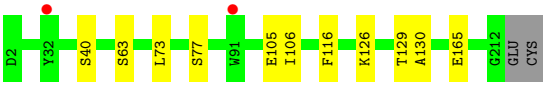
Chain A:



• Molecule 1: MORAb-009 FAB light chain

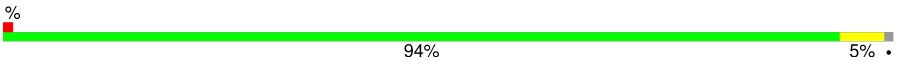
Chain C:





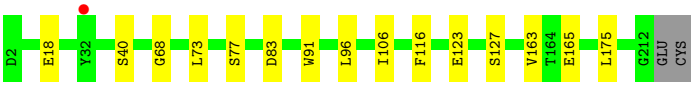
• Molecule 1: MORAb-009 FAB light chain

Chain E:



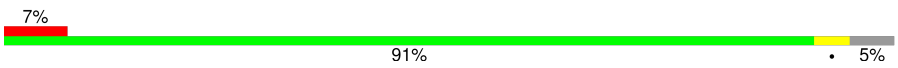
• Molecule 1: MORAb-009 FAB light chain

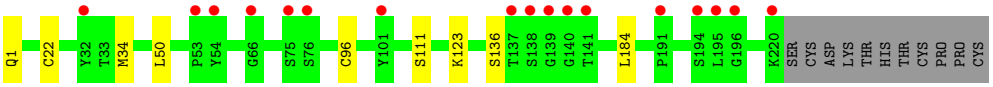
Chain G:



• Molecule 2: MORAb-009 FAB heavy chain

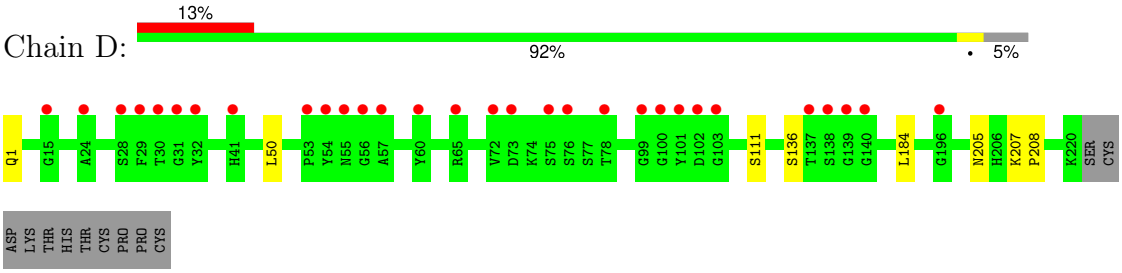
Chain B:





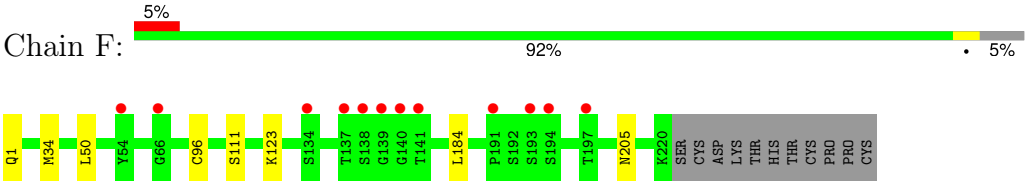
• Molecule 2: MORAb-009 FAB heavy chain

Chain D:



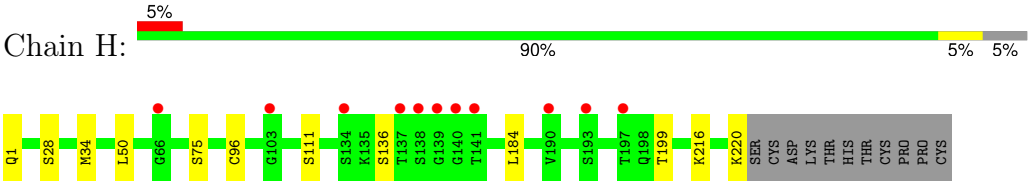
• Molecule 2: MORAb-009 FAB heavy chain

Chain F:



• Molecule 2: MORAb-009 FAB heavy chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.31Å 141.31Å 281.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.82 – 1.75 39.19 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.0 (38.82-1.75) 85.3 (39.19-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_965)	Depositor
R, R_{free}	0.208 , 0.234 0.201 , 0.221	Depositor DCC
R_{free} test set	2312 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27005	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7127e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PCA, PG4

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	0.51	0/1652	0.63	0/2241
1	C	0.49	0/1652	0.60	0/2241
1	E	0.48	0/1652	0.60	0/2241
1	G	0.49	0/1652	0.61	0/2241
2	B	0.48	0/1681	0.59	0/2288
2	D	0.41	0/1675	0.55	0/2280
2	F	0.48	0/1681	0.58	0/2288
2	H	0.46	0/1681	0.58	0/2288
All	All	0.48	0/13326	0.59	0/18108

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

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	1615	1551	1551	6	0
1	C	1615	1551	1551	8	0
1	E	1615	1551	1551	6	0
1	G	1615	1551	1551	11	0
2	B	1641	1608	1607	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1638	1602	1602	4	0
2	F	1641	1608	1607	6	0
2	H	1641	1607	1607	8	0
3	A	26	36	36	1	0
3	C	26	36	36	0	0
3	E	39	54	54	2	0
3	G	39	54	54	1	0
4	A	154	0	0	2	0
4	B	125	0	0	0	0
4	C	130	0	0	0	0
4	D	86	0	0	0	0
4	E	140	0	0	1	0
4	F	151	0	0	0	0
4	G	140	0	0	2	0
4	H	119	0	0	0	0
All	All	14196	12809	12807	52	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 2.

All (52) 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)
2:F:34:MET:SD	2:F:96[B]:CYS:SG	2.79	0.80
2:B:34:MET:SD	2:B:96[B]:CYS:SG	2.83	0.76
2:F:34:MET:CG	2:F:96[B]:CYS:SG	2.86	0.64
2:H:34:MET:SD	2:H:96[B]:CYS:SG	2.99	0.60
2:B:34:MET:CG	2:B:96[B]:CYS:SG	2.91	0.59
1:G:73:LEU:C	1:G:73:LEU:HD23	2.25	0.57
2:F:50:LEU:HD12	2:F:50:LEU:C	2.30	0.52
2:D:50:LEU:C	2:D:50:LEU:HD12	2.30	0.52
1:C:73:LEU:C	1:C:73:LEU:HD23	2.31	0.50
2:F:34:MET:HG3	2:F:96[B]:CYS:SG	2.52	0.50
1:C:63:SER:HB3	2:H:28:SER:HB3	1.94	0.49
1:E:73:LEU:C	1:E:73:LEU:HD23	2.33	0.49
2:F:184:LEU:C	2:F:184:LEU:HD12	2.33	0.49
2:H:50:LEU:C	2:H:50:LEU:HD12	2.33	0.49
2:B:50:LEU:HD12	2:B:50:LEU:C	2.33	0.49
2:H:184:LEU:HD12	2:H:184:LEU:C	2.33	0.48
2:B:184:LEU:C	2:B:184:LEU:HD12	2.34	0.48
2:H:199:THR:HG23	2:H:216:LYS:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:SER:HB2	1:E:165:GLU:HG3	1.96	0.47
2:D:184:LEU:C	2:D:184:LEU:HD12	2.35	0.47
2:B:34:MET:HG3	2:B:96[B]:CYS:SG	2.54	0.47
1:A:73:LEU:C	1:A:73:LEU:HD23	2.36	0.46
1:G:116:PHE:HD1	2:H:136:SER:HA	1.80	0.46
2:B:123:LYS:HA	1:G:123:GLU:HG3	1.97	0.46
1:G:68:GLY:N	4:G:442:HOH:O	2.48	0.46
2:H:34:MET:CG	2:H:96[B]:CYS:SG	3.04	0.46
1:G:40:SER:HB2	1:G:165:GLU:HG3	1.97	0.46
1:C:116:PHE:HD1	2:D:136:SER:HA	1.81	0.45
3:A:501:PG4:H31	4:A:752:HOH:O	2.17	0.45
1:C:40:SER:HB2	1:C:165:GLU:HG3	2.00	0.44
1:G:127:SER:HB2	4:G:474:HOH:O	2.17	0.43
1:A:105:GLU:HG2	1:A:106:ILE:N	2.33	0.43
1:G:40:SER:HA	3:G:301:PG4:H71	1.99	0.43
1:G:163:VAL:HG22	1:G:175:LEU:HD12	2.01	0.43
2:B:22:CYS:SG	2:B:96[B]:CYS:SG	3.16	0.43
1:A:83:ASP:HB3	1:A:106:ILE:HG12	2.01	0.42
1:G:83:ASP:HB3	1:G:106:ILE:HG12	2.01	0.42
1:A:40:SER:HB2	1:A:165:GLU:HG3	2.01	0.42
1:E:140:TYR:CG	1:E:141:PRO:HA	2.55	0.42
1:A:116:PHE:HD1	2:B:136:SER:HA	1.84	0.42
1:E:83:ASP:HB3	1:E:106:ILE:HG12	2.01	0.42
1:G:18:GLU:O	1:G:77:SER:HA	2.20	0.42
1:G:91:TRP:HA	1:G:96:LEU:HD22	2.02	0.41
3:E:301:PG4:H61	4:E:540:HOH:O	2.20	0.41
1:E:84:ALA:HA	3:E:301:PG4:H31	2.03	0.41
1:E:91:TRP:HA	1:E:96:LEU:HD22	2.01	0.41
1:C:126:LYS:HD3	2:F:123:LYS:HB2	2.03	0.41
1:C:129:THR:HG22	1:C:130:ALA:N	2.36	0.41
2:D:207:LYS:N	2:D:208:PRO:CD	2.84	0.41
1:C:77:SER:HB3	2:H:75:SER:HA	2.03	0.41
1:C:105:GLU:HG2	1:C:106:ILE:N	2.36	0.41
1:A:199:GLN:HB2	4:A:730:HOH:O	2.21	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	209/213 (98%)	204 (98%)	5 (2%)	0	100	100
1	C	209/213 (98%)	204 (98%)	5 (2%)	0	100	100
1	E	209/213 (98%)	204 (98%)	5 (2%)	0	100	100
1	G	209/213 (98%)	204 (98%)	5 (2%)	0	100	100
2	B	220/231 (95%)	217 (99%)	3 (1%)	0	100	100
2	D	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
2	F	220/231 (95%)	216 (98%)	4 (2%)	0	100	100
2	H	220/231 (95%)	217 (99%)	3 (1%)	0	100	100
All	All	1715/1776 (97%)	1681 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	185/187 (99%)	185 (100%)	0	100	100
1	C	185/187 (99%)	185 (100%)	0	100	100
1	E	185/187 (99%)	185 (100%)	0	100	100
1	G	185/187 (99%)	185 (100%)	0	100	100
2	B	186/195 (95%)	185 (100%)	1 (0%)	88	83
2	D	185/195 (95%)	183 (99%)	2 (1%)	73	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	186/195 (95%)	184 (99%)	2 (1%)	73 59
2	H	186/195 (95%)	184 (99%)	2 (1%)	73 59
All	All	1483/1528 (97%)	1476 (100%)	7 (0%)	88 83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	111	SER
2	D	111	SER
2	D	205	ASN
2	F	111	SER
2	F	205	ASN
2	H	111	SER
2	H	220	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PCA	D	1	2	7,8,9	1.83	1 (14%)	9,10,12	1.71	4 (44%)
2	PCA	B	1	2	7,8,9	1.82	1 (14%)	9,10,12	2.05	4 (44%)
2	PCA	F	1	2	7,8,9	1.92	1 (14%)	9,10,12	1.99	4 (44%)
2	PCA	H	1	2	7,8,9	1.90	1 (14%)	9,10,12	1.58	3 (33%)

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
2	PCA	D	1	2	-	0/0/11/13	0/1/1/1
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1
2	PCA	F	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	PCA	CD-N	4.81	1.46	1.34
2	H	1	PCA	CD-N	4.78	1.46	1.34
2	B	1	PCA	CD-N	4.68	1.46	1.34
2	D	1	PCA	CD-N	4.66	1.46	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	PCA	CB-CA-C	-4.03	107.12	112.66
2	F	1	PCA	CB-CA-C	-3.92	107.27	112.66
2	D	1	PCA	CB-CA-N	2.48	110.05	103.24
2	H	1	PCA	CB-CA-C	-2.42	109.34	112.66
2	D	1	PCA	CB-CA-C	-2.30	109.50	112.66
2	B	1	PCA	OE-CD-CG	-2.29	122.63	126.72
2	B	1	PCA	CB-CA-N	2.26	109.46	103.24
2	F	1	PCA	O-C-CA	-2.23	119.04	124.77
2	B	1	PCA	CA-N-CD	-2.20	106.04	113.58
2	D	1	PCA	CA-N-CD	-2.18	106.12	113.58
2	D	1	PCA	OE-CD-CG	-2.17	122.84	126.72
2	H	1	PCA	OE-CD-CG	-2.09	122.98	126.72
2	H	1	PCA	CB-CA-N	2.06	108.91	103.24
2	F	1	PCA	CB-CA-N	2.01	108.78	103.24
2	F	1	PCA	CA-N-CD	-2.01	106.70	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
3	PG4	C	302	-	12,12,12	0.63	0	11,11,11	0.96	0
3	PG4	E	303	-	12,12,12	0.66	0	11,11,11	0.94	1 (9%)
3	PG4	C	301	-	12,12,12	0.61	0	11,11,11	0.82	0
3	PG4	G	302	-	12,12,12	0.62	0	11,11,11	1.09	1 (9%)
3	PG4	G	301	-	12,12,12	0.59	0	11,11,11	0.78	0
3	PG4	E	301	-	12,12,12	0.60	0	11,11,11	0.99	1 (9%)
3	PG4	A	502	-	12,12,12	0.69	0	11,11,11	0.88	0
3	PG4	A	501	-	12,12,12	0.60	0	11,11,11	0.79	0
3	PG4	G	303	-	12,12,12	0.62	0	11,11,11	0.90	0
3	PG4	E	302	-	12,12,12	0.67	0	11,11,11	0.99	1 (9%)

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	PG4	C	302	-	-	4/10/10/10	-
3	PG4	E	303	-	-	2/10/10/10	-
3	PG4	C	301	-	-	1/10/10/10	-
3	PG4	G	302	-	-	6/10/10/10	-
3	PG4	G	301	-	-	5/10/10/10	-
3	PG4	E	301	-	-	4/10/10/10	-
3	PG4	A	502	-	-	3/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	A	501	-	-	4/10/10/10	-
3	PG4	G	303	-	-	4/10/10/10	-
3	PG4	E	302	-	-	1/10/10/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	302	PG4	C3-O2-C2	2.44	123.94	113.26
3	E	301	PG4	C5-O3-C4	2.27	123.20	113.26
3	E	303	PG4	C7-O4-C6	2.10	122.46	113.26
3	E	302	PG4	C3-O2-C2	2.06	122.29	113.26

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	302	PG4	C4-C3-O2-C2
3	G	301	PG4	O3-C5-C6-O4
3	G	302	PG4	O2-C3-C4-O3
3	G	302	PG4	O3-C5-C6-O4
3	C	301	PG4	O2-C3-C4-O3
3	C	302	PG4	O4-C7-C8-O5
3	E	301	PG4	O4-C7-C8-O5
3	A	501	PG4	O4-C7-C8-O5
3	G	303	PG4	O4-C7-C8-O5
3	E	302	PG4	O4-C7-C8-O5
3	A	501	PG4	O2-C3-C4-O3
3	G	303	PG4	O1-C1-C2-O2
3	A	502	PG4	O3-C5-C6-O4
3	G	303	PG4	O3-C5-C6-O4
3	C	302	PG4	O2-C3-C4-O3
3	C	302	PG4	O3-C5-C6-O4
3	G	301	PG4	C8-C7-O4-C6
3	E	301	PG4	C1-C2-O2-C3
3	C	302	PG4	C3-C4-O3-C5
3	A	501	PG4	C6-C5-O3-C4
3	E	301	PG4	C8-C7-O4-C6
3	G	301	PG4	C6-C5-O3-C4
3	G	301	PG4	O1-C1-C2-O2
3	G	302	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	G	303	PG4	C5-C6-O4-C7
3	A	502	PG4	C1-C2-O2-C3
3	E	303	PG4	O4-C7-C8-O5
3	G	301	PG4	O2-C3-C4-O3
3	A	501	PG4	C3-C4-O3-C5
3	G	302	PG4	C8-C7-O4-C6
3	G	302	PG4	C3-C4-O3-C5
3	E	303	PG4	O3-C5-C6-O4
3	E	301	PG4	O3-C5-C6-O4
3	A	502	PG4	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	301	PG4	1	0
3	E	301	PG4	2	0
3	A	501	PG4	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^{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	211/213 (99%)	0.12	2 (0%)	84	88	30, 42, 66, 92	0
1	C	211/213 (99%)	0.18	2 (0%)	84	88	35, 46, 69, 95	0
1	E	211/213 (99%)	0.13	3 (1%)	75	81	33, 46, 68, 111	0
1	G	211/213 (99%)	0.11	1 (0%)	91	93	33, 45, 69, 93	0
2	B	219/231 (94%)	0.47	17 (7%)	13	17	30, 44, 76, 114	0
2	D	219/231 (94%)	0.74	30 (13%)	3	3	34, 52, 85, 154	0
2	F	219/231 (94%)	0.25	12 (5%)	25	30	31, 41, 73, 113	0
2	H	219/231 (94%)	0.32	11 (5%)	28	33	32, 46, 77, 111	0
All	All	1720/1776 (96%)	0.29	78 (4%)	33	38	30, 45, 75, 154	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	101	TYR	8.8
2	D	54	TYR	6.4
2	B	139	GLY	6.4
2	B	54	TYR	6.1
2	B	101	TYR	5.9
2	F	193	SER	5.3
2	D	139	GLY	4.9
2	D	138	SER	4.8
2	F	139	GLY	4.8
1	G	32	TYR	4.8
2	D	75	SER	4.7
2	B	138	SER	4.7
1	C	32	TYR	4.5
2	F	137	THR	4.4
2	H	197	THR	4.0
2	F	138	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	91	TRP	3.6
2	D	76	SER	3.6
2	F	197	THR	3.6
2	D	73	ASP	3.6
2	F	141	THR	3.5
2	D	55	ASN	3.5
2	D	28	SER	3.5
2	D	100	GLY	3.5
2	H	138	SER	3.5
2	D	31	GLY	3.4
2	F	140	GLY	3.3
2	B	140	GLY	3.3
2	F	191	PRO	3.3
2	H	137	THR	3.3
2	D	32	TYR	3.1
2	D	196	GLY	3.1
2	H	139	GLY	3.0
2	D	103	GLY	3.0
2	F	54	TYR	2.9
2	H	140	GLY	2.9
2	D	72	VAL	2.9
2	D	99	GLY	2.9
2	D	65	ARG	2.8
2	D	60	TYR	2.8
2	B	75	SER	2.7
2	B	220	LYS	2.7
2	D	137	THR	2.7
2	H	141	THR	2.7
2	D	24	ALA	2.7
2	B	195	LEU	2.6
2	H	103	GLY	2.6
2	D	41	HIS	2.6
2	D	29	PHE	2.6
2	F	134	SER	2.6
2	D	56	GLY	2.6
2	F	66	GLY	2.6
1	E	32	TYR	2.6
2	F	194	SER	2.5
2	H	193	SER	2.5
1	A	91	TRP	2.5
2	D	15	GLY	2.5
2	D	102	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	57	ALA	2.4
2	D	53	PRO	2.3
2	B	76	SER	2.3
2	H	66	GLY	2.3
2	B	141	THR	2.3
1	E	152	ASN	2.3
2	B	191	PRO	2.2
1	E	168	SER	2.2
2	B	196	GLY	2.2
2	H	134	SER	2.2
2	B	66	GLY	2.1
2	B	53	PRO	2.1
2	H	190	VAL	2.1
2	B	137	THR	2.0
2	D	78	THR	2.0
2	B	194	SER	2.0
2	B	32	TYR	2.0
2	D	30	THR	2.0
1	A	212	GLY	2.0
2	D	140	GLY	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
2	PCA	D	1	8/9	0.79	0.32	68,93,103,107	0
2	PCA	B	1	8/9	0.91	0.29	55,72,95,102	0
2	PCA	H	1	8/9	0.94	0.20	48,72,88,88	0
2	PCA	F	1	8/9	0.96	0.13	34,62,85,92	0

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
3	PG4	E	302	13/13	0.76	0.28	61,84,113,114	0
3	PG4	G	302	13/13	0.80	0.26	71,87,114,115	0
3	PG4	E	301	13/13	0.84	0.20	54,76,91,104	0
3	PG4	G	303	13/13	0.84	0.16	58,83,110,133	0
3	PG4	C	302	13/13	0.86	0.26	54,86,141,147	0
3	PG4	A	501	13/13	0.88	0.19	55,76,96,105	0
3	PG4	G	301	13/13	0.88	0.15	59,81,99,102	0
3	PG4	A	502	13/13	0.89	0.19	52,70,163,174	0
3	PG4	C	301	13/13	0.90	0.17	55,78,98,113	0
3	PG4	E	303	13/13	0.91	0.12	54,80,121,125	0

6.5 Other polymers (i)

There are no such residues in this entry.