Full wwPDB X-ray Structure Validation Report (i)

Apr 3, 2016 – 11:48 PM EDT

PDB ID	:	4YO0
Title	:	Crystal structure of monoclonal anti-human podoplanin antibody NZ-1 with bound PA peptide
Authors	:	Fujii, Y.; Kitago, Y.; Arimori, T.; Takagi, J.
Deposited on	:	2015-03-11
Resolution	:	1.56 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

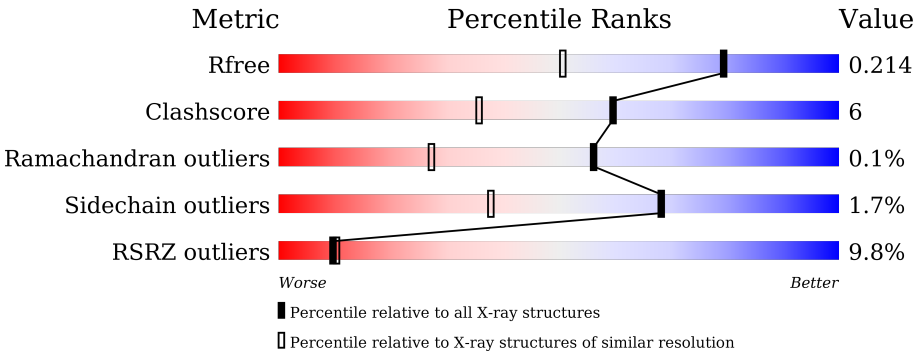
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 1.56 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	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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 >=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 <=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	238	6% 74% 13% • 12%
1	C	238	11% 76% 7% 17%
2	B	233	9% 78% 12% 10%
2	D	233	9% 83% 7% 10%
3	E	14	7% 79% 7% 14%
3	F	14	7% 64% 14% 21%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7078 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 Heavy chain of antigen binding fragment, Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	9	0
			1629	1035	271	312	11			
1	C	198	Total	C	N	O	S	0	3	0
			1508	958	247	294	9			

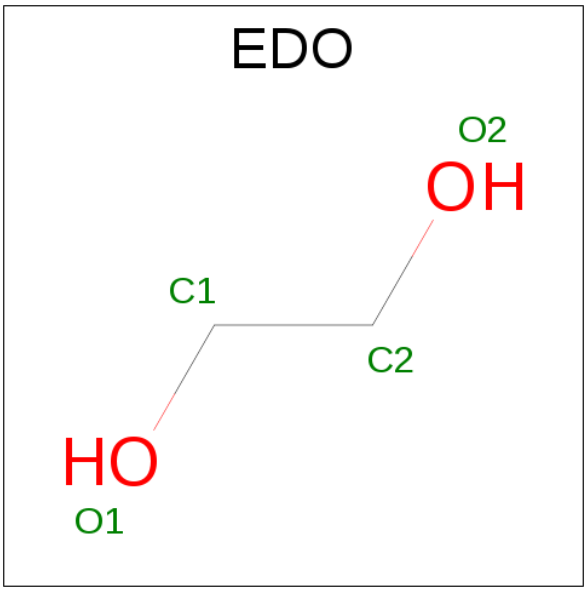
- Molecule 2 is a protein called Light chain of antigen binding fragment, Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	4	0
			1635	1016	284	330	5			
2	D	210	Total	C	N	O	S	0	3	0
			1632	1014	284	329	5			

- Molecule 3 is a protein called PA14 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	12	Total	C	N	O	S	0	2	0
			91	57	13	19	2			
3	F	11	Total	C	N	O	S	0	1	0
			80	50	11	17	2			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

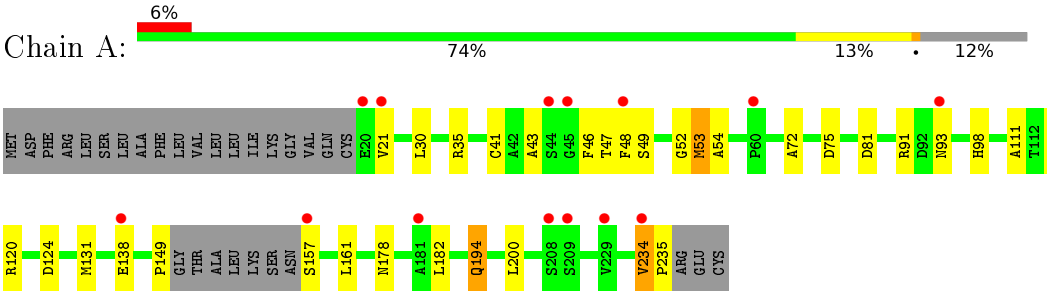
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	128	Total O 128 128	0	0
5	B	128	Total O 128 128	0	0
5	C	87	Total O 87 87	0	0
5	D	141	Total O 141 141	0	0
5	E	7	Total O 7 7	0	0
5	F	8	Total O 8 8	0	0

3 Residue-property plots

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.

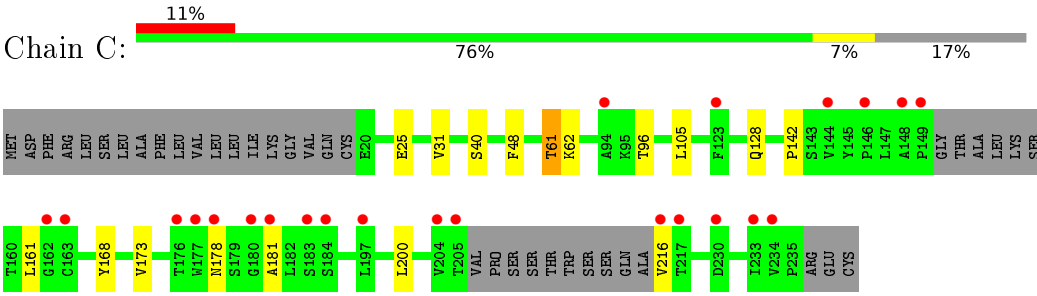
- Molecule 1: Heavy chain of antigen binding fragment, Fab

Chain A:



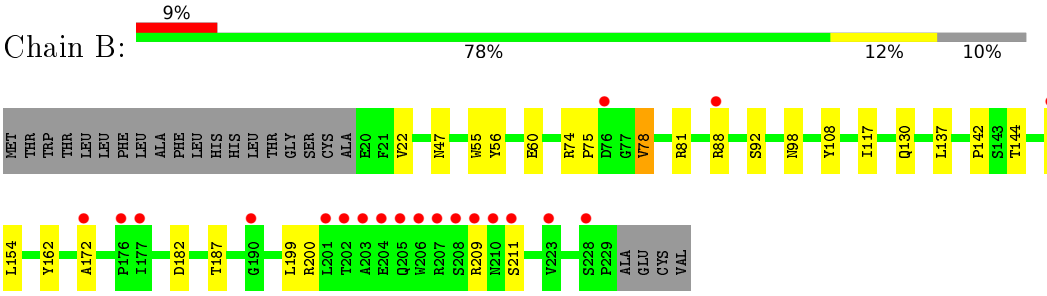
- Molecule 1: Heavy chain of antigen binding fragment, Fab

Chain C:



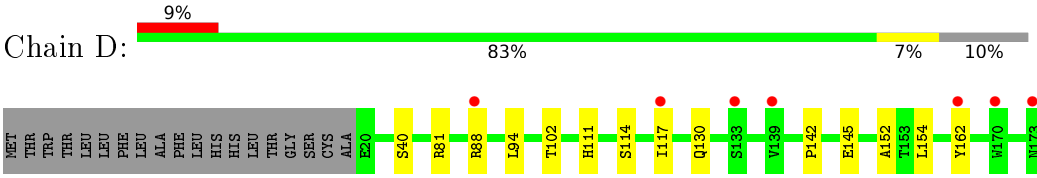
- Molecule 2: Light chain of antigen binding fragment, Fab

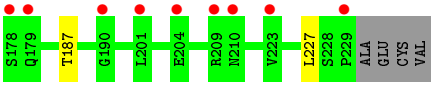
Chain B:



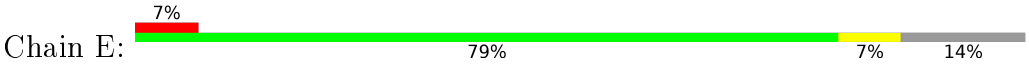
- Molecule 2: Light chain of antigen binding fragment, Fab

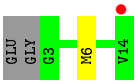
Chain D:



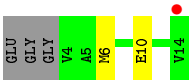


• Molecule 3: PA14 peptide





• Molecule 3: PA14 peptide



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.18Å 80.01Å 132.52Å 90.00° 96.61° 90.00°	Depositor
Resolution (Å)	40.00 – 1.56 40.01 – 1.56	Depositor EDS
% Data completeness (in resolution range)	97.5 (40.00-1.56) 97.6 (40.01-1.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.56Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.179 , 0.214 0.178 , 0.214	Depositor DCC
R_{free} test set	6032 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.1	EDS
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 121232 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7078	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, EDO

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	0.91	0/1687	0.91	2/2296 (0.1%)
1	C	0.83	0/1549	0.83	0/2108
2	B	0.88	5/1675 (0.3%)	0.83	0/2283
2	D	0.85	0/1669	0.86	0/2271
3	E	1.07	0/93	1.04	0/125
3	F	0.99	1/83 (1.2%)	0.87	0/113
All	All	0.87	6/6756 (0.1%)	0.86	2/9196 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	55	TRP	CE3-CZ3	6.35	1.49	1.38
2	B	108	TYR	CG-CD1	6.06	1.47	1.39
2	B	92	SER	CA-CB	5.48	1.61	1.52
3	F	10	GLU	CD-OE1	5.46	1.31	1.25
2	B	108	TYR	CE2-CZ	5.33	1.45	1.38
2	B	56	TYR	CD2-CE2	5.33	1.47	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	124	ASP	CB-CG-OD2	-5.53	113.32	118.30

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	1629	0	1613	35	1
1	C	1508	0	1479	10	0
2	B	1635	0	1584	19	0
2	D	1632	0	1582	11	0
3	E	91	0	90	1	0
3	F	80	0	78	2	0
4	D	4	0	6	0	0
5	A	128	0	0	4	0
5	B	128	0	0	3	0
5	C	87	0	0	0	0
5	D	141	0	0	2	0
5	E	7	0	0	0	0
5	F	8	0	0	0	0
All	All	7078	0	6432	74	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 6.

All (74) 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:53[A]:MET:HG3	1:A:98[A]:HIS:NE2	1.80	0.95
1:A:53[B]:MET:HG2	1:A:98[B]:HIS:CE1	2.12	0.83
1:C:61:THR:HG22	1:C:62:LYS:HG3	1.63	0.80
1:A:72:ALA:O	1:A:91[B]:ARG:NH1	2.14	0.79
1:A:48:PHE:CZ	1:A:98[A]:HIS:CD2	2.71	0.78
2:D:102:THR:HG21	2:D:130:GLN:HE21	1.54	0.72
1:A:53[B]:MET:HG2	1:A:98[B]:HIS:NE2	2.08	0.67
1:A:48:PHE:HZ	1:A:98[A]:HIS:CD2	2.12	0.67
2:B:182:ASP:OD2	2:B:200:ARG:NH1	2.29	0.66
1:A:53[A]:MET:HG3	1:A:98[A]:HIS:CD2	2.31	0.65
2:B:172:ALA:HB1	2:B:209:ARG:HD3	1.81	0.63
1:A:49:SER:HB3	1:A:93:ASN:ND2	2.15	0.62
1:A:53[B]:MET:CG	1:A:98[B]:HIS:CE1	2.83	0.62
2:D:145:GLU:HG3	5:D:427:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:THR:CG2	2:D:130:GLN:HE21	2.15	0.59
2:D:117:ILE:HG12	3:F:6[B]:MET:HE2	1.84	0.58
1:A:53[B]:MET:HG2	1:A:98[B]:HIS:CD2	2.38	0.58
1:A:53[B]:MET:HG3	1:A:54:ALA:N	2.18	0.57
2:B:60:GLU:HG2	2:B:187:THR:HG23	1.86	0.56
1:A:138:GLU:OE1	1:A:138:GLU:N	2.37	0.56
2:B:130:GLN:HB3	2:B:162:TYR:CE1	2.41	0.56
2:B:130:GLN:HB3	2:B:162:TYR:CZ	2.40	0.55
1:A:91[A]:ARG:CZ	1:A:98[A]:HIS:CE1	2.90	0.55
1:A:98[B]:HIS:HB2	5:A:344:HOH:O	2.07	0.55
2:B:74[A]:ARG:NH2	5:B:301:HOH:O	2.26	0.55
1:C:168:TYR:CE2	1:C:173:VAL:HG13	2.42	0.55
2:B:47[B]:ASN:ND2	2:B:88:ARG:HH21	2.06	0.54
1:A:91[B]:ARG:NH2	1:A:93:ASN:ND2	2.56	0.54
2:B:154:LEU:HD12	2:B:199:LEU:HD23	1.90	0.54
2:B:117:ILE:HG12	3:E:6[A]:MET:HE2	1.90	0.53
1:A:53[A]:MET:HG3	1:A:98[A]:HIS:CE1	2.44	0.52
1:A:98[B]:HIS:CE1	1:A:115:CYS:HB2	2.45	0.52
2:B:142:PRO:HD3	2:B:154:LEU:CD2	2.41	0.51
1:A:43:ALA:HB3	1:A:48:PHE:CD1	2.45	0.51
2:B:75:PRO:O	2:B:78[A]:VAL:HG13	2.11	0.50
1:C:178:ASN:HB3	1:C:181:ALA:HB3	1.92	0.50
1:A:43:ALA:HB3	1:A:48:PHE:CE1	2.48	0.49
1:C:161:LEU:HD12	1:C:216:VAL:HG21	1.95	0.48
1:A:149:PRO:HD3	1:A:161:LEU:HD23	1.96	0.47
1:A:120:ARG:NH2	5:A:301:HOH:O	2.30	0.47
2:D:111:HIS:NE2	3:F:6[B]:MET:CE	2.78	0.46
1:C:31:VAL:HG11	1:C:105:LEU:HD13	1.98	0.46
2:B:81:ARG:HD2	2:B:98:ASN:O	2.16	0.46
2:D:154:LEU:HD13	2:D:227:LEU:HD12	1.98	0.46
1:A:41:CYS:SG	1:A:98[B]:HIS:NE2	2.88	0.45
1:C:25[B]:GLU:OE1	1:C:128:GLN:OE1	2.34	0.45
1:A:21:VAL:HG13	1:A:46:PHE:CD1	2.51	0.45
2:B:200:ARG:HD3	5:B:303:HOH:O	2.15	0.45
1:A:131[B]:MET:HE3	5:A:388:HOH:O	2.16	0.45
1:A:200:LEU:HD12	1:A:200:LEU:C	2.36	0.45
2:B:144:THR:O	2:B:148:GLN:HG3	2.17	0.45
2:D:102:THR:HG21	2:D:130:GLN:NE2	2.26	0.45
2:D:130:GLN:HB2	2:D:162:TYR:CD1	2.52	0.45
2:D:81[A]:ARG:HG3	5:D:408:HOH:O	2.16	0.45
2:B:142:PRO:HD3	2:B:154:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASP:HB2	5:A:389:HOH:O	2.16	0.44
2:B:74[A]:ARG:HG2	2:B:78[A]:VAL:HG22	1.99	0.44
1:C:48:PHE:CD2	1:C:96:THR:HA	2.53	0.43
1:A:178:ASN:HB2	1:A:182:LEU:HG	2.01	0.43
1:A:53[A]:MET:HB2	1:A:98[A]:HIS:CE1	2.54	0.43
1:A:52:GLY:C	1:A:53[A]:MET:HG2	2.39	0.42
1:A:111:ALA:HB3	1:A:113:TYR:CE1	2.54	0.42
1:A:53[B]:MET:CG	1:A:98[B]:HIS:NE2	2.80	0.42
2:D:40:SER:HA	2:D:94:LEU:HD23	2.01	0.42
1:A:194:GLN:HG3	2:B:200:ARG:NH1	2.34	0.42
1:A:91[A]:ARG:CZ	1:A:98[A]:HIS:NE2	2.83	0.42
2:B:74[A]:ARG:HD3	5:B:301:HOH:O	2.20	0.42
1:A:53[B]:MET:HG2	1:A:98[B]:HIS:CG	2.55	0.41
1:C:173:VAL:HG22	1:C:200:LEU:HD21	2.02	0.41
2:B:60:GLU:HG2	2:B:187:THR:CG2	2.50	0.41
2:D:142:PRO:HG3	2:D:152:ALA:HB1	2.02	0.41
1:C:142:PRO:HB3	1:C:168:TYR:HB3	2.02	0.41
1:C:25[B]:GLU:HA	1:C:40:SER:O	2.20	0.41
1:A:234:VAL:HA	1:A:235:PRO:HD3	1.86	0.41

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)
1:A:35[B]:ARG:NH2	1:A:47:THR:OG1[1_655]	2.11	0.09

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	214/238 (90%)	209 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	195/238 (82%)	191 (98%)	4 (2%)	0	100 100
2	B	212/233 (91%)	206 (97%)	6 (3%)	0	100 100
2	D	211/233 (91%)	205 (97%)	5 (2%)	1 (0%)	34 9
3	E	11/14 (79%)	11 (100%)	0	0	100 100
3	F	10/14 (71%)	10 (100%)	0	0	100 100
All	All	853/970 (88%)	832 (98%)	20 (2%)	1 (0%)	56 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	114	SER

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	184/200 (92%)	178 (97%)	6 (3%)	45 13
1	C	168/200 (84%)	167 (99%)	1 (1%)	90 78
2	B	188/203 (93%)	183 (97%)	5 (3%)	52 19
2	D	187/203 (92%)	185 (99%)	2 (1%)	80 58
3	E	10/9 (111%)	10 (100%)	0	100 100
3	F	9/9 (100%)	9 (100%)	0	100 100
All	All	746/824 (90%)	732 (98%)	14 (2%)	68 33

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

Mol	Chain	Res	Type
1	A	30	LEU
1	A	53[A]	MET
1	A	53[B]	MET
1	A	157	SER
1	A	194	GLN

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Mol	Chain	Res	Type
1	A	234	VAL
2	B	22	VAL
2	B	78[A]	VAL
2	B	78[B]	VAL
2	B	137	LEU
2	B	211	SER
1	C	61	THR
2	D	88	ARG
2	D	187	THR

Some 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)

2 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	B	20	2	7,8,9	1.97	2 (28%)	9,10,12	3.03	5 (55%)
2	PCA	D	20	2	7,8,9	2.58	2 (28%)	9,10,12	1.67	2 (22%)

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	B	20	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	D	20	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	B	20	PCA	CA-N	2.24	1.49	1.46
2	D	20	PCA	CA-N	3.92	1.51	1.46
2	B	20	PCA	CD-N	4.54	1.47	1.33
2	D	20	PCA	CD-N	4.93	1.48	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	20	PCA	CB-CA-C	-7.09	102.28	112.80
2	B	20	PCA	OE-CD-CG	-3.62	119.68	126.85
2	D	20	PCA	CB-CA-C	-3.04	108.29	112.80
2	B	20	PCA	CA-N-CD	-2.45	104.81	113.53
2	D	20	PCA	OE-CD-CG	-2.15	122.59	126.85
2	B	20	PCA	O-C-CA	-2.09	119.97	125.69
2	B	20	PCA	CB-CA-N	2.19	109.97	103.34

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
4	EDO	D	301	-	3,3,3	0.71	0	2,2,2	0.25	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	EDO	D	301	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	209/238 (87%)	0.53	14 (6%) 21 21	21, 36, 59, 84	0
1	C	198/238 (83%)	0.83	25 (12%) 5 5	21, 43, 76, 98	0
2	B	209/233 (89%)	0.64	22 (10%) 8 8	21, 39, 75, 107	0
2	D	209/233 (89%)	0.82	20 (9%) 10 10	20, 41, 73, 85	0
3	E	12/14 (85%)	0.60	1 (8%) 14 14	25, 33, 55, 65	0
3	F	11/14 (78%)	1.07	1 (9%) 11 12	26, 30, 57, 69	0
All	All	848/970 (87%)	0.71	83 (9%) 10 10	20, 39, 73, 107	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	159	VAL	11.2
2	B	208	SER	8.4
1	C	234	VAL	7.3
3	F	14	VAL	6.9
1	C	148	ALA	6.6
1	C	216	VAL	5.9
2	D	175	ALA	5.9
1	C	94	ALA	5.6
2	B	202	THR	5.6
2	B	210	ASN	5.5
1	C	233	ILE	5.2
1	C	180	GLY	4.3
2	D	190	GLY	4.3
1	C	183	SER	4.2
1	C	158	MET	4.1
2	D	177	ILE	4.1
2	B	207	ARG	4.1
2	B	150	ASN	4.1
2	B	228	SER	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	190	GLY	3.8
2	D	178	SER	3.8
2	D	176	PRO	3.7
2	B	204	GLU	3.7
1	C	205	THR	3.7
1	A	45	GLY	3.6
2	B	203	ALA	3.5
2	D	229	PRO	3.5
2	B	209	ARG	3.4
2	B	205	GLN	3.4
1	A	234	VAL	3.2
1	C	149	PRO	3.2
2	B	201	LEU	3.2
1	C	162	GLY	3.2
2	B	206	TRP	3.1
1	C	177	TRP	3.1
1	C	230	ASP	3.0
2	D	117	ILE	3.0
2	B	211	SER	3.0
1	A	21	VAL	3.0
1	A	44	SER	2.9
2	D	223	VAL	2.8
2	B	177	ILE	2.8
1	C	184	SER	2.7
1	C	217	THR	2.6
1	A	20	GLU	2.6
2	D	209	ARG	2.6
1	C	163	CYS	2.5
1	A	209	SER	2.5
2	D	133	SER	2.5
1	A	181	ALA	2.5
2	D	174	GLY	2.5
2	D	204	GLU	2.4
1	A	138	GLU	2.4
2	D	201	LEU	2.4
1	C	146	PRO	2.4
2	D	210	ASN	2.4
2	D	162	TYR	2.4
1	A	208	SER	2.3
1	C	144	VAL	2.3
1	C	178	ASN	2.3
1	A	93	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	123	PHE	2.3
2	B	88	ARG	2.3
2	D	139	VAL	2.3
1	A	48	PHE	2.3
2	B	172	ALA	2.3
2	D	173	ASN	2.3
2	D	170	TRP	2.3
1	A	229	VAL	2.3
2	B	148	GLN	2.2
2	B	176	PRO	2.2
2	D	179	GLN	2.2
2	B	223	VAL	2.2
1	A	157	SER	2.2
1	C	197	LEU	2.2
1	C	176	THR	2.1
1	C	181	ALA	2.1
2	B	76	ASP	2.1
2	D	88	ARG	2.1
3	E	14[A]	VAL	2.0
2	B	149	GLY	2.0
1	C	204	VAL	2.0
1	A	60	PRO	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. 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^{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	LLDF	B-factors(Å^2)	Q<0.9
2	PCA	D	20	8/9	0.76	0.20	-	39,47,53,54	0
2	PCA	B	20	8/9	0.85	0.10	-	36,40,43,44	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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^{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	LLDF	B-factors(Å^2)	Q<0.9
4	EDO	D	301	4/4	0.76	0.11	-1.29	47,55,61,62	0

6.5 Other polymers

There are no such residues in this entry.