Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:10 PM GMT

PDB ID	:	4V3D
Title	:	The CIDRa domain from HB3var03 PfEMP1 bound to endothelial protein C receptor
Authors	:	Lau, C.K.Y.; Turner, L.; Jespersen, J.S.; Lowe, E.D.; Petersen, B.; Wang, C.W.; Petersen, J.E.V.; Lusingu, J.; Theander, T.G.; Lavstsen, T.; Higgins, M.K.
Deposited on	:	2014-10-17
Resolution	:	2.65 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:

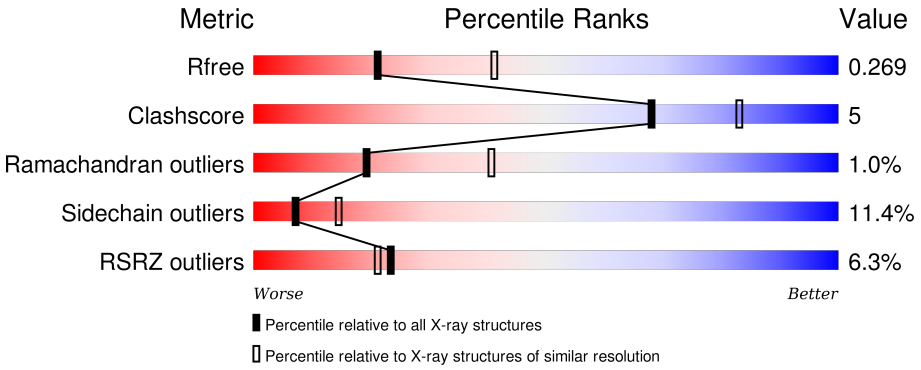
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	251	6% 66% 16% • 16%
1	C	251	10% 55% 14% • 26%
2	B	170	% 84% 14% ••
2	D	170	3% 83% 14% ••

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PTY	B	200	-	-	-	X
3	PTY	D	200	-	-	-	X
4	NAG	D	201	-	-	-	X
5	MAN	B	207	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6397 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.

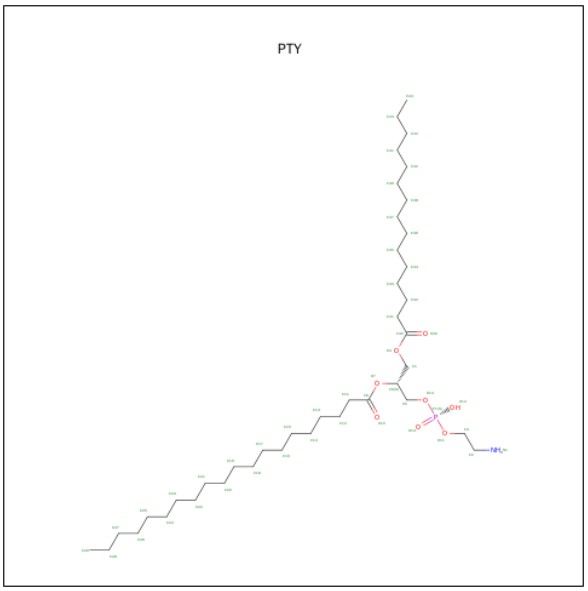
- Molecule 1 is a protein called HB3VAR03 CIDRA DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1755	1116	289	339	11			
1	C	186	Total	C	N	O	S	0	0	0
			1578	1016	256	295	11			

- Molecule 2 is a protein called ENDOTHELIAL PROTEIN C RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1384	884	246	250	4			
2	D	168	Total	C	N	O	S	0	0	0
			1376	878	245	249	4			

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
3	D	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

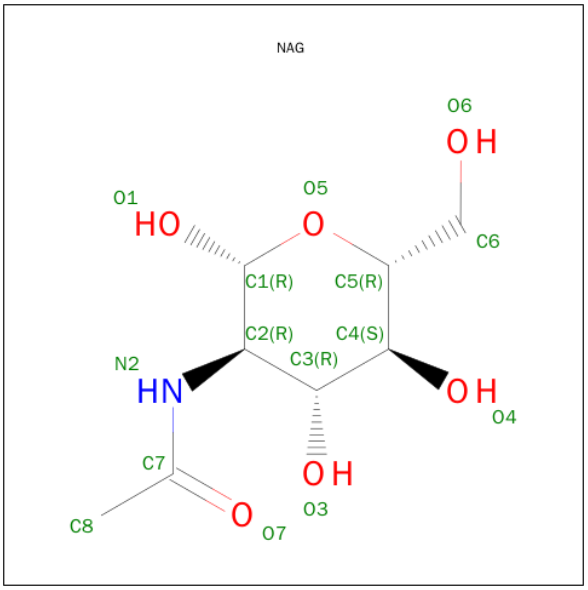
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

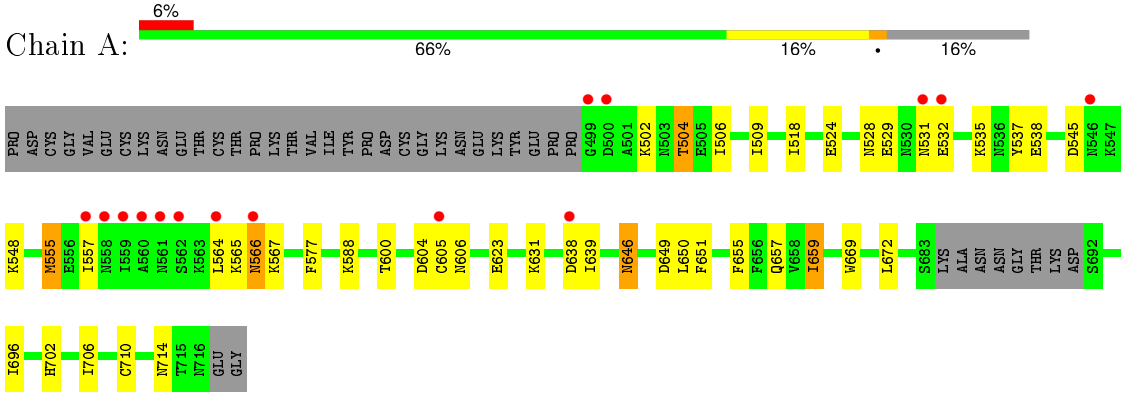
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	3	Total C N O 39 22 2 15	0	0

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.

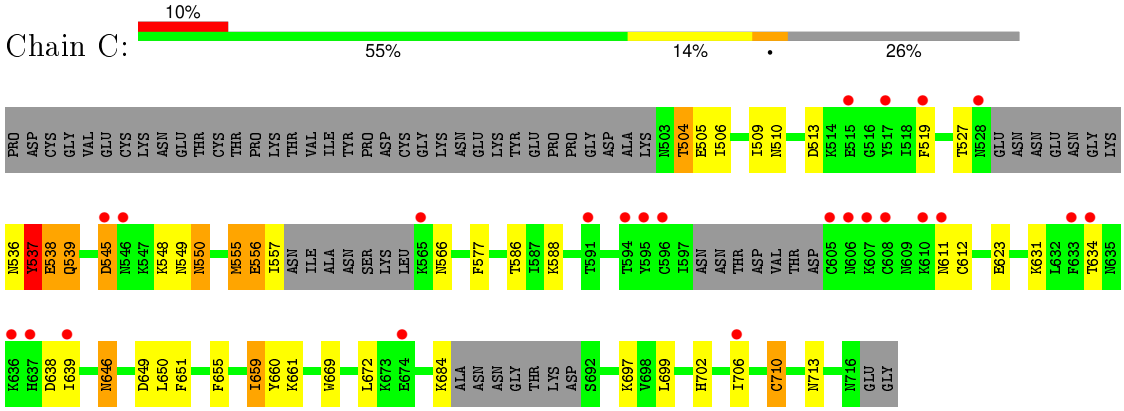
- Molecule 1: HB3VAR03 CIDRA DOMAIN

Chain A:



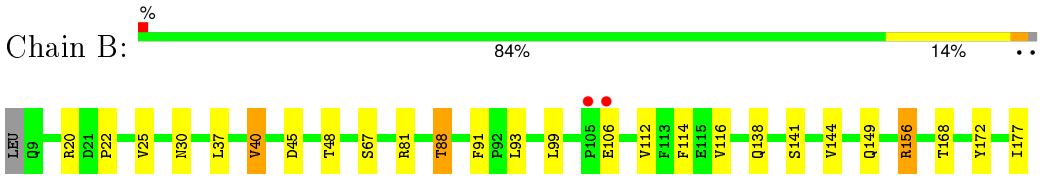
- Molecule 1: HB3VAR03 CIDRA DOMAIN

Chain C:



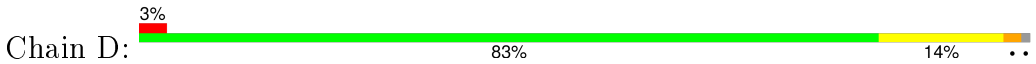
- Molecule 2: ENDOTHELIAL PROTEIN C RECEPTOR

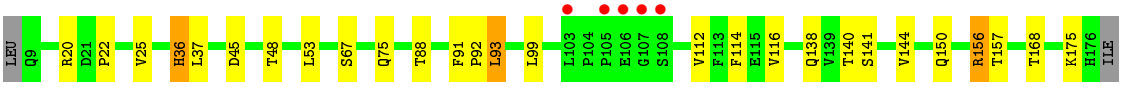
Chain B:



- Molecule 2: ENDOTHELIAL PROTEIN C RECEPTOR

Chain D:




LEU
Q9
R20
D21
P22
V25
H36
L37
D45
T48
L53
S67
Q75
T88
F91
P92
L93
L99
L103
P104
P105
E106
G107
S108
V112
F113
F114
E115
V116
Q138
V139
T140
S141
V144
Q150
R156
T157
T168
K175
H176
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	66.13Å 94.67Å 290.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.29 – 2.65 50.79 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.0 (53.29-2.65) 94.0 (50.79-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.222 , 0.255 0.230 , 0.269	Depositor DCC
R_{free} test set	1287 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 25427 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6397	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: NAG, PTY, MAN

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	0.53	0/1790	0.76	0/2406
1	C	0.48	0/1610	0.79	3/2157 (0.1%)
2	B	0.50	0/1422	0.74	2/1936 (0.1%)
2	D	0.45	0/1414	0.72	2/1925 (0.1%)
All	All	0.49	0/6236	0.75	7/8424 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	93	LEU	N-CA-CB	-6.30	97.80	110.40
2	B	93	LEU	N-CA-CB	-6.12	98.17	110.40
2	B	93	LEU	CA-CB-CG	5.67	128.34	115.30
2	D	93	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	537	TYR	C-N-CA	5.42	135.26	121.70
1	C	556	GLU	C-N-CA	5.24	134.80	121.70
1	C	538	GLU	N-CA-C	5.12	124.83	111.00

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	1755	0	1690	14	0
1	C	1578	0	1529	21	0
2	B	1384	0	1335	11	0
2	D	1376	0	1324	19	0
3	B	50	0	79	3	0
3	D	50	0	79	3	0
4	B	28	0	25	1	0
4	D	56	0	50	1	0
5	B	39	0	34	0	0
6	B	28	0	26	1	0
6	D	14	0	13	0	0
7	D	39	0	34	2	0
All	All	6397	0	6218	59	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 5.

All (59) 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:696:ILE:CD1	1:A:696:ILE:CG1	1.75	1.62
1:A:538:GLU:HB2	1:A:555:MET:HE1	1.62	0.82
1:C:537:TYR:N	1:C:537:TYR:CD1	2.54	0.74
1:C:537:TYR:N	1:C:537:TYR:HD1	1.87	0.73
1:C:536:ASN:C	1:C:537:TYR:CD1	2.65	0.69
1:C:660:TYR:HD1	2:D:150:GLN:HE22	1.42	0.68
2:B:172:TYR:CD2	3:B:200:PTY:H282	2.33	0.62
1:C:505:GLU:HG2	1:C:539:GLN:HE22	1.66	0.61
2:D:93:LEU:HD23	7:D:206:NAG:H82	1.83	0.60
1:C:555:MET:O	1:C:566:ASN:HB2	2.03	0.59
6:B:205:NAG:H81	2:D:36:HIS:CE1	2.38	0.59
4:B:202:NAG:H5	4:D:201:NAG:H81	1.87	0.57
2:B:37:LEU:CD2	2:D:37:LEU:HD22	2.35	0.56
1:A:545:ASP:HB3	1:A:548:LYS:HB2	1.87	0.56
2:B:37:LEU:HD23	2:D:37:LEU:HD22	1.88	0.55
1:C:510:ASN:O	1:C:537:TYR:CD2	2.59	0.55
1:A:555:MET:HB3	1:A:567:LYS:HB3	1.88	0.55
1:C:655:PHE:O	1:C:659:ILE:HB	2.07	0.55
1:A:655:PHE:O	1:A:659:ILE:HB	2.08	0.54
2:B:168:THR:HG22	3:B:200:PTY:H281	1.89	0.54
2:D:75:GLN:HE22	2:D:156:ARG:HH11	1.56	0.53
1:C:536:ASN:C	1:C:537:TYR:HD1	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:THR:HG21	1:A:631:LYS:HB2	1.92	0.52
1:C:504:THR:HG21	1:C:631:LYS:HB2	1.92	0.52
1:C:660:TYR:CD1	2:D:150:GLN:NE2	2.78	0.50
1:A:555:MET:O	1:A:566:ASN:HA	2.11	0.50
2:D:25:VAL:CG1	2:D:45:ASP:HB3	2.43	0.49
1:A:646:ASN:ND2	1:A:649:ASP:H	2.11	0.49
1:C:538:GLU:HB3	1:C:555:MET:CE	2.44	0.48
2:D:36:HIS:CG	2:D:37:LEU:H	2.32	0.48
1:C:510:ASN:O	1:C:537:TYR:HD2	1.95	0.48
2:B:116:VAL:HG21	3:B:200:PTY:H372	1.95	0.48
1:C:646:ASN:ND2	1:C:649:ASP:H	2.11	0.47
2:D:22:PRO:HG3	2:D:91:PHE:CE2	2.49	0.47
2:B:22:PRO:HG3	2:B:91:PHE:CE2	2.49	0.47
2:D:168:THR:HG22	3:D:200:PTY:H272	1.97	0.46
1:C:519:PHE:HB2	1:C:611:ASN:OD1	2.15	0.46
2:B:40:VAL:HG11	2:D:53:LEU:HD21	1.98	0.45
2:D:156:ARG:HE	2:D:156:ARG:HB2	1.51	0.45
1:A:657:GLN:OE1	2:B:81:ARG:NH1	2.50	0.45
2:D:116:VAL:HG21	3:D:200:PTY:H371	1.99	0.44
2:D:92:PRO:O	7:D:206:NAG:H3	2.18	0.44
1:C:706:ILE:O	1:C:710:CYS:HB3	2.17	0.44
1:A:706:ILE:O	1:A:710:CYS:HB2	2.18	0.43
1:C:545:ASP:HB3	1:C:548:LYS:HB2	2.00	0.43
1:C:586:THR:HG21	1:C:699:LEU:HD11	2.01	0.43
1:A:524:GLU:O	1:A:528:ASN:HB3	2.19	0.43
1:C:651:PHE:HA	1:C:669:TRP:CZ2	2.54	0.42
2:B:25:VAL:CG1	2:B:45:ASP:HB3	2.50	0.42
2:B:141:SER:OG	2:B:144:VAL:HG23	2.19	0.42
1:A:651:PHE:HA	1:A:669:TRP:CZ2	2.54	0.42
2:D:157:THR:HG22	3:D:200:PTY:H321	2.02	0.42
1:A:518:ILE:HB	1:A:588:LYS:HG2	2.03	0.41
2:D:141:SER:OG	2:D:144:VAL:HG23	2.21	0.41
2:B:156:ARG:HE	2:B:156:ARG:HB2	1.55	0.41
1:C:660:TYR:HD1	2:D:150:GLN:NE2	2.14	0.40
2:D:25:VAL:HG12	2:D:45:ASP:HB3	2.02	0.40
1:A:702:HIS:NE2	1:A:706:ILE:HD11	2.36	0.40
1:C:702:HIS:NE2	1:C:706:ILE:HD11	2.36	0.40

There are no symmetry-related clashes.

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	206/251 (82%)	189 (92%)	13 (6%)	4 (2%)	10 22
1	C	176/251 (70%)	168 (96%)	7 (4%)	1 (1%)	30 54
2	B	167/170 (98%)	159 (95%)	7 (4%)	1 (1%)	30 54
2	D	166/170 (98%)	158 (95%)	7 (4%)	1 (1%)	30 54
All	All	715/842 (85%)	674 (94%)	34 (5%)	7 (1%)	19 41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	606	ASN
1	A	535	LYS
1	A	565	LYS
1	C	550	ASN
1	A	566	ASN
2	B	88	THR
2	D	88	THR

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	198/234 (85%)	175 (88%)	23 (12%)	7 14
1	C	178/234 (76%)	149 (84%)	29 (16%)	3 6
2	B	151/152 (99%)	137 (91%)	14 (9%)	11 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	150/152 (99%)	139 (93%)	11 (7%)	17 36
All	All	677/772 (88%)	600 (89%)	77 (11%)	7 14

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	502	LYS
1	A	504	THR
1	A	506	ILE
1	A	509	ILE
1	A	529	GLU
1	A	531	ASN
1	A	532	GLU
1	A	537	TYR
1	A	555	MET
1	A	557	ILE
1	A	564	LEU
1	A	577	PHE
1	A	600	THR
1	A	604	ASP
1	A	605	CYS
1	A	623	GLU
1	A	638	ASP
1	A	639	ILE
1	A	646	ASN
1	A	650	LEU
1	A	659	ILE
1	A	672	LEU
1	A	714	ASN
2	B	20	ARG
2	B	30	ASN
2	B	40	VAL
2	B	48	THR
2	B	67	SER
2	B	88	THR
2	B	99	LEU
2	B	106	GLU
2	B	112	VAL
2	B	114	PHE
2	B	138	GLN
2	B	149	GLN
2	B	156	ARG

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Mol	Chain	Res	Type
2	B	177	ILE
1	C	504	THR
1	C	506	ILE
1	C	509	ILE
1	C	513	ASP
1	C	527	THR
1	C	537	TYR
1	C	539	GLN
1	C	545	ASP
1	C	549	ASN
1	C	550	ASN
1	C	555	MET
1	C	556	GLU
1	C	557	ILE
1	C	577	PHE
1	C	588	LYS
1	C	612	CYS
1	C	623	GLU
1	C	634	THR
1	C	638	ASP
1	C	639	ILE
1	C	646	ASN
1	C	650	LEU
1	C	659	ILE
1	C	661	LYS
1	C	672	LEU
1	C	684	LYS
1	C	697	LYS
1	C	710	CYS
1	C	713	ASN
2	D	20	ARG
2	D	36	HIS
2	D	48	THR
2	D	67	SER
2	D	99	LEU
2	D	112	VAL
2	D	114	PHE
2	D	138	GLN
2	D	140	THR
2	D	156	ARG
2	D	175	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	558	ASN
1	A	646	ASN
1	A	714	ASN
2	B	54	GLN
2	B	57	GLN
2	B	70	GLN
2	B	134	GLN
2	B	174	GLN
1	C	539	GLN
1	C	646	ASN
2	D	39	HIS
2	D	57	GLN
2	D	70	GLN
2	D	138	GLN
2	D	174	GLN

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

12 carbohydrates 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	$\#\|Z\| > 2$
4	NAG	B	201	4	14,14,15	0.32	0	15,19,21	0.74	1 (6%)
4	NAG	B	202	2,4	14,14,15	0.34	0	15,19,21	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	203	2,5	14,14,15	0.36	0	15,19,21	1.07	1 (6%)
5	NAG	B	204	5	14,14,15	0.37	0	15,19,21	0.79	1 (6%)
5	MAN	B	207	5	11,11,12	0.34	0	14,15,17	1.65	1 (7%)
4	NAG	D	201	4	14,14,15	0.26	0	15,19,21	0.55	0
4	NAG	D	202	2,4	14,14,15	0.32	0	15,19,21	1.52	1 (6%)
7	MAN	D	203	7	11,11,12	0.44	0	14,15,17	1.26	2 (14%)
4	NAG	D	204	4	14,14,15	0.27	0	15,19,21	0.54	0
4	NAG	D	205	2,4	14,14,15	0.39	0	15,19,21	1.72	3 (20%)
7	NAG	D	206	2,7	14,14,15	0.36	0	15,19,21	0.83	1 (6%)
7	NAG	D	207	7	14,14,15	0.30	0	15,19,21	0.71	1 (6%)

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	B	201	4	-	0/6/23/26	0/1/1/1
4	NAG	B	202	2,4	-	0/6/23/26	0/1/1/1
5	NAG	B	203	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	204	5	-	0/6/23/26	0/1/1/1
5	MAN	B	207	5	-	0/2/19/22	0/1/1/1
4	NAG	D	201	4	-	0/6/23/26	0/1/1/1
4	NAG	D	202	2,4	-	0/6/23/26	0/1/1/1
7	MAN	D	203	7	-	0/2/19/22	0/1/1/1
4	NAG	D	204	4	-	0/6/23/26	0/1/1/1
4	NAG	D	205	2,4	-	0/6/23/26	0/1/1/1
7	NAG	D	206	2,7	-	0/6/23/26	0/1/1/1
7	NAG	D	207	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	205	NAG	C2-N2-C7	2.38	126.10	123.04
4	D	205	NAG	C3-C4-C5	2.41	114.39	110.20
7	D	203	MAN	C1-C2-C3	2.47	112.46	109.54
4	B	201	NAG	C1-O5-C5	2.48	115.40	112.25
5	B	204	NAG	C1-O5-C5	2.49	115.41	112.25
7	D	207	NAG	C1-O5-C5	2.52	115.44	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	206	NAG	C1-O5-C5	2.77	115.77	112.25
4	B	202	NAG	C1-O5-C5	3.19	116.30	112.25
5	B	203	NAG	C1-O5-C5	3.33	116.47	112.25
7	D	203	MAN	C1-O5-C5	3.82	117.09	112.25
5	B	207	MAN	C1-O5-C5	5.28	118.95	112.25
4	D	202	NAG	C1-O5-C5	5.35	119.04	112.25
4	D	205	NAG	C1-O5-C5	5.52	119.26	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	NAG	1	0
4	D	201	NAG	1	0
7	D	206	NAG	2	0

5.6 Ligand geometry

5 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	PTY	B	200	-	48,49,49	0.41	0	49,54,54	0.63	1 (2%)
6	NAG	B	205	2	14,14,15	0.39	0	15,19,21	0.51	0
6	NAG	B	206	2	14,14,15	0.30	0	15,19,21	1.22	1 (6%)
3	PTY	D	200	-	48,49,49	0.45	0	49,54,54	0.61	2 (4%)
6	NAG	D	208	2	14,14,15	0.28	0	15,19,21	0.87	1 (6%)

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	PTY	B	200	-	-	0/53/53/53	0/0/0/0
6	NAG	B	205	2	-	0/6/23/26	0/1/1/1
6	NAG	B	206	2	-	0/6/23/26	0/1/1/1
3	PTY	D	200	-	-	0/53/53/53	0/0/0/0
6	NAG	D	208	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	200	PTY	O14-P1-O13	-2.81	98.70	109.62
3	D	200	PTY	O14-P1-O13	-2.31	100.65	109.62
3	D	200	PTY	O11-P1-O13	-2.24	100.91	109.62
6	D	208	NAG	C2-N2-C7	2.15	125.81	123.04
6	B	206	NAG	C1-O5-C5	3.94	117.24	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	200	PTY	3	0
6	B	205	NAG	1	0
3	D	200	PTY	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	210/251 (83%)	0.27	15 (7%) 19 16	27, 56, 110, 123	0
1	C	186/251 (74%)	0.78	24 (12%) 5 3	41, 81, 131, 155	0
2	B	169/170 (99%)	-0.04	2 (1%) 81 80	25, 44, 80, 126	0
2	D	168/170 (98%)	0.17	5 (2%) 54 52	38, 61, 98, 147	0
All	All	733/842 (87%)	0.31	46 (6%) 23 21	25, 61, 116, 155	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	559	ILE	8.3
1	C	595	TYR	6.6
1	A	560	ALA	6.6
1	C	633	PHE	6.3
1	C	634	THR	5.8
1	C	607	LYS	5.5
1	A	561	ASN	5.4
1	C	565	LYS	4.8
1	A	562	SER	4.5
1	A	558	ASN	4.4
1	C	545	ASP	4.2
1	A	557	ILE	4.1
1	A	564	LEU	3.9
1	C	519	PHE	3.8
1	C	517	TYR	3.8
1	C	610	LYS	3.4
1	C	594	THR	3.3
1	C	611	ASN	3.2
1	C	637	HIS	3.2
1	C	606	ASN	3.1
1	A	532	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	639	ILE	3.0
2	D	106	GLU	3.0
2	B	105	PRO	3.0
1	A	499	GLY	2.9
2	D	108	SER	2.9
2	D	105	PRO	2.8
1	C	528	ASN	2.7
1	C	515	GLU	2.6
1	C	674	GLU	2.6
1	C	636	LYS	2.5
1	C	596	CYS	2.5
1	C	605	CYS	2.5
1	C	546	ASN	2.5
1	A	546	ASN	2.4
2	D	107	GLY	2.3
1	A	638	ASP	2.2
2	D	103	LEU	2.2
1	A	566	ASN	2.2
1	A	500	ASP	2.1
1	C	706	ILE	2.1
1	A	605	CYS	2.1
1	C	608	CYS	2.1
1	C	591	THR	2.0
1	A	531	ASN	2.0
2	B	106	GLU	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)

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
5	MAN	B	207	11/12	0.63	0.35	5.72	77,82,93,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	D	201	14/15	0.81	0.30	4.21	91,97,104,107	0
4	NAG	D	205	14/15	0.85	0.22	1.37	94,101,104,106	0
7	NAG	D	206	14/15	0.92	0.17	-0.58	53,64,72,82	0
5	NAG	B	203	14/15	0.97	0.14	-0.87	35,42,46,49	0
5	NAG	B	204	14/15	0.96	0.12	-1.15	42,45,52,63	0
4	NAG	D	202	14/15	0.81	0.30	-	101,103,113,114	0
7	MAN	D	203	11/12	0.66	0.25	-	119,122,132,135	0
7	NAG	D	207	14/15	0.92	0.14	-	87,95,105,113	0
4	NAG	D	204	14/15	0.88	0.16	-	106,112,118,118	0
4	NAG	B	202	14/15	0.73	0.32	-	141,148,153,156	0
4	NAG	B	201	14/15	0.50	0.42	-	148,160,169,172	0

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
3	PTY	D	200	50/50	0.87	0.29	4.42	36,61,118,118	0
3	PTY	B	200	50/50	0.92	0.22	2.11	29,41,76,82	0
6	NAG	B	205	14/15	0.91	0.14	-1.20	39,46,52,57	0
6	NAG	B	206	14/15	0.71	0.23	-	88,97,102,102	0
6	NAG	D	208	14/15	0.71	0.23	-	103,109,115,120	0

6.5 Other polymers

There are no such residues in this entry.