Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:40 AM GMT

PDB ID	:	2DW1
Title	:	Crystal structure of VAP2 from Crotalus atrox venom (Form 2-2 crystal)
Authors	:	Takeda, S.; Igarashi, T.; Araki, S.
Deposited on	:	2006-08-02
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references (i)) 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 2.50 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	Percentile Ranks	Value
Rfree		0.286
Clashscore		13
Ramachandran outliers		0.4%
Sidechain outliers		2.9%
RSRZ outliers		1.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
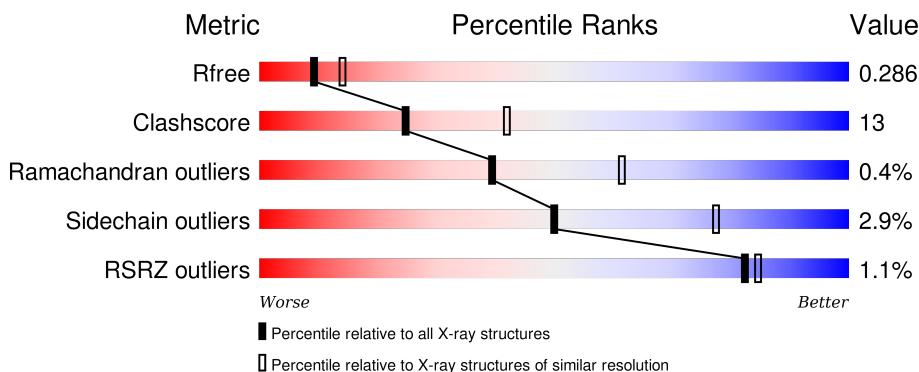
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	419	78% 20% ··
1	B	419	70% 27% ··

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6801 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 Catrocollastatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total 3219	C 1990	N 545	O 637	S 47	0	0	0
1	B	415	Total 3219	C 1990	N 545	O 637	S 47	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	VAL	PHE	SEE REMARK 999	UNP Q90282
B	203	VAL	PHE	SEE REMARK 999	UNP Q90282

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	4	Total 49	C 28	N 2	O 19	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Zn 1	0	0
4	A	1	Total 1	Zn 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total 3	Ca 3	0	0
5	A	3	Total 3	Ca 3	0	0

- Molecule 6 is 3-(N-HYDROXYCARBOXAMIDO)-2-ISOBUTYLPROPANOYL-TRP-MET HYLAMIDE (three-letter code: GM6) (formula: $C_{20}H_{28}N_4O_4$).
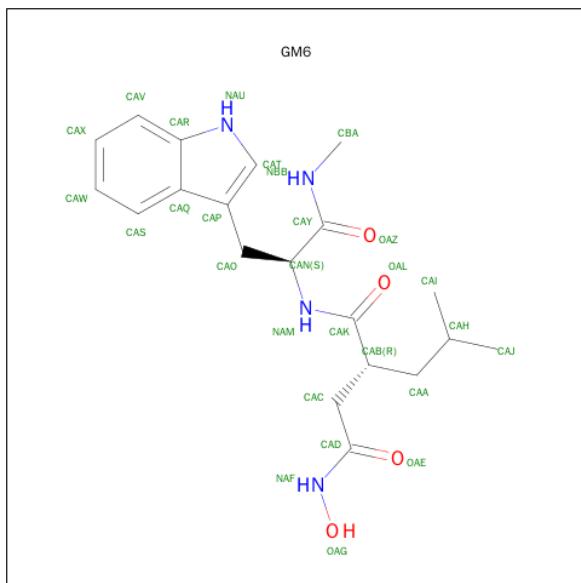
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total 28	C 20	N 4	O 4	0	0
6	A	1	Total 28	C 20	N 4	O 4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	121	Total 121	O 121	0	0
7	B	90	Total 90	O 90	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: Catrocollastatin
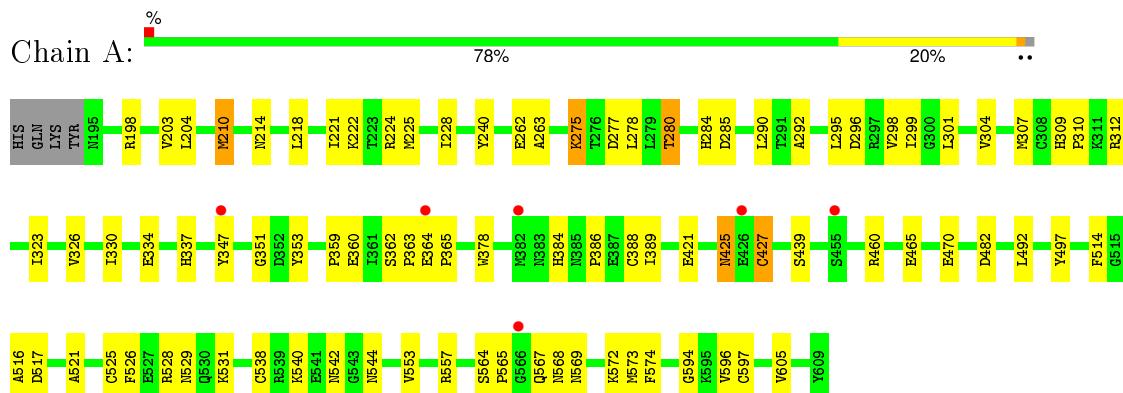
- Molecule 1: Catrocollastatin
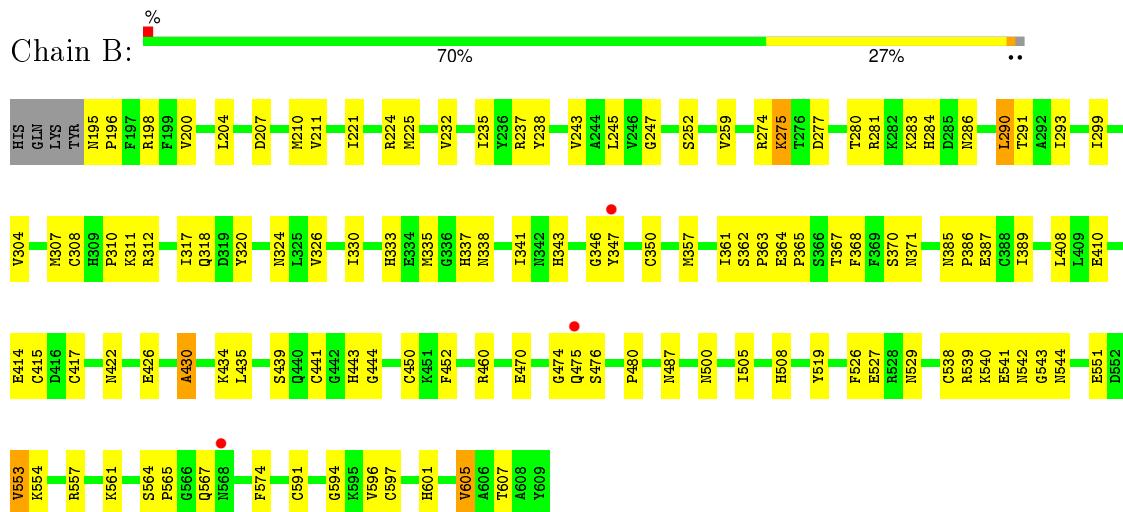
4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.67Å 118.18Å 138.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.54 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 98.1 (48.54-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.286 0.231 , 0.286	Depositor DCC
R_{free} test set	1650 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.6	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 33228 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6801	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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 68.78 % 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 4.1288e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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.

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5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CA, FUC, GM6, 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	0.33	0/3291	0.60	0/4453
1	B	0.32	0/3291	0.60	0/4453
All	All	0.33	0/6582	0.60	0/8906

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3219	0	2986	64	0
1	B	3219	0	2986	95	0
2	A	39	0	34	3	0
3	B	49	0	43	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	28	0	28	1	0
6	B	28	0	27	2	0
7	A	121	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	90	0	0	5	0
All	All	6801	0	6104	162	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 13.

All (162) 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:B:529:ASN:HD21	1:B:557:ARG:HB3	1.39	0.87
3:B:801:NAG:H61	3:B:809:FUC:O2	1.80	0.81
1:B:195:ASN:HB2	1:B:196:PRO:HD2	1.63	0.80
1:A:309:HIS:HD2	1:A:312:ARG:H	1.29	0.80
1:B:307:MET:HE3	1:B:308:CYS:H	1.46	0.79
2:A:801:NAG:H62	2:A:802:NAG:O5	1.83	0.79
1:A:526:PHE:HB3	1:A:553:VAL:HG13	1.65	0.79
1:A:529:ASN:HD21	1:A:557:ARG:HB3	1.47	0.78
1:B:542:ASN:HB2	1:B:544:ASN:ND2	2.01	0.75
1:A:198:ARG:HD2	1:A:389:ILE:HG13	1.69	0.73
1:A:204:LEU:HD13	1:A:225:MET:HE3	1.71	0.73
1:B:259:VAL:HG12	1:B:293:ILE:HD13	1.71	0.72
1:A:567:GLN:HG3	1:A:568:ASN:H	1.55	0.72
1:A:204:LEU:HD13	1:A:225:MET:CE	2.20	0.71
1:A:364:GLU:HG2	1:A:364:GLU:O	1.90	0.71
1:B:363:PRO:C	1:B:365:PRO:HD3	2.13	0.69
1:A:594:GLY:O	1:A:605:VAL:HG23	1.93	0.69
1:B:439:SER:CB	1:B:450:CYS:HB3	2.24	0.68
1:B:299:ILE:HG12	6:B:1:GM6:OAL	1.92	0.67
1:B:224:ARG:HE	1:B:324:ASN:ND2	1.93	0.67
1:B:526:PHE:O	1:B:553:VAL:HG22	1.95	0.66
1:A:309:HIS:CD2	1:A:312:ARG:H	2.11	0.65
1:B:596:VAL:HG21	7:B:810:HOH:O	1.98	0.64
1:B:237:ARG:NH2	1:B:422:ASN:HB3	2.14	0.62
1:B:259:VAL:HG12	1:B:293:ILE:CD1	2.29	0.61
1:B:415:CYS:SG	1:B:435:LEU:HD23	2.39	0.61
1:B:307:MET:HE3	1:B:308:CYS:N	2.14	0.61
1:A:384:HIS:O	1:A:386:PRO:HD3	2.03	0.59
1:B:362:SER:O	1:B:365:PRO:HG3	2.03	0.59
1:B:439:SER:HB3	1:B:450:CYS:HB3	1.84	0.59
1:A:521:ALA:HB1	1:A:525:CYS:SG	2.43	0.58
1:B:198:ARG:HD2	1:B:389:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ILE:HG12	6:A:2:GM6:OAL	2.04	0.58
1:B:539:ARG:HH11	1:B:539:ARG:HG2	1.68	0.58
1:B:225:MET:CE	1:B:290:LEU:HD22	2.35	0.57
1:A:203:VAL:HG11	1:A:278:LEU:HD21	1.85	0.57
1:A:363:PRO:C	1:A:365:PRO:HD3	2.25	0.57
1:B:200:VAL:HG11	1:B:335:MET:CE	2.34	0.57
1:B:470:GLU:HB3	1:B:480:PRO:HG2	1.87	0.57
1:B:204:LEU:HD13	1:B:225:MET:CE	2.35	0.56
1:B:551:GLU:HG2	7:B:835:HOH:O	2.05	0.56
1:B:235:ILE:HG12	1:B:367:THR:HB	1.88	0.56
1:A:514:PHE:CD2	1:A:572:LYS:HD3	2.41	0.56
1:B:487:ASN:HD21	1:B:500:ASN:H	1.52	0.55
1:B:326:VAL:O	1:B:330:ILE:HG12	2.06	0.55
1:B:368:PHE:HA	7:B:891:HOH:O	2.08	0.54
1:B:540:LYS:HA	1:B:544:ASN:O	2.08	0.54
1:A:594:GLY:C	1:A:605:VAL:HG23	2.28	0.54
1:B:277:ASP:O	1:B:280:THR:HG22	2.07	0.54
1:A:362:SER:O	1:A:365:PRO:HG3	2.08	0.53
1:B:542:ASN:HB2	1:B:544:ASN:HD21	1.72	0.53
1:A:526:PHE:CB	1:A:553:VAL:HG13	2.37	0.53
1:B:281:ARG:HH11	1:B:281:ARG:HG3	1.74	0.53
1:B:386:PRO:O	1:B:389:ILE:HG12	2.09	0.53
1:A:224:ARG:O	1:A:228:ILE:HG13	2.09	0.52
1:B:204:LEU:HD13	1:B:225:MET:HE2	1.90	0.52
1:A:285:ASP:HB3	1:A:388:CYS:SG	2.50	0.52
1:A:421:GLU:N	1:A:421:GLU:OE2	2.40	0.52
1:B:487:ASN:ND2	1:B:500:ASN:H	2.08	0.52
1:B:211:VAL:HG21	1:B:252:SER:HA	1.93	0.51
1:B:317:ILE:HG23	1:B:330:ILE:CG2	2.41	0.51
1:A:347:TYR:O	2:A:801:NAG:H3	2.10	0.51
1:A:351:GLY:C	1:A:353:TYR:H	2.13	0.51
1:B:210:MET:CE	1:B:290:LEU:HD23	2.41	0.51
1:B:304:VAL:HA	1:B:337:HIS:O	2.11	0.50
1:B:408:LEU:O	1:B:410:GLU:HG3	2.11	0.50
1:A:278:LEU:HG	1:A:284:HIS:CE1	2.46	0.50
1:A:263:ALA:HB1	1:A:301:LEU:HD22	1.94	0.50
1:A:204:LEU:HD13	1:A:225:MET:HE2	1.93	0.50
1:B:317:ILE:HG23	1:B:330:ILE:HG21	1.94	0.49
1:B:291:THR:OG1	1:B:293:ILE:HG12	2.12	0.49
1:A:425:ASN:C	1:A:425:ASN:HD22	2.17	0.48
1:B:347:TYR:CD2	3:B:802:NAG:H4	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:THR:HG22	1:B:607:THR:O	2.12	0.48
1:B:274:ARG:HH21	1:B:284:HIS:CD2	2.32	0.48
1:B:475:GLN:HA	1:B:475:GLN:HE21	1.79	0.48
1:A:225:MET:HE1	1:A:290:LEU:HD13	1.95	0.48
1:B:439:SER:HB2	1:B:450:CYS:HB3	1.93	0.48
1:A:240:TYR:HB2	1:A:378:TRP:HZ2	1.77	0.48
1:B:210:MET:HE2	1:B:290:LEU:HD23	1.95	0.48
1:B:307:MET:O	1:B:308:CYS:HB2	2.14	0.47
1:A:427:CYS:HB3	1:A:439:SER:HB2	1.95	0.47
1:A:210:MET:HG2	1:A:292:ALA:HB2	1.96	0.47
1:B:221:ILE:O	1:B:225:MET:HG2	2.15	0.47
1:B:460:ARG:NH1	1:B:470:GLU:HG2	2.30	0.47
1:A:564:SER:HB2	1:A:565:PRO:HD2	1.95	0.47
1:A:514:PHE:CG	1:A:572:LYS:HD3	2.50	0.47
1:B:245:LEU:HD11	1:B:247:GLY:O	2.14	0.47
1:B:286:ASN:HB2	1:B:307:MET:HE1	1.97	0.47
1:A:567:GLN:HG3	1:A:568:ASN:N	2.24	0.47
1:B:225:MET:HE1	1:B:290:LEU:HD22	1.96	0.46
1:B:200:VAL:HG11	1:B:335:MET:HE1	1.97	0.46
1:B:341:ILE:HG21	1:B:357:MET:HG3	1.97	0.46
1:A:596:VAL:CG1	1:A:597:CYS:N	2.78	0.46
1:A:334:GLU:HA	1:A:334:GLU:OE1	2.15	0.46
1:A:240:TYR:HB2	1:A:378:TRP:CZ2	2.51	0.46
1:A:516:ALA:HB1	7:A:921:HOH:O	2.15	0.46
1:B:350:CYS:HB3	1:B:370:SER:HA	1.96	0.46
1:B:237:ARG:HA	7:B:874:HOH:O	2.14	0.46
1:A:364:GLU:N	1:A:365:PRO:HD3	2.30	0.46
1:B:422:ASN:N	1:B:422:ASN:HD22	2.12	0.46
1:A:574:PHE:CD1	1:A:574:PHE:C	2.90	0.46
1:A:277:ASP:O	1:A:280:THR:HB	2.16	0.45
1:B:460:ARG:HH12	1:B:470:GLU:HG2	1.80	0.45
1:B:361:ILE:HG12	1:B:362:SER:H	1.82	0.45
1:B:364:GLU:N	1:B:365:PRO:HD3	2.32	0.45
1:B:541:GLU:C	1:B:543:GLY:H	2.20	0.45
1:A:540:LYS:HA	1:A:544:ASN:O	2.15	0.45
1:B:475:GLN:HA	1:B:475:GLN:NE2	2.31	0.45
1:B:574:PHE:CD2	1:B:574:PHE:C	2.89	0.45
1:B:554:LYS:HB2	7:B:887:HOH:O	2.18	0.44
1:B:343:HIS:HA	1:B:357:MET:O	2.17	0.44
1:A:304:VAL:HA	1:A:337:HIS:O	2.18	0.44
1:A:516:ALA:O	1:A:517:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ARG:HA	1:A:531:LYS:HE3	1.99	0.44
1:A:567:GLN:CG	1:A:568:ASN:H	2.28	0.43
1:B:607:THR:O	1:B:607:THR:CG2	2.65	0.43
1:B:505:ILE:HD11	1:B:508:HIS:CD2	2.52	0.43
1:B:281:ARG:NH1	1:B:281:ARG:HG3	2.34	0.43
1:B:591:CYS:HB3	1:B:597:CYS:SG	2.59	0.43
1:B:597:CYS:HA	1:B:601:HIS:O	2.18	0.43
1:B:363:PRO:O	1:B:365:PRO:HD3	2.18	0.43
1:A:295:LEU:HB2	1:A:298:VAL:O	2.19	0.43
1:B:474:GLY:C	1:B:476:SER:H	2.22	0.43
1:B:539:ARG:HG2	1:B:539:ARG:NH1	2.33	0.43
1:B:275:LYS:CG	1:B:310:PRO:HB2	2.48	0.43
1:B:594:GLY:O	1:B:605:VAL:HG23	2.19	0.43
1:B:564:SER:HB2	1:B:565:PRO:HD2	2.01	0.43
1:B:195:ASN:HB2	1:B:196:PRO:CD	2.43	0.42
1:A:460:ARG:NH1	1:A:482:ASP:HA	2.34	0.42
1:B:311:LYS:HG3	1:B:312:ARG:N	2.34	0.42
1:B:414:GLU:OE2	1:B:434:LYS:HD2	2.19	0.42
1:B:318:GLN:C	1:B:320:TYR:H	2.22	0.42
1:B:207:ASP:OD1	1:B:291:THR:HA	2.20	0.42
1:B:443:HIS:ND1	1:B:444:GLY:N	2.67	0.42
1:B:527:GLU:HA	1:B:553:VAL:HG21	2.01	0.42
1:B:232:VAL:HG12	1:B:243:VAL:HG21	2.02	0.42
1:A:218:LEU:O	1:A:222:LYS:HG3	2.18	0.42
1:A:326:VAL:O	1:A:330:ILE:HG12	2.20	0.42
1:B:417:CYS:SG	1:B:430:ALA:HB2	2.59	0.42
1:A:275:LYS:HG2	1:A:310:PRO:HB2	2.02	0.42
1:B:441:CYS:HB3	1:B:452:PHE:HE2	1.84	0.42
1:B:333:HIS:CE1	6:B:1:GM6:HAI2	2.55	0.41
1:B:475:GLN:O	1:B:475:GLN:HG3	2.20	0.41
1:A:497:TYR:CZ	1:A:605:VAL:HG21	2.55	0.41
1:B:326:VAL:HG13	1:B:361:ILE:CD1	2.50	0.41
1:A:573:MET:C	1:A:573:MET:SD	2.99	0.41
1:A:347:TYR:CE2	2:A:802:NAG:H3	2.55	0.41
1:A:465:GLU:CD	1:A:492:LEU:H	2.23	0.41
1:B:361:ILE:HG12	1:B:362:SER:N	2.36	0.41
1:B:237:ARG:HG2	1:B:237:ARG:HH11	1.86	0.41
1:B:519:TYR:O	1:B:561:LYS:N	2.37	0.41
1:A:359:PRO:HG2	1:A:360:GLU:OE2	2.20	0.41
1:A:542:ASN:ND2	1:A:542:ASN:N	2.69	0.41
1:A:542:ASN:HD22	1:A:542:ASN:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:MET:O	1:B:338:ASN:HB2	2.21	0.40
1:A:323:ILE:HB	1:A:326:VAL:HG23	2.03	0.40
1:A:386:PRO:O	1:A:389:ILE:HG12	2.22	0.40
3:B:801:NAG:C6	3:B:809:FUC:O2	2.59	0.40
1:A:517:ASP:CB	1:A:564:SER:HA	2.51	0.40
1:A:460:ARG:HD2	1:A:470:GLU:OE2	2.20	0.40
1:A:214:ASN:HB2	1:A:221:ILE:HD11	2.03	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	413/419 (99%)	390 (94%)	22 (5%)	1 (0%)	52	75
1	B	413/419 (99%)	374 (91%)	37 (9%)	2 (0%)	34	55
All	All	826/838 (99%)	764 (92%)	59 (7%)	3 (0%)	39	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	ASP
1	B	346	GLY
1	B	430	ALA

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	361/365 (99%)	352 (98%)	9 (2%)	55	82
1	B	361/365 (99%)	349 (97%)	12 (3%)	45	73
All	All	722/730 (99%)	701 (97%)	21 (3%)	50	77

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	MET
1	A	262	GLU
1	A	275	LYS
1	A	280	THR
1	A	307	MET
1	A	425	ASN
1	A	427	CYS
1	A	538	CYS
1	A	569	ASN
1	B	238	TYR
1	B	275	LYS
1	B	283	LYS
1	B	290	LEU
1	B	371	ASN
1	B	385	ASN
1	B	387	GLU
1	B	426	GLU
1	B	538	CYS
1	B	553	VAL
1	B	567	GLN
1	B	605	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	230	ASN
1	A	288	GLN
1	A	309	HIS
1	A	385	ASN
1	A	425	ASN
1	A	440	GLN

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Mol	Chain	Res	Type
1	A	475	GLN
1	A	500	ASN
1	A	529	ASN
1	A	542	ASN
1	A	569	ASN
1	A	599	ASN
1	B	288	GLN
1	B	324	ASN
1	B	385	ASN
1	B	475	GLN
1	B	487	ASN
1	B	500	ASN
1	B	529	ASN
1	B	542	ASN
1	B	544	ASN
1	B	563	ASN
1	B	568	ASN
1	B	599	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

7 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	#$|Z| > 2$
2	NAG	A	801	1,2	14,14,15	0.80	0	15,19,21	1.54	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	802	2	14,14,15	1.11	1 (7%)	15,19,21	1.40	4 (26%)
2	MAN	A	803	2	11,11,12	0.77	0	14,15,17	0.51	0
3	NAG	B	801	1,3	14,14,15	0.72	0	15,19,21	1.16	2 (13%)
3	NAG	B	802	3	14,14,15	0.57	0	15,19,21	0.69	0
3	BMA	B	803	3	11,11,12	0.65	0	14,15,17	0.45	0
3	FUC	B	809	3	10,10,11	0.67	0	14,14,16	0.85	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
2	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	MAN	A	803	2	-	0/2/19/22	0/1/1/1
3	NAG	B	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	802	3	-	2/6/23/26	0/1/1/1
3	BMA	B	803	3	-	0/2/19/22	0/1/1/1
3	FUC	B	809	3	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	NAG	C1-C2	3.36	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	NAG	C4-C3-C2	-3.77	105.37	111.23
2	A	802	NAG	C2-N2-C7	-2.46	119.88	123.04
2	A	801	NAG	C2-N2-C7	-2.39	119.96	123.04
3	B	801	NAG	C2-N2-C7	-2.38	119.99	123.04
2	A	802	NAG	C3-C4-C5	-2.33	106.14	110.20
2	A	802	NAG	C4-C3-C2	-2.30	107.66	111.23
2	A	801	NAG	C1-O5-C5	2.33	115.20	112.25
2	A	802	NAG	C1-O5-C5	2.43	115.33	112.25
2	A	801	NAG	O4-C4-C5	2.55	116.00	109.24
3	B	801	NAG	C3-C4-C5	2.71	114.92	110.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	NAG	C8-C7-N2-C2
3	B	802	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	2	0
2	A	802	NAG	2	0
3	B	801	NAG	2	0
3	B	802	NAG	1	0
3	B	809	FUC	2	0

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 8 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	GM6	A	2	4	28,29,29	1.25	3 (10%)	25,39,39	0.82	0
6	GM6	B	1	4	28,29,29	1.25	3 (10%)	25,39,39	0.87	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
6	GM6	A	2	4	-	0/27/28/28	0/2/2/2
6	GM6	B	1	4	-	0/27/28/28	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2	GM6	OAG-NAF	-2.12	1.36	1.39
6	B	1	GM6	CAT-CAP	-2.08	1.34	1.38
6	A	2	GM6	CAW-CAS	2.40	1.42	1.36
6	B	1	GM6	CAW-CAS	2.44	1.42	1.36
6	B	1	GM6	CAX-CAV	2.56	1.42	1.36
6	A	2	GM6	CAX-CAV	2.76	1.43	1.36

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2	GM6	1	0
6	B	1	GM6	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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(Å²)	Q<0.9
1	A	415/419 (99%)	-0.30	6 (1%)	78	80	13, 33, 59, 70	0
1	B	415/419 (99%)	-0.15	3 (0%)	89	90	18, 39, 68, 83	0
All	All	830/838 (99%)	-0.23	9 (1%)	82	84	13, 36, 65, 83	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	347	TYR	5.3
1	B	475	GLN	2.9
1	A	347	TYR	2.8
1	A	364	GLU	2.2
1	A	426	GLU	2.1
1	A	566	GLY	2.1
1	B	568	ASN	2.1
1	A	382	MET	2.0
1	A	455	SER	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, 95th 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	NAG	B	801	14/15	0.89	0.24	0.23	59,63,66,66	0
2	NAG	A	801	14/15	0.87	0.16	0.03	58,61,67,77	0
3	BMA	B	803	11/12	0.64	0.20	-	77,79,80,81	0
2	MAN	A	803	11/12	0.48	0.34	-	103,104,106,106	0
2	NAG	A	802	14/15	0.75	0.34	-	85,90,93,100	0
3	NAG	B	802	14/15	0.86	0.25	-	67,71,73,76	0
3	FUC	B	809	10/11	0.88	0.34	-	61,62,63,63	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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
6	GM6	B	1	28/28	0.94	0.17	1.54	31,36,45,55	0
6	GM6	A	2	28/28	0.96	0.15	0.26	16,34,46,49	0
5	CA	A	702	1/1	0.98	0.10	-0.57	38,38,38,38	0
5	CA	A	701	1/1	0.99	0.10	-0.83	35,35,35,35	0
5	CA	B	713	1/1	0.96	0.10	-0.98	42,42,42,42	0
5	CA	A	703	1/1	0.96	0.07	-1.60	40,40,40,40	0
5	CA	B	712	1/1	0.90	0.05	-3.76	52,52,52,52	0
5	CA	B	711	1/1	0.94	0.06	-4.55	43,43,43,43	0
4	ZN	A	700	1/1	0.99	0.12	-	22,22,22,22	0
4	ZN	B	700	1/1	0.99	0.08	-	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.