Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:37 AM GMT

PDB ID	:	3FCS
Title	:	Structure of complete ectodomain of integrin aIIBb3
Authors	:	Zhu, J.; Luo, B.-H.; Xiao, T.; Zhang, C.; Nishida, N.; Springer, T.A.
Deposited on	:	2008-11-22
Resolution	:	2.55 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:

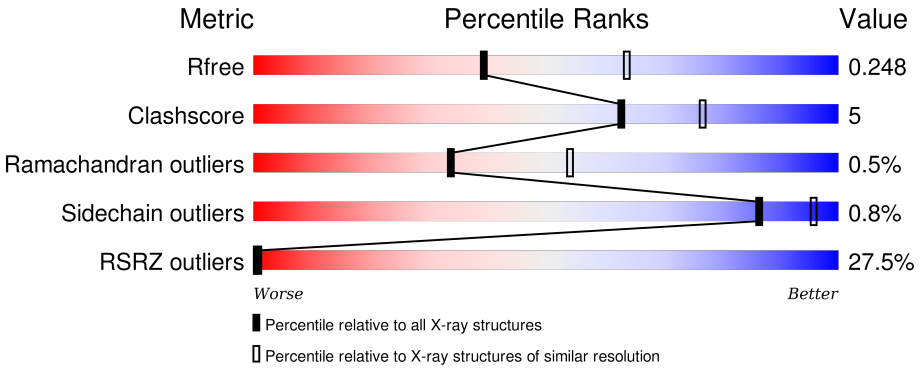
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	959	20% 83% 12% 5%
1	C	959	35% 82% 11% • 6%
2	B	690	27% 87% 12% •
2	D	690	21% 78% 9% 13%

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
10	MAN	B	3561	X	-	-	-
4	NAG	A	3570	-	-	-	X
4	NAG	C	3570	X	-	-	X
4	NAG	D	3099	X	-	-	-
8	MAN	B	3322	X	-	-	-
9	MAN	B	3373	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24961 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 Integrin, alpha 2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	914	Total	C	N	O	S	0	7	3
			7033	4446	1231	1326	30			
1	C	904	Total	C	N	O	S	0	8	2
			6953	4387	1224	1312	30			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	959	CYS	-	EXPRESSION TAG	UNP Q17R67
C	959	CYS	-	EXPRESSION TAG	UNP Q17R67

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	680	Total	C	N	O	S	0	1	0
			5220	3207	890	1052	71			
2	D	603	Total	C	N	O	S	0	3	0
			4615	2839	790	923	63			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	688	CYS	PRO	ENGINEERED	UNP P05106
D	688	CYS	PRO	ENGINEERED	UNP P05106

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	5	Total	Ca	0	0
			5	5		

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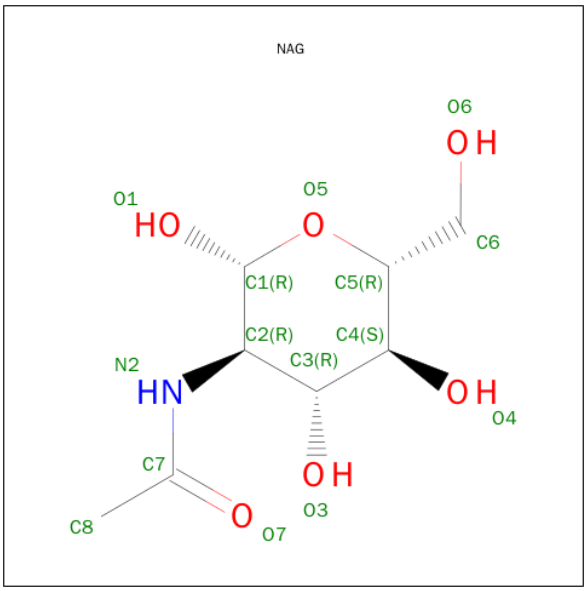
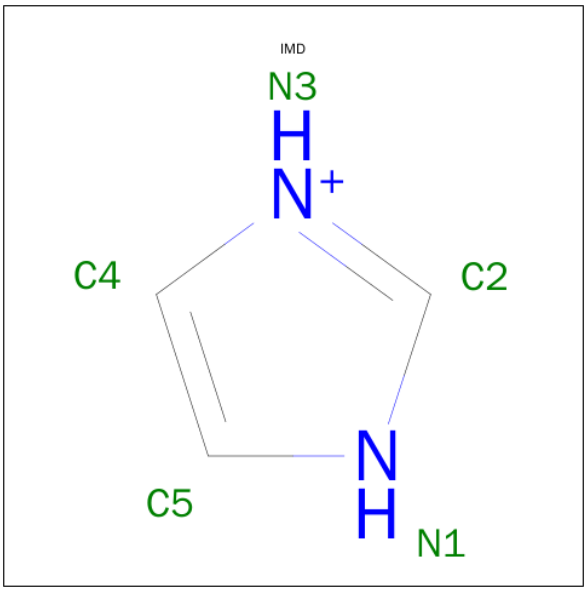
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Ca 2 2	0	0
3	C	5	Total Ca 5 5	0	0

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0
5	C	1	Total C N 5 3 2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

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

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	4	Total C N O 50 28 2 20	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 10 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	5	Total C N O 61 34 2 25	0	0

- Molecule 11 is water.

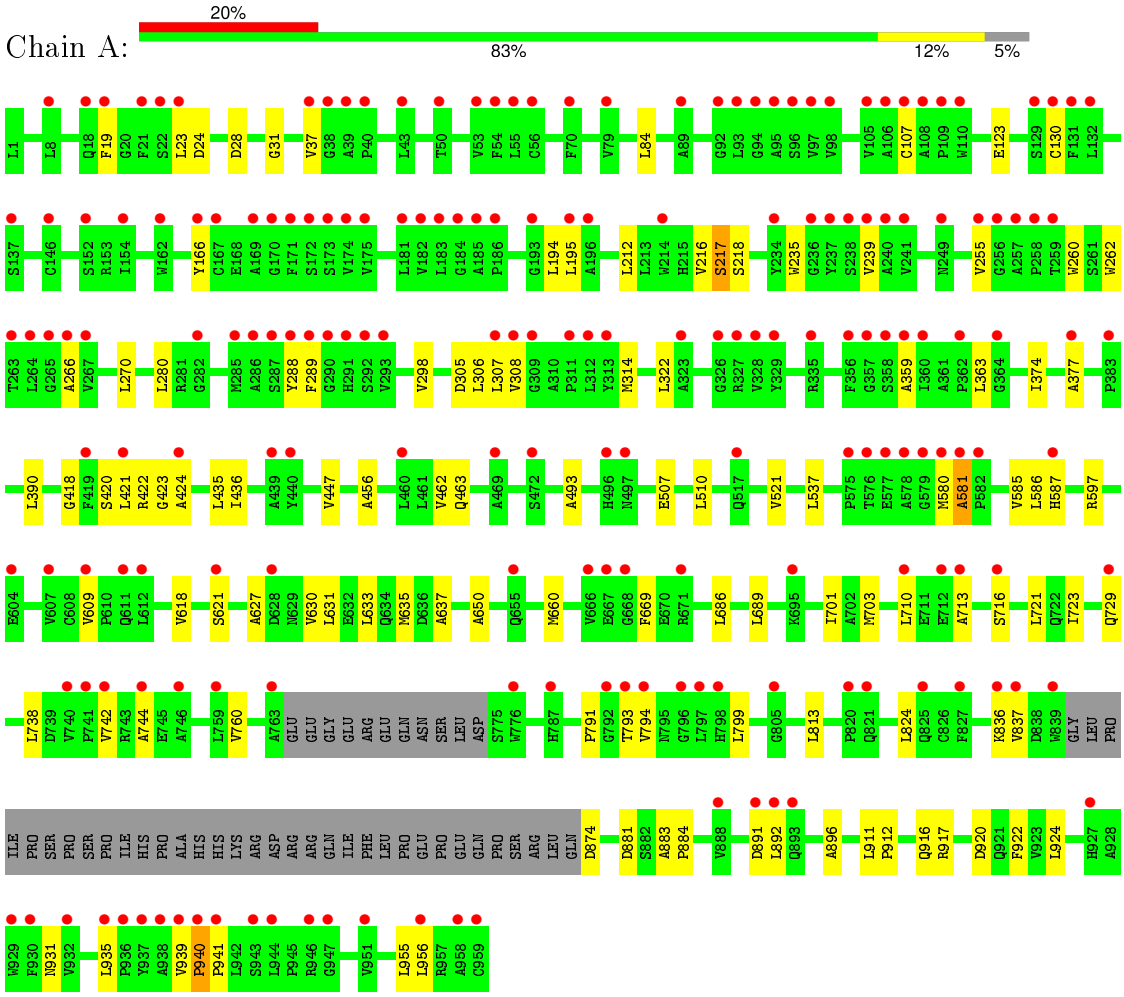
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	232	Total O 232 232	0	0
11	B	73	Total O 73 73	0	0
11	C	270	Total O 270 270	0	0
11	D	103	Total O 103 103	0	0

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.

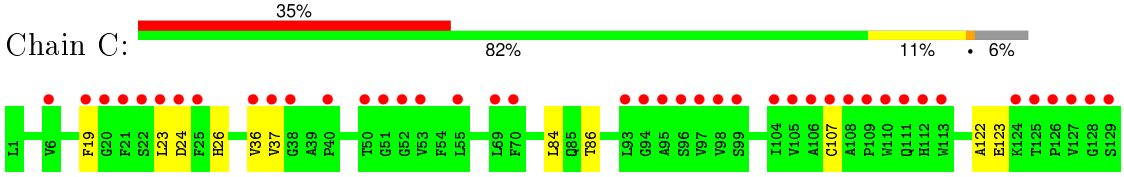
- Molecule 1: Integrin, alpha 2b

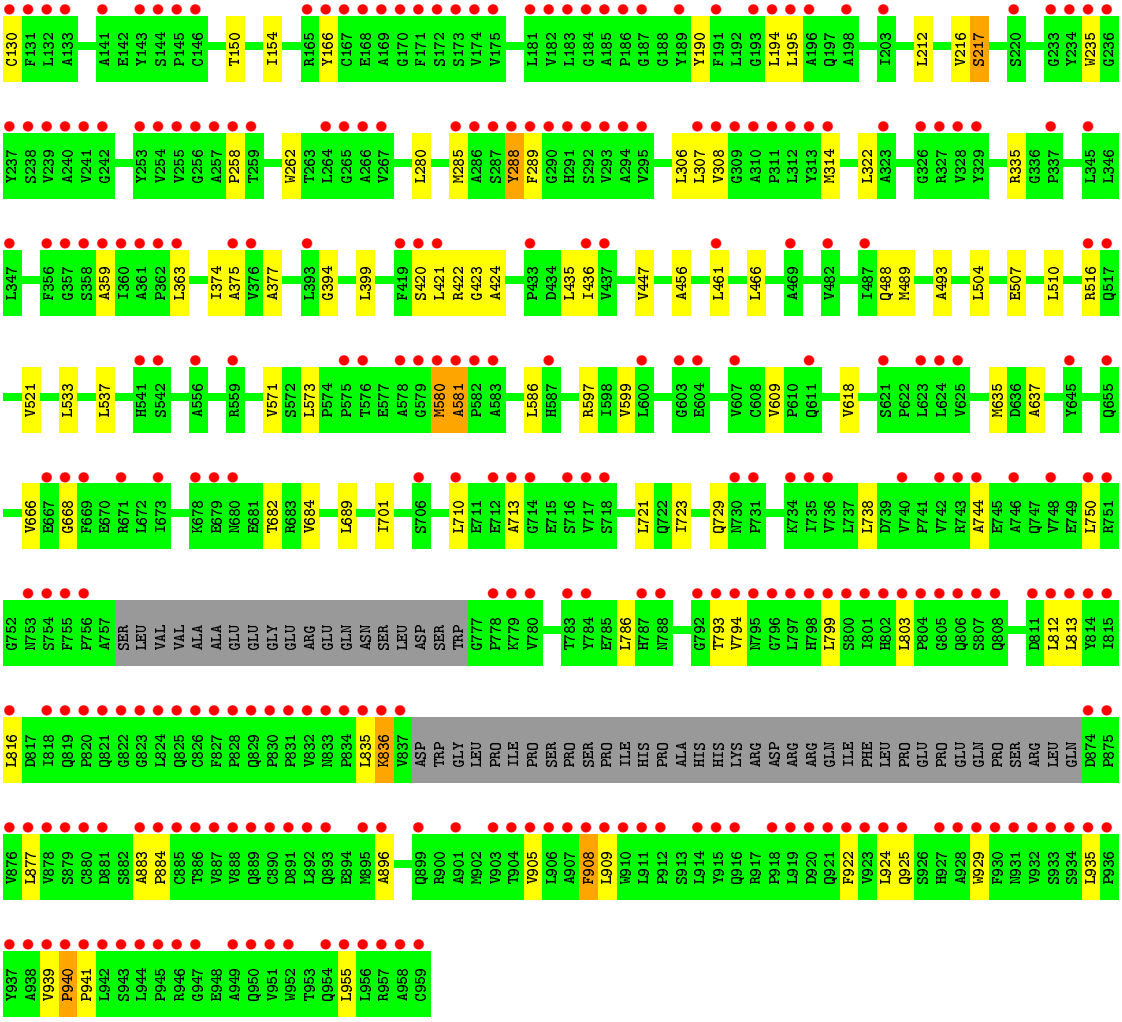
Chain A:



- Molecule 1: Integrin, alpha 2b

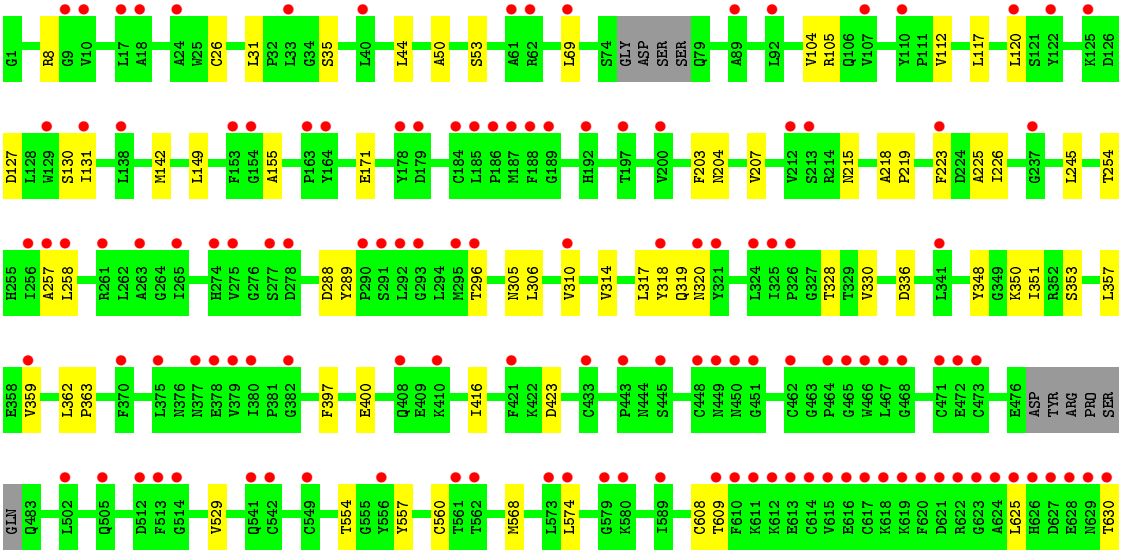
Chain C:

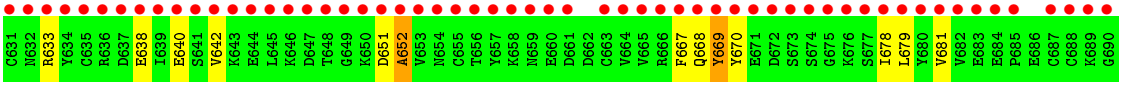




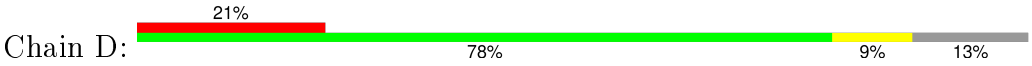
• Molecule 2: Integrin beta-3

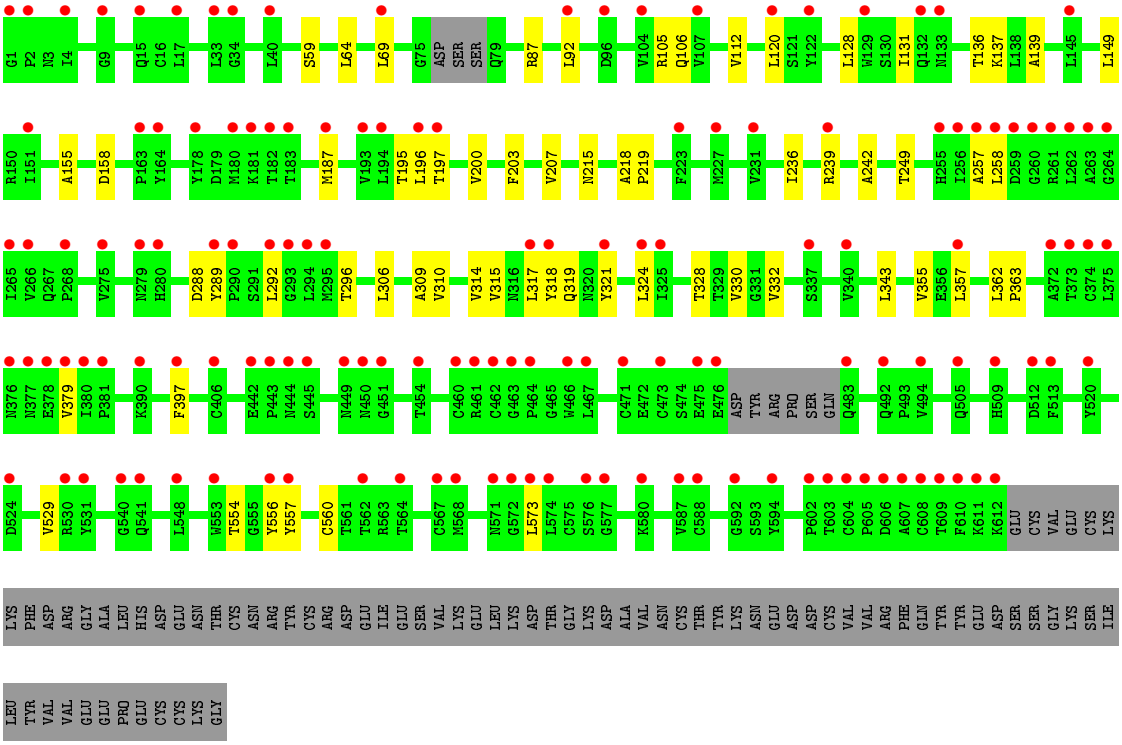
Chain B:





• Molecule 2: Integrin beta-3





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	81.30Å 81.30Å 654.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.31 – 2.55 45.30 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.31-2.55) 98.6 (45.30-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.233 , 0.268 0.226 , 0.248	Depositor DCC
R_{free} test set	1785 reflections (1.34%)	DCC
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 61.8	EDS
Estimated twinning fraction	0.155 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 135027 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	24961	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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: MG, MAN, CA, NAG, IMD

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	0.24	0/7209	0.43	0/9823
1	C	0.25	0/7124	0.43	0/9705
2	B	0.23	0/5314	0.40	0/7182
2	D	0.24	0/4704	0.41	0/6362
All	All	0.24	0/24351	0.42	0/33072

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	B	1	0
9	B	1	0
10	B	1	0
All	All	3	0

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	3322	MAN	C1
9	B	3373	MAN	C1
10	B	3561	MAN	C1

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	7033	0	6875	80	0
1	C	6953	0	6797	79	0
2	B	5220	0	4964	53	0
2	D	4615	0	4405	42	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
3	C	5	0	0	0	0
3	D	2	0	0	0	0
4	A	28	0	26	1	0
4	C	28	0	26	2	0
4	D	14	0	13	0	0
5	A	5	0	5	0	0
5	C	25	0	25	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	56	0	50	1	0
7	C	28	0	25	0	0
7	D	112	0	100	0	0
8	B	50	0	43	1	0
9	B	39	0	34	2	0
10	B	61	0	52	4	0
11	A	232	0	0	3	0
11	B	73	0	0	0	0
11	C	270	0	0	1	0
11	D	103	0	0	3	0
All	All	24961	0	23440	251	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 (251) 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:C:507:GLU:HB2	4:C:3570:NAG:H82	1.38	1.02
1:C:816:LEU:HD11	1:C:908:PHE:CZ	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:573:LEU:O	11:D:693:HOH:O	2.05	0.74
2:B:320:ASN:HD22	8:B:3320:NAG:H83	1.51	0.73
1:C:314:MET:CE	1:C:322:LEU:HD22	2.20	0.72
1:C:516:ARG:O	11:C:1134:HOH:O	2.08	0.70
1:C:507:GLU:CB	4:C:3570:NAG:H82	2.21	0.68
1:A:195:LEU:HD11	1:A:255:VAL:CG2	2.24	0.67
1:A:618:VAL:HG23	1:A:738:LEU:HD13	1.77	0.67
1:C:580:MET:O	1:C:581:ALA:HB3	1.96	0.66
2:D:310:VAL:HG11	2:D:318:TYR:CD2	2.30	0.66
1:A:580:MET:O	1:A:581:ALA:HB3	1.95	0.65
2:D:319[A]:GLN:HA	2:D:330:VAL:HG21	1.79	0.64
1:A:216:VAL:O	1:A:218:SER:N	2.31	0.64
2:D:69:LEU:HD13	2:D:105:ARG:HB3	1.79	0.64
2:B:69:LEU:HD13	2:B:105:ARG:HB3	1.80	0.63
2:B:203:PHE:O	2:B:207:VAL:HG13	1.98	0.63
2:D:319[B]:GLN:HA	2:D:330:VAL:HG21	1.81	0.63
1:A:813:LEU:HD11	1:A:924:LEU:CD1	2.29	0.63
1:C:420:SER:C	1:C:421:LEU:HD12	2.20	0.62
2:D:195:THR:O	2:D:197:THR:HG23	2.01	0.61
1:C:813:LEU:HD13	1:C:924:LEU:HD13	1.84	0.60
1:A:813:LEU:HD11	1:A:924:LEU:HD13	1.82	0.60
1:A:420:SER:C	1:A:421:LEU:HD12	2.22	0.60
2:B:120:LEU:HD12	2:B:155:ALA:HB1	1.83	0.60
1:C:618:VAL:HG23	1:C:738:LEU:HD13	1.83	0.59
1:C:744:ALA:HB3	1:C:940:PRO:HB3	1.83	0.59
1:A:195:LEU:HD11	1:A:255:VAL:HG22	1.83	0.59
1:C:909:LEU:HD21	1:C:924:LEU:HD11	1.85	0.59
1:A:580:MET:O	1:A:581:ALA:CB	2.50	0.58
1:A:931:ASN:ND2	11:A:1035:HOH:O	2.35	0.58
2:D:288:ASP:OD1	2:D:289:TYR:N	2.36	0.58
1:A:883:ALA:HB1	1:A:884:PRO:HD2	1.86	0.58
1:C:150:THR:HG23	1:C:154:ILE:HD12	1.86	0.57
2:D:362:LEU:HD12	2:D:363:PRO:HD2	1.85	0.57
2:D:315:VAL:HG21	2:D:332:VAL:HG22	1.87	0.57
1:A:939:VAL:HG12	1:A:941:PRO:HD3	1.86	0.57
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.87	0.57
1:A:195:LEU:HD12	1:A:235:TRP:CH2	2.40	0.56
1:C:939:VAL:HG12	1:C:941:PRO:HD3	1.87	0.56
1:C:721:LEU:HD12	1:C:721:LEU:N	2.20	0.56
2:B:625:LEU:HD13	2:B:630:THR:O	2.06	0.56
2:D:529:VAL:CG1	2:D:557:TYR:CE1	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LEU:HD21	1:A:701:ILE:HD11	1.88	0.56
2:B:625:LEU:HD22	2:B:630:THR:HB	1.87	0.55
2:B:400:GLU:HB2	9:B:3371:NAG:H83	1.89	0.55
1:A:881:ASP:O	11:A:1183:HOH:O	2.18	0.55
1:C:883:ALA:HB1	1:C:884:PRO:HD2	1.89	0.55
1:A:195:LEU:HD11	1:A:255:VAL:HG21	1.88	0.54
2:D:529:VAL:HG11	2:D:557:TYR:CE1	2.42	0.54
1:C:710:LEU:HD23	1:C:713:ALA:HB2	1.90	0.54
1:A:744:ALA:HB3	1:A:940:PRO:HB3	1.90	0.54
2:B:319:GLN:HA	2:B:330:VAL:HG21	1.89	0.54
1:A:314:MET:CE	1:A:322:LEU:HD22	2.37	0.54
1:C:289:PHE:CZ	1:C:308:VAL:HG11	2.42	0.54
1:C:580:MET:O	1:C:581:ALA:CB	2.55	0.53
2:B:638:GLU:HB2	2:B:678:ILE:HG23	1.90	0.53
1:C:489:MET:CE	1:C:533:LEU:HD12	2.39	0.52
1:C:793:THR:HG22	1:C:896:ALA:HA	1.90	0.52
1:A:650:ALA:HA	1:A:686:LEU:HD23	1.92	0.52
1:A:760:VAL:HG12	1:A:956:LEU:HB2	1.90	0.52
2:B:305:ASN:HB3	2:B:351:ILE:HD13	1.91	0.52
1:A:618:VAL:CG1	1:A:631:LEU:HD22	2.39	0.52
2:B:630:THR:O	2:B:630:THR:HG22	2.10	0.52
1:C:423:GLY:O	1:C:424:ALA:HB3	2.09	0.52
1:A:510:LEU:HB3	1:A:521:VAL:HG23	1.92	0.52
1:C:510:LEU:HB3	1:C:521:VAL:HG23	1.91	0.52
2:B:131:ILE:CG2	2:B:131:ILE:O	2.58	0.51
2:B:669:TYR:HB3	2:B:679:LEU:HD23	1.92	0.51
2:B:667:PHE:CB	2:B:681:VAL:HG22	2.40	0.51
1:C:635:MET:SD	1:C:721:LEU:HD23	2.50	0.51
1:A:710:LEU:HD23	1:A:713:ALA:HB2	1.91	0.51
1:A:436:ILE:HG22	1:A:447:VAL:HG22	1.92	0.51
2:D:218:ALA:HB3	2:D:219:PRO:HD3	1.93	0.51
1:A:660:MET:CE	10:B:3560:NAG:H83	2.40	0.51
1:C:314:MET:HE3	1:C:322:LEU:HD22	1.90	0.51
2:B:117:LEU:CD2	2:B:225:ALA:HB1	2.41	0.51
2:D:343:LEU:C	2:D:343:LEU:HD23	2.31	0.50
1:A:689:LEU:CD2	1:A:701:ILE:HD11	2.42	0.50
1:C:436:ILE:HG22	1:C:447:VAL:HG22	1.92	0.50
1:C:609:VAL:HG22	1:C:729:GLN:HB2	1.94	0.50
2:D:257:ALA:O	2:D:258:LEU:HB2	2.12	0.50
1:A:456:ALA:HB2	1:A:586:LEU:HD11	1.94	0.50
1:A:423:GLY:O	1:A:424:ALA:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ALA:CB	1:A:421:LEU:HD13	2.42	0.50
2:B:310:VAL:HG11	2:B:318:TYR:CD2	2.47	0.50
1:A:721:LEU:HD12	1:A:721:LEU:N	2.27	0.50
1:A:322:LEU:HD12	2:B:296:THR:HG21	1.93	0.49
2:B:131:ILE:HG22	2:B:131:ILE:O	2.10	0.49
2:D:314:VAL:HG22	2:D:314:VAL:O	2.12	0.49
2:B:652:ALA:HB3	2:B:668:GLN:NE2	2.27	0.49
2:D:120:LEU:HD12	2:D:155:ALA:HB1	1.93	0.49
2:D:529:VAL:HG21	2:D:556:TYR:CE1	2.47	0.49
2:D:59:SER:HB3	2:D:92:LEU:HD23	1.94	0.49
2:B:26:CYS:SG	2:B:31:LEU:HD12	2.52	0.49
2:B:306:LEU:HB3	2:B:328:THR:HG22	1.94	0.49
2:D:249:THR:HG22	2:D:309:ALA:HB3	1.95	0.49
1:A:359:ALA:HB3	1:A:377:ALA:HB3	1.94	0.49
1:A:390:LEU:N	1:A:390:LEU:HD12	2.28	0.49
1:A:793:THR:HG23	1:A:896:ALA:HA	1.95	0.49
2:D:158:ASP:HB3	2:D:187:MET:CE	2.43	0.48
2:B:630:THR:HG23	2:B:633:ARG:HD3	1.94	0.48
1:A:635:MET:SD	1:A:721:LEU:HD23	2.53	0.48
2:D:137:LYS:NZ	11:D:1190:HOH:O	2.45	0.48
1:A:716:SER:HA	1:A:742:VAL:HG23	1.96	0.48
1:C:24:ASP:HA	1:C:422:ARG:HG3	1.95	0.48
1:A:507:GLU:HB2	4:A:3570:NAG:H82	1.96	0.48
1:A:794:VAL:HG12	1:A:935:LEU:CD2	2.44	0.48
1:C:359:ALA:CB	1:C:421:LEU:HD13	2.43	0.48
1:C:19:PHE:CZ	1:C:37:VAL:HG11	2.49	0.48
1:C:258:PRO:HB2	1:C:288:TYR:CD2	2.49	0.48
1:C:195:LEU:CD1	1:C:235:TRP:CZ3	2.97	0.48
1:C:750:LEU:HD13	1:C:786:LEU:CD2	2.43	0.48
1:C:394:GLY:HA2	1:C:399:LEU:HD23	1.96	0.48
1:C:504:LEU:HD13	1:C:571:VAL:CG1	2.43	0.47
2:D:64:LEU:HD12	2:D:87:ARG:HG2	1.95	0.47
1:C:86:THR:HG21	1:C:212:LEU:HD22	1.95	0.47
1:C:285:MET:HE2	2:D:321:TYR:CE1	2.49	0.47
1:A:216:VAL:O	1:A:217:SER:C	2.52	0.47
1:C:794:VAL:HG12	1:C:935:LEU:CD2	2.44	0.47
1:C:504:LEU:HD23	1:C:573:LEU:HD23	1.95	0.47
1:A:824:LEU:HD12	1:A:891:ASP:O	2.14	0.47
2:D:239:ARG:HB2	2:D:242:ALA:HB3	1.97	0.47
2:B:257:ALA:O	2:B:258:LEU:HB2	2.15	0.47
1:C:909:LEU:HD11	1:C:955:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:LEU:O	1:C:599:VAL:HG23	2.15	0.47
1:C:195:LEU:HD13	1:C:235:TRP:CH2	2.50	0.46
1:C:909:LEU:CD2	1:C:924:LEU:HD11	2.44	0.46
10:B:3560:NAG:H4	10:B:3561:MAN:H2	1.77	0.46
2:B:218:ALA:HB3	2:B:219:PRO:HD3	1.97	0.46
2:B:529:VAL:HG11	2:B:557:TYR:CE1	2.49	0.46
2:B:203:PHE:CE2	2:B:207:VAL:HG11	2.50	0.46
1:A:883:ALA:HB1	1:A:884:PRO:CD	2.45	0.46
1:C:363:LEU:HD21	1:C:435:LEU:HD13	1.97	0.46
1:C:799:LEU:HD12	1:C:929:TRP:O	2.15	0.46
1:C:922:PHE:HB2	1:C:955:LEU:HD12	1.97	0.46
2:B:171:GLU:OE1	2:B:171:GLU:N	2.49	0.46
2:D:249:THR:HA	2:D:309:ALA:O	2.16	0.45
1:C:280:LEU:CD1	1:C:306:LEU:HD23	2.45	0.45
1:A:637:ALA:HB1	1:A:723:ILE:HD11	1.99	0.45
2:B:117:LEU:HD21	2:B:225:ALA:HB1	1.99	0.45
1:C:195:LEU:HD13	1:C:235:TRP:CZ3	2.52	0.45
1:A:289:PHE:CZ	1:A:308:VAL:HG11	2.52	0.45
2:D:357:LEU:HD11	2:D:397:PHE:CD2	2.51	0.45
1:A:260:TRP:CE3	1:A:266:ALA:HB2	2.51	0.45
2:B:359:VAL:HG22	2:B:416:ILE:CD1	2.47	0.45
2:D:292:LEU:HD21	2:D:324:LEU:HD12	1.98	0.45
1:A:107:CYS:HA	1:A:130:CYS:HA	1.98	0.45
1:A:493:ALA:HB2	1:A:537:LEU:HD13	1.99	0.45
2:D:379:VAL:O	2:D:379:VAL:HG13	2.17	0.45
1:A:307:LEU:HD11	1:A:374:ILE:HG21	1.98	0.45
2:B:667:PHE:HB3	2:B:681:VAL:HG22	1.98	0.45
1:A:24:ASP:HA	1:A:422:ARG:HG3	1.99	0.45
2:B:568:MET:HB2	2:B:574:LEU:HD23	1.98	0.45
1:A:307:LEU:CD1	1:A:374:ILE:HG21	2.47	0.45
1:A:633:LEU:HD22	1:A:703:MET:CE	2.47	0.45
1:C:489:MET:HE2	1:C:533:LEU:HD12	1.98	0.44
1:A:920:ASP:OD1	11:A:1153:HOH:O	2.21	0.44
1:C:456:ALA:HB2	1:C:586:LEU:HD11	1.99	0.44
1:C:835:LEU:O	1:C:836:LYS:C	2.56	0.44
1:C:377:ALA:HB2	1:C:421:LEU:HD11	1.98	0.44
1:C:363:LEU:HD11	1:C:375:ALA:HB2	1.98	0.44
1:C:359:ALA:HB1	1:C:421:LEU:HD13	1.98	0.44
2:D:529:VAL:HG11	2:D:557:TYR:CZ	2.53	0.44
1:C:803:LEU:CD1	1:C:905:VAL:HG11	2.47	0.44
1:A:363:LEU:HD21	1:A:435:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD21	1:A:239:VAL:HG11	1.99	0.44
1:C:461:LEU:HD12	1:C:488:GLN:OE1	2.17	0.44
2:B:69:LEU:HD13	2:B:105:ARG:CB	2.45	0.44
2:B:50:ALA:HB3	2:B:53:SER:HB3	2.00	0.44
1:C:493:ALA:HB2	1:C:537:LEU:HD13	2.00	0.44
1:A:359:ALA:HB3	1:A:421:LEU:HD13	2.00	0.43
1:A:689:LEU:HD12	1:A:723:ILE:HG23	1.99	0.43
1:C:216:VAL:O	1:C:217:SER:C	2.56	0.43
2:B:223:PHE:CE1	2:B:254:THR:HG21	2.53	0.43
2:B:26:CYS:HB2	2:B:44:LEU:HD13	1.99	0.43
1:C:666:VAL:HG12	1:C:668:GLY:CA	2.48	0.43
1:A:19:PHE:CE1	1:A:37:VAL:HG11	2.53	0.43
2:B:112:VAL:O	2:B:149:LEU:HD12	2.18	0.43
2:B:226:ILE:HD13	2:B:306:LEU:HD21	2.01	0.43
1:A:377:ALA:HB1	1:A:418:GLY:O	2.18	0.43
2:B:554:THR:HG22	2:B:560:CYS:O	2.18	0.43
1:C:504:LEU:HD13	1:C:571:VAL:HG11	1.99	0.43
2:D:139:ALA:HB2	2:D:200:VAL:HG11	2.00	0.43
1:A:922:PHE:HB2	1:A:955:LEU:HD12	2.01	0.43
2:D:136:THR:HG22	2:D:200:VAL:HG23	2.00	0.43
1:A:813:LEU:HD11	1:A:924:LEU:HD11	2.01	0.43
1:A:660:MET:HE2	10:B:3560:NAG:H83	2.01	0.43
1:A:824:LEU:HD13	1:A:892:LEU:HB2	2.00	0.43
1:A:916:GLN:O	1:A:917:ARG:HB2	2.19	0.43
1:C:637:ALA:HB1	1:C:723:ILE:HD11	2.01	0.43
1:C:883:ALA:HB1	1:C:884:PRO:CD	2.49	0.42
1:C:689:LEU:CD2	1:C:701:ILE:HD11	2.49	0.42
1:C:689:LEU:HD21	1:C:701:ILE:HD11	1.99	0.42
1:C:19:PHE:CE1	1:C:37:VAL:HG11	2.53	0.42
1:A:194:LEU:C	1:A:194:LEU:HD12	2.39	0.42
1:C:107:CYS:HA	1:C:130:CYS:HA	2.00	0.42
2:B:357:LEU:HD11	2:B:397:PHE:CD2	2.54	0.42
1:C:122:ALA:O	1:C:123:GLU:HB2	2.19	0.42
2:B:130:SER:OG	2:B:336:ASP:O	2.30	0.42
2:B:31:LEU:HD21	2:B:35:SER:HB2	2.02	0.42
1:A:585:VAL:HG12	1:A:587[A]:HIS:CD2	2.54	0.42
2:B:245:LEU:HD11	2:B:348:TYR:CD1	2.54	0.42
2:B:350:LYS:O	2:B:353:SER:HB3	2.18	0.42
2:B:204:ASN:O	2:B:207:VAL:HG22	2.20	0.42
2:D:106:GLN:NE2	2:D:355:VAL:HG22	2.34	0.42
1:A:627:ALA:HB2	1:A:791:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:3099:NAG:H81	9:B:3371:NAG:H2	2.02	0.42
1:A:84:LEU:HB2	1:A:212:LEU:HD12	2.00	0.42
1:C:314:MET:HE1	1:C:322:LEU:HD22	2.01	0.42
1:A:618:VAL:HG11	1:A:631:LEU:HD22	2.00	0.42
2:B:142:MET:HB3	2:B:149:LEU:HD22	2.01	0.42
2:D:128:LEU:O	2:D:131:ILE:HG22	2.19	0.42
1:C:194:LEU:HD12	1:C:194:LEU:C	2.41	0.42
1:A:794:VAL:HG12	1:A:935:LEU:HD22	2.01	0.42
2:B:314:VAL:HG22	2:B:314:VAL:O	2.18	0.42
1:A:195:LEU:CD1	1:A:255:VAL:HG21	2.49	0.41
1:C:877:LEU:HD11	1:C:925:GLN:OE1	2.20	0.41
1:C:322:LEU:HD12	2:D:296:THR:HG21	2.02	0.41
2:D:529:VAL:HG12	2:D:557:TYR:CE1	2.55	0.41
2:B:667:PHE:HB2	2:B:681:VAL:HG22	2.02	0.41
1:C:262:TRP:HB3	2:D:317:LEU:HD13	2.03	0.41
1:A:609:VAL:HG22	1:A:729:GLN:HB2	2.01	0.41
2:B:529:VAL:CG1	2:B:557:TYR:CE1	3.03	0.41
2:D:196:LEU:HD13	2:D:236:ILE:O	2.20	0.41
2:D:203:PHE:O	2:D:207:VAL:HG13	2.20	0.41
1:A:195:LEU:HD21	1:A:239:VAL:CG1	2.50	0.41
1:A:911:LEU:HB2	1:A:912:PRO:HD3	2.03	0.41
1:A:462:VAL:HG22	1:A:463:GLN:N	2.35	0.41
2:D:306:LEU:HB3	2:D:328:THR:HG22	2.03	0.41
1:C:812:LEU:CD2	1:C:909:LEU:HD22	2.51	0.41
2:B:362:LEU:HD12	2:B:363:PRO:HD2	2.02	0.41
1:C:682:THR:O	1:C:684:VAL:HG23	2.21	0.41
1:A:28:ASP:OD1	1:A:31:GLY:N	2.54	0.41
1:A:280:LEU:CD1	1:A:306:LEU:HD23	2.51	0.41
1:C:195:LEU:HD12	1:C:235:TRP:CZ3	2.56	0.41
1:A:298:VAL:HG22	1:A:305:ASP:OD2	2.21	0.41
1:C:26:HIS:HB2	1:C:36:VAL:HG23	2.03	0.41
1:C:803:LEU:HD13	1:C:905:VAL:HG11	2.03	0.40
2:D:112:VAL:HG22	11:D:737:HOH:O	2.21	0.40
1:C:359:ALA:HB3	1:C:377:ALA:HB3	2.03	0.40
2:B:104:VAL:HG21	2:B:357:LEU:HD21	2.02	0.40
1:A:637:ALA:HB1	1:A:723:ILE:CD1	2.51	0.40
1:A:630:VAL:HG21	10:B:3560:NAG:O3	2.21	0.40
2:B:640:GLU:HG2	2:B:642:VAL:HG13	2.02	0.40
1:C:307:LEU:CD1	1:C:374:ILE:HG21	2.51	0.40
1:C:84:LEU:HB2	1:C:212:LEU:HD12	2.03	0.40
2:D:112:VAL:O	2:D:149:LEU:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:ASP:OD1	2:B:289:TYR:N	2.55	0.40
2:D:554:THR:HG22	2:D:560:CYS:O	2.20	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	913/959 (95%)	864 (95%)	41 (4%)	8 (1%)	21	36
1	C	904/959 (94%)	863 (96%)	37 (4%)	4 (0%)	39	60
2	B	675/690 (98%)	613 (91%)	58 (9%)	4 (1%)	30	48
2	D	600/690 (87%)	559 (93%)	41 (7%)	0	100	100
All	All	3092/3298 (94%)	2899 (94%)	177 (6%)	16 (0%)	34	54

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	SER
1	A	837	VAL
1	A	940	PRO
1	A	581	ALA
1	A	836	LYS
1	C	217	SER
1	C	836	LYS
1	C	940	PRO
2	B	670	TYR
1	A	669[A]	PHE
1	A	669[B]	PHE
2	B	609	THR
2	B	652	ALA

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Mol	Chain	Res	Type
1	C	581	ALA
1	A	123	GLU
2	B	8	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	762/799 (95%)	755 (99%)	7 (1%)	84	95
1	C	753/799 (94%)	745 (99%)	8 (1%)	80	93
2	B	604/612 (99%)	598 (99%)	6 (1%)	82	94
2	D	534/612 (87%)	533 (100%)	1 (0%)	95	99
All	All	2653/2822 (94%)	2631 (99%)	22 (1%)	86	96

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	270	LEU
1	A	288	TYR
1	A	597	ARG
1	A	621	SER
1	A	874	ASP
2	B	127	ASP
2	B	215	ASN
2	B	423	ASP
2	B	608	CYS
2	B	651	ASP
2	B	669	TYR
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	288	TYR
1	C	335	ARG

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Mol	Chain	Res	Type
1	C	580	MET
1	C	597	ARG
1	C	908	PHE
2	D	215	ASN

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

Mol	Chain	Res	Type
1	A	197	GLN
1	A	534	ASN
1	A	676	GLN
1	A	680	ASN
1	A	795	ASN
1	A	916	GLN
2	B	106	GLN
2	B	668	GLN
1	C	7	GLN
1	C	197	GLN
1	C	676	GLN
1	C	680	ASN
1	C	921	GLN
2	D	14	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

26 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	$\#\|Z\| > 2$
7	NAG	B	3099	2,7	14,14,15	0.58	0	15,19,21	1.13	1 (6%)
7	NAG	B	3100	7	14,14,15	0.57	0	15,19,21	0.81	1 (6%)
8	NAG	B	3320	8,2	14,14,15	0.48	0	15,19,21	0.65	0
8	NAG	B	3321	8	14,14,15	0.51	0	15,19,21	0.56	0
8	MAN	B	3322	8	11,11,12	0.58	0	14,15,17	0.69	0
8	MAN	B	3323	8	11,11,12	0.49	0	14,15,17	2.73	3 (21%)
9	NAG	B	3371	9,2	14,14,15	0.61	0	15,19,21	0.56	0
9	NAG	B	3372	9	14,14,15	0.49	0	15,19,21	0.68	0
9	MAN	B	3373	9	11,11,12	0.61	0	14,15,17	0.60	0
7	NAG	B	3452	2,7	14,14,15	0.64	0	15,19,21	0.65	0
7	NAG	B	3453	7	14,14,15	0.51	0	15,19,21	0.61	0
10	NAG	B	3559	10,2	14,14,15	0.59	0	15,19,21	0.78	0
10	NAG	B	3560	10	14,14,15	0.45	0	15,19,21	0.93	0
10	MAN	B	3561	10	11,11,12	0.54	0	14,15,17	0.87	0
10	MAN	B	3562	10	11,11,12	0.54	0	14,15,17	0.69	0
10	MAN	B	3563	10	11,11,12	0.60	0	14,15,17	0.73	0
7	NAG	C	3249	1,7	14,14,15	0.48	0	15,19,21	1.27	2 (13%)
7	NAG	C	3250	7	14,14,15	0.62	0	15,19,21	0.82	0
7	NAG	D	3320	2,7	14,14,15	0.58	0	15,19,21	0.65	0
7	NAG	D	3321	7	14,14,15	0.54	0	15,19,21	0.59	0
7	NAG	D	3371	2,7	14,14,15	0.53	0	15,19,21	0.56	0
7	NAG	D	3372	7	14,14,15	0.51	0	15,19,21	0.59	0
7	NAG	D	3452	2,7	14,14,15	0.55	0	15,19,21	0.51	0
7	NAG	D	3453	7	14,14,15	0.55	0	15,19,21	0.66	0
7	NAG	D	3559	2,7	14,14,15	0.53	0	15,19,21	0.57	0
7	NAG	D	3560	7	14,14,15	0.58	0	15,19,21	0.60	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
7	NAG	B	3099	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	3100	7	-	0/6/23/26	0/1/1/1
8	NAG	B	3320	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	3321	8	-	0/6/23/26	0/1/1/1
8	MAN	B	3322	8	1/1/4/5	0/2/19/22	0/1/1/1
8	MAN	B	3323	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	3371	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	3372	9	-	0/6/23/26	0/1/1/1
9	MAN	B	3373	9	1/1/4/5	0/2/19/22	0/1/1/1
7	NAG	B	3452	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	3453	7	-	0/6/23/26	0/1/1/1
10	NAG	B	3559	10,2	-	0/6/23/26	0/1/1/1
10	NAG	B	3560	10	-	0/6/23/26	0/1/1/1
10	MAN	B	3561	10	1/1/4/5	0/2/19/22	0/1/1/1
10	MAN	B	3562	10	-	0/2/19/22	0/1/1/1
10	MAN	B	3563	10	-	0/2/19/22	0/1/1/1
7	NAG	C	3249	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	3250	7	-	0/6/23/26	0/1/1/1
7	NAG	D	3320	2,7	-	0/6/23/26	0/1/1/1
7	NAG	D	3321	7	-	0/6/23/26	0/1/1/1
7	NAG	D	3371	2,7	-	0/6/23/26	0/1/1/1
7	NAG	D	3372	7	-	0/6/23/26	0/1/1/1
7	NAG	D	3452	2,7	-	0/6/23/26	0/1/1/1
7	NAG	D	3453	7	-	0/6/23/26	0/1/1/1
7	NAG	D	3559	2,7	-	0/6/23/26	0/1/1/1
7	NAG	D	3560	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	3100	NAG	C4-C3-C2	2.09	114.48	111.23
7	C	3249	NAG	C1-O5-C5	2.53	115.46	112.25
7	C	3249	NAG	O4-C4-C5	3.04	117.29	109.24
7	B	3099	NAG	C4-C3-C2	3.14	116.11	111.23
8	B	3323	MAN	O5-C1-C2	3.90	117.19	110.86
8	B	3323	MAN	C1-C2-C3	4.89	115.33	109.54
8	B	3323	MAN	C1-O5-C5	7.78	122.12	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	B	3373	MAN	C1
10	B	3561	MAN	C1
8	B	3322	MAN	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3099	NAG	1	0
8	B	3320	NAG	1	0
9	B	3371	NAG	2	0
10	B	3560	NAG	4	0
10	B	3561	MAN	1	0

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 16 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
4	NAG	A	3015	1	14,14,15	0.46	0	15,19,21	0.56	0
4	NAG	A	3570	1	14,14,15	0.65	0	15,19,21	1.63	1 (6%)
5	IMD	A	5001	-	3,5,5	0.52	0	4,5,5	0.58	0
4	NAG	C	3015	1	14,14,15	0.55	0	15,19,21	0.67	0
4	NAG	C	3570	1	14,14,15	0.54	0	15,19,21	0.59	0
5	IMD	C	5001	-	3,5,5	0.53	0	4,5,5	0.60	0
5	IMD	C	5002	-	3,5,5	0.54	0	4,5,5	0.59	0
5	IMD	C	5003	-	3,5,5	0.53	0	4,5,5	0.60	0
5	IMD	C	5004	-	3,5,5	0.52	0	4,5,5	0.57	0
5	IMD	C	960	-	3,5,5	0.53	0	4,5,5	0.58	0
4	NAG	D	3099	2	14,14,15	0.54	0	15,19,21	0.56	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	NAG	A	3015	1	-	0/6/23/26	0/1/1/1
4	NAG	A	3570	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IMD	A	5001	-	-	0/0/0/0	0/1/1/1
4	NAG	C	3015	1	-	0/6/23/26	0/1/1/1
4	NAG	C	3570	1	1/1/5/7	0/6/23/26	0/1/1/1
5	IMD	C	5001	-	-	0/0/0/0	0/1/1/1
5	IMD	C	5002	-	-	0/0/0/0	0/1/1/1
5	IMD	C	5003	-	-	0/0/0/0	0/1/1/1
5	IMD	C	5004	-	-	0/0/0/0	0/1/1/1
5	IMD	C	960	-	-	0/0/0/0	0/1/1/1
4	NAG	D	3099	2	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3570	NAG	C1-O5-C5	5.72	119.51	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	3570	NAG	C1
4	D	3099	NAG	C1

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
4	A	3570	NAG	1	0
4	C	3570	NAG	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

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	914/959 (95%)	1.28	193 (21%)	1	1	23, 27, 53, 90	0
1	C	904/959 (94%)	1.92	331 (36%)	0	0	23, 27, 52, 90	16 (1%)
2	B	680/690 (98%)	1.87	186 (27%)	1	0	23, 46, 62, 72	84 (12%)
2	D	603/690 (87%)	1.42	142 (23%)	1	1	23, 44, 63, 72	0
All	All	3101/3298 (94%)	1.62	852 (27%)	1	0	23, 35, 59, 90	100 (3%)

All (852) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	634	TYR	16.8
2	B	628	GLU	14.7
2	B	624	ALA	13.7
2	B	652	ALA	12.9
2	B	682	VAL	12.7
2	B	664	VAL	12.5
2	B	625	LEU	12.5
2	B	681	VAL	12.0
2	B	614	CYS	11.9
2	B	641	SER	11.7
2	B	646	LYS	10.4
1	C	959	CYS	10.3
2	B	680	TYR	10.3
1	C	937	TYR	10.2
2	B	688	CYS	10.2
2	B	466	TRP	10.1
2	B	631	CYS	10.0
2	B	627	ASP	9.9
1	C	820	PRO	9.8
2	B	677	SER	9.6
2	B	650	LYS	9.5

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Mol	Chain	Res	Type	RSRZ
1	C	932	VAL	9.5
1	C	813	LEU	9.4
1	C	887	VAL	9.3
2	B	666	ARG	9.0
2	B	629	ASN	8.9
2	B	665	VAL	8.7
1	C	832	VAL	8.4
2	D	610	PHE	8.4
1	A	579	GLY	8.0
1	C	930	PHE	8.0
1	A	578	ALA	8.0
2	B	617	CYS	7.9
2	B	670	TYR	7.9
1	C	800	SER	7.9
1	C	938	ALA	7.9
1	C	794	VAL	7.8
2	B	676	LYS	7.8
2	B	618	LYS	7.7
1	C	956	LEU	7.7
2	D	612	LYS	7.7
1	C	824	LEU	7.7
1	A	941	PRO	7.6
1	C	578	ALA	7.6
1	C	958	ALA	7.6
1	C	755	PHE	7.5
2	D	573	LEU	7.5
2	B	647	ASP	7.4
2	B	651	ASP	7.4
1	C	909	LEU	7.4
2	B	379	VAL	7.4
1	C	914	LEU	7.4
1	C	936	PRO	7.3
1	C	579	GLY	7.3
1	C	919	LEU	7.3
2	B	640	GLU	7.3
2	B	623	GLY	7.2
2	B	669	TYR	7.2
1	C	920	ASP	7.0
1	A	713	ALA	6.9
1	C	878	VAL	6.9
2	B	656	THR	6.8
1	A	580	MET	6.8

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Mol	Chain	Res	Type	RSRZ
1	C	885	CYS	6.8
1	C	933	SER	6.8
1	C	801	ILE	6.7
2	D	466	TRP	6.7
1	C	833	ASN	6.6
2	B	679	LEU	6.6
2	B	467	LEU	6.5
2	D	379	VAL	6.5
2	B	690	GLY	6.5
2	B	643	LYS	6.5
2	B	621	ASP	6.4
1	C	877	LEU	6.4
2	B	615	VAL	6.4
2	B	610	PHE	6.3
2	B	633	ARG	6.3
2	D	609	THR	6.3
2	B	626	HIS	6.2
2	B	10	VAL	6.2
1	C	829	GLN	6.2
1	C	804	PRO	6.2
2	B	642	VAL	6.2
2	B	667	PHE	6.2
2	B	674	SER	6.2
2	B	655	CYS	6.2
1	C	802	HIS	6.1
1	C	793	THR	6.1
2	B	630	THR	6.1
1	C	834	PRO	6.0
2	B	675	GLY	6.0
1	C	941	PRO	5.9
1	C	827	PHE	5.8
2	B	672	ASP	5.8
1	C	906	LEU	5.8
1	C	931	ASN	5.8
2	B	689	LYS	5.7
1	C	822	GLY	5.7
1	C	783	THR	5.7
2	D	182	THR	5.7
2	B	645	LEU	5.6
1	C	915	TYR	5.6
1	C	908	PHE	5.6
1	C	876	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	922	PHE	5.5
1	C	814	TYR	5.5
2	B	673	SER	5.5
1	C	778	PRO	5.5
1	C	934	SER	5.5
2	B	377	ASN	5.5
2	D	129	TRP	5.5
1	A	792	GLY	5.5
1	C	886	THR	5.4
1	C	952	TRP	5.4
1	C	712	GLU	5.4
1	A	939	VAL	5.4
1	C	910	TRP	5.3
1	C	826	CYS	5.3
1	C	929	TRP	5.3
2	B	684	GLU	5.2
2	B	678	ILE	5.2
2	B	622	ARG	5.2
1	C	798	HIS	5.2
1	A	710	LEU	5.2
2	B	685	PRO	5.2
1	C	710	LEU	5.2
2	D	33	LEU	5.1
2	B	661	ASP	5.1
1	C	903	VAL	5.1
1	C	891	ASP	5.1
1	C	907	ALA	5.0
1	C	779	LYS	5.0
1	C	935	LEU	4.9
2	B	683	GLU	4.9
2	B	635	CYS	4.9
1	C	784	TYR	4.9
2	B	129	TRP	4.9
1	C	746	ALA	4.9
1	C	890	CYS	4.9
1	C	888	VAL	4.9
1	C	949	ALA	4.8
1	C	580	MET	4.8
1	C	797	LEU	4.8
1	A	668	GLY	4.8
2	B	639	ILE	4.8
1	C	836	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	815	ILE	4.8
2	B	275	VAL	4.8
2	D	574	LEU	4.7
1	C	895	MET	4.7
2	D	572	GLY	4.7
2	B	644	GLU	4.7
1	C	884	PRO	4.7
1	C	240	ALA	4.7
2	B	649	GLY	4.7
1	C	517	GLN	4.7
1	C	950	GLN	4.7
2	B	668	GLN	4.7
2	B	659	ASN	4.6
2	D	275	VAL	4.6
2	B	378	GLU	4.6
1	A	97	VAL	4.6
1	A	776	TRP	4.6
2	B	632	ASN	4.6
1	C	744	ALA	4.5
2	D	373	THR	4.5
2	B	471	CYS	4.5
1	A	107	CYS	4.5
2	B	445	SER	4.5
1	C	939	VAL	4.4
2	B	473	CYS	4.4
2	B	654	ASN	4.4
1	A	959	CYS	4.4
2	B	653	VAL	4.4
2	D	257	ALA	4.4
1	C	173	SER	4.3
1	A	621	SER	4.3
1	C	811	ASP	4.3
1	C	905	VAL	4.3
1	C	828	PRO	4.3
1	C	795	ASN	4.3
1	C	880	CYS	4.3
2	D	608	CYS	4.3
2	D	443	PRO	4.2
2	D	9	GLY	4.2
1	C	879	SER	4.2
1	A	288	TYR	4.2
1	C	945	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	107	VAL	4.2
1	C	874	ASP	4.2
2	D	571	ASN	4.1
1	C	940	PRO	4.1
2	D	464	PRO	4.1
2	D	261	ARG	4.1
1	A	234	TYR	4.1
1	A	655	GLN	4.1
1	A	893	GLN	4.1
1	C	816	LEU	4.1
1	C	823	GLY	4.1
1	C	921	GLN	4.1
1	A	581	ALA	4.1
1	C	237	TYR	4.1
2	B	184	CYS	4.1
2	B	619	LYS	4.1
1	A	667	GLU	4.1
1	C	98	VAL	4.1
1	C	892	LEU	4.1
2	D	337	SER	4.0
2	B	185	LEU	4.0
1	C	516	ARG	4.0
1	C	837	VAL	4.0
1	A	936	PRO	4.0
1	A	105	VAL	4.0
1	C	239	VAL	4.0
1	A	576	THR	4.0
2	B	579	GLY	4.0
1	C	812	LEU	4.0
2	D	467	LEU	4.0
1	C	954	GLN	4.0
2	D	377	ASN	3.9
1	C	288	TYR	3.9
2	B	638	GLU	3.9
2	D	483	GLN	3.9
2	D	194	LEU	3.9
1	C	582	PRO	3.9
1	C	944	LEU	3.9
2	D	374	CYS	3.9
1	C	169	ALA	3.9
1	C	916	GLN	3.9
2	D	492	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	105	VAL	3.9
1	A	794	VAL	3.9
1	C	255	VAL	3.9
1	C	360	ILE	3.9
1	A	940	PRO	3.8
1	C	942	LEU	3.8
1	C	171	PHE	3.8
1	A	820	PRO	3.8
1	A	171	PHE	3.8
1	C	328	VAL	3.8
2	B	613	GLU	3.8
1	C	106	ALA	3.8
1	C	806	GLN	3.8
2	B	277	SER	3.8
2	D	462	CYS	3.8
1	C	195	LEU	3.8
1	C	927	HIS	3.8
1	C	359	ALA	3.8
1	C	172	SER	3.8
1	C	792	GLY	3.8
1	A	938	ALA	3.7
2	D	4	ILE	3.7
1	C	170	GLY	3.7
1	C	186	PRO	3.7
2	D	587	VAL	3.7
1	C	95	ALA	3.7
1	C	183	LEU	3.7
1	C	184	GLY	3.7
2	B	636	ARG	3.7
1	C	951	VAL	3.7
1	A	712	GLU	3.7
2	D	606	ASP	3.7
1	C	290	GLY	3.6
1	C	96	SER	3.6
2	D	256	ILE	3.6
1	C	667	GLU	3.6
1	A	839	TRP	3.6
2	B	611	LYS	3.6
2	B	687	CYS	3.6
2	D	473	CYS	3.6
2	D	494	VAL	3.6
1	C	889	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	97	VAL	3.5
1	A	582	PRO	3.5
1	C	875	PRO	3.5
2	B	321	TYR	3.5
1	C	289	PHE	3.5
1	A	716	SER	3.5
1	C	819	GLN	3.5
2	D	557	TYR	3.5
1	C	896	ALA	3.5
2	D	376	ASN	3.5
1	C	821[A]	GLN	3.5
1	C	604	GLU	3.5
1	A	258	PRO	3.5
1	C	893	GLN	3.5
1	A	183	LEU	3.5
1	C	294	ALA	3.5
1	A	671[A]	ARG	3.5
1	C	624	LEU	3.5
2	B	616	GLU	3.5
1	C	196	ALA	3.5
1	A	93	LEU	3.5
1	A	956	LEU	3.5
1	C	924	LEU	3.5
1	A	98	VAL	3.4
1	A	38	GLY	3.4
2	D	325	ILE	3.4
1	C	713	ALA	3.4
1	A	827	PHE	3.4
1	C	234	TYR	3.4
1	C	575	PRO	3.4
1	C	831	PRO	3.4
1	C	104	ILE	3.4
2	B	107	VAL	3.4
2	B	212	VAL	3.4
1	C	835	LEU	3.4
1	C	108	ALA	3.4
1	C	541	HIS	3.4
2	D	262	LEU	3.4
2	B	257	ALA	3.4
1	C	309	GLY	3.4
2	B	648	THR	3.4
1	A	958	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	263	ALA	3.4
1	A	172	SER	3.4
1	A	239	VAL	3.3
1	C	107	CYS	3.4
1	C	109	PRO	3.3
1	C	185	ALA	3.3
2	B	657	TYR	3.3
1	C	559[A]	ARG	3.3
2	D	451	GLY	3.3
2	D	607	ALA	3.3
1	C	235	TRP	3.3
1	C	286	ALA	3.3
2	B	612	LYS	3.3
2	D	390	LYS	3.3
1	C	254	VAL	3.3
1	A	173	SER	3.3
1	C	167	CYS	3.3
2	D	541	GLN	3.3
2	D	577	GLY	3.3
1	A	96	SER	3.3
2	D	122	TYR	3.3
2	D	180	MET	3.3
2	D	592	GLY	3.2
1	A	237	TYR	3.2
1	C	291	HIS	3.2
2	B	620	PHE	3.2
2	B	382	GLY	3.2
1	A	837	VAL	3.2
2	B	213	SER	3.2
2	D	602	PRO	3.2
2	D	321	TYR	3.2
1	A	796	GLY	3.2
1	C	955	LEU	3.2
2	B	197	THR	3.2
1	C	266	ALA	3.2
2	B	513	PHE	3.2
1	A	797	LEU	3.2
2	B	186	PRO	3.2
1	A	95	ALA	3.2
1	C	241	VAL	3.2
2	B	178	TYR	3.2
1	C	130	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	359	ALA	3.1
1	C	174	VAL	3.1
1	C	292	SER	3.1
1	A	944	LEU	3.1
1	A	94	GLY	3.1
1	A	360	ILE	3.1
1	C	668	GLY	3.1
2	B	9	GLY	3.1
2	B	541	GLN	3.1
1	C	253	TYR	3.1
2	B	122	TYR	3.1
1	A	110	TRP	3.1
1	A	607	VAL	3.1
2	D	178	TYR	3.1
1	C	311	PRO	3.1
1	C	803	LEU	3.1
1	C	911	LEU	3.1
1	A	286	ALA	3.1
1	C	928	ALA	3.1
1	C	145	PRO	3.1
1	C	947	GLY	3.1
2	D	564	THR	3.1
2	D	380	ILE	3.1
1	C	357	GLY	3.1
1	C	146	CYS	3.1
2	B	324	LEU	3.1
2	D	471	CYS	3.1
1	A	162	TRP	3.1
2	B	443	PRO	3.0
2	D	295	MET	3.0
1	C	93	LEU	3.0
2	D	258	LEU	3.0
1	A	729	GLN	3.0
1	C	808	GLN	3.0
1	A	240	ALA	3.0
1	A	469	ALA	3.0
1	C	581	ALA	3.0
1	C	293	VAL	3.0
1	C	38	GLY	3.0
1	C	337	PRO	3.0
2	D	239	ARG	3.0
1	C	238	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	947	GLY	3.0
1	C	308	VAL	3.0
2	B	502	LEU	3.0
1	A	937	TYR	3.0
1	C	143	TYR	3.0
1	A	238	SER	3.0
1	C	326	GLY	3.0
1	A	37	VAL	3.0
1	C	295	VAL	3.0
1	C	825	GLN	3.0
1	A	929[A]	TRP	3.0
1	C	110	TRP	3.0
2	D	280	HIS	3.0
2	B	410	LYS	3.0
1	A	106	ALA	3.0
2	B	514	GLY	3.0
1	A	285	MET	3.0
1	C	129	SER	3.0
1	A	241	VAL	3.0
1	A	289	PHE	3.0
2	D	324	LEU	3.0
1	C	287	SER	3.0
1	C	904	THR	3.0
1	A	169	ALA	3.0
1	C	883	ALA	3.0
1	A	55	LEU	2.9
1	C	23	LEU	2.9
1	C	264	LEU	2.9
1	C	750	LEU	2.9
1	C	310	ALA	2.9
1	C	901	ALA	2.9
2	D	444	ASN	2.9
1	C	127	VAL	2.9
1	C	671	ARG	2.9
1	C	259	THR	2.9
2	D	197	THR	2.9
1	A	184	GLY	2.9
1	C	194	LEU	2.9
1	C	233	GLY	2.9
1	C	285	MET	2.9
1	C	314	MET	2.9
2	B	671	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	259	ASP	2.9
1	A	293	VAL	2.9
1	C	788	ASN	2.9
2	B	61	ALA	2.9
1	A	891	ASP	2.9
1	C	267	VAL	2.9
1	C	780	VAL	2.9
2	D	445	SER	2.9
2	B	574	LEU	2.9
1	A	40	PRO	2.9
1	C	918	PRO	2.9
1	C	53	VAL	2.9
2	D	378	GLU	2.8
2	B	375	LEU	2.8
1	C	112	HIS	2.8
1	C	50	THR	2.8
1	A	290	GLY	2.8
1	C	313	TYR	2.8
1	C	753	ASN	2.8
1	C	182	VAL	2.8
1	C	734	LYS	2.8
1	A	19	PHE	2.8
2	B	291	SER	2.8
2	B	462	CYS	2.8
2	D	406	CYS	2.8
1	C	587[A]	HIS	2.8
1	C	419	PHE	2.8
2	D	183	THR	2.8
1	A	92	GLY	2.8
1	A	695	LYS	2.8
1	A	292	SER	2.8
1	A	943	SER	2.8
1	A	167	CYS	2.8
1	C	799	LEU	2.8
1	C	175	VAL	2.8
2	D	193	VAL	2.8
1	C	312	LEU	2.8
2	B	69	LEU	2.8
2	D	567	CYS	2.8
2	B	237	GLY	2.8
1	C	669	PHE	2.8
1	A	186	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	258	PRO	2.8
1	C	830	PRO	2.8
1	C	730	ASN	2.8
2	D	580	LYS	2.8
1	C	132	LEU	2.8
1	C	957	ARG	2.8
2	B	179	ASP	2.8
2	B	637	ASP	2.8
1	A	611	GLN	2.7
1	A	264	LEU	2.7
1	C	236	GLY	2.7
1	C	740	VAL	2.7
2	D	454	THR	2.7
1	C	556	ALA	2.7
1	A	170	GLY	2.7
1	C	242	GLY	2.7
1	A	759	LEU	2.7
1	C	70	PHE	2.7
2	D	556	TYR	2.7
1	C	220	SER	2.7
1	C	899	GLN	2.7
2	B	274	HIS	2.7
2	D	292	LEU	2.7
2	D	442	GLU	2.7
2	D	104	VAL	2.7
2	D	381	PRO	2.7
2	B	188	PHE	2.7
1	C	678	LYS	2.7
2	D	40	LEU	2.7
2	D	163	PRO	2.7
2	B	451	GLY	2.7
1	C	600	LEU	2.7
2	B	120	LEU	2.7
1	C	362	PRO	2.7
2	B	261	ARG	2.7
1	A	174	VAL	2.7
1	C	748	VAL	2.7
1	C	256	GLY	2.7
2	B	542	CYS	2.7
2	D	260	GLY	2.7
1	C	946	ARG	2.6
2	B	131	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	2.6
1	C	307	LEU	2.6
1	A	517	GLN	2.6
1	C	376	VAL	2.6
1	A	109	PRO	2.6
1	C	113	TRP	2.6
1	C	166	TYR	2.6
1	A	291	HIS	2.6
1	C	754	SER	2.6
2	B	258	LEU	2.6
1	C	257	ALA	2.6
2	D	513	PHE	2.6
1	A	195	LEU	2.6
2	B	380	ILE	2.6
2	B	464	PRO	2.6
2	D	17	LEU	2.6
1	A	628	ASP	2.6
1	C	128	GLY	2.6
1	A	53	VAL	2.6
1	A	666	VAL	2.6
1	A	362	PRO	2.6
1	A	182	VAL	2.6
1	C	607	VAL	2.6
2	B	110	TYR	2.6
2	B	164	TYR	2.6
2	D	576	SER	2.6
1	A	575	PRO	2.6
1	C	356	PHE	2.6
2	B	663	CYS	2.6
2	D	461	ARG	2.5
1	C	603	GLY	2.5
1	A	312	LEU	2.5
1	A	421	LEU	2.5
2	B	33	LEU	2.5
2	D	120	LEU	2.5
1	C	925	GLN	2.5
1	C	361	ALA	2.5
1	A	308	VAL	2.5
2	B	448	CYS	2.5
2	B	326	PRO	2.5
1	A	8	LEU	2.5
2	D	164	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	263	THR	2.5
1	C	735	ILE	2.5
1	C	743	ARG	2.5
1	A	39	ALA	2.5
1	A	266	ALA	2.5
1	C	265	GLY	2.5
1	C	420	SER	2.5
1	C	796	GLY	2.5
2	D	530	ARG	2.5
1	A	798	HIS	2.5
1	C	731	PRO	2.5
1	C	421	LEU	2.5
2	B	17	LEU	2.5
2	D	611	LYS	2.5
1	C	126	PRO	2.5
2	D	2	PRO	2.5
2	B	293	GLY	2.5
2	D	187	MET	2.5
1	C	706	SER	2.5
2	B	92	LEU	2.5
1	A	256	GLY	2.5
1	C	94	GLY	2.5
2	B	318	TYR	2.5
2	D	264	GLY	2.5
2	D	293	GLY	2.5
1	A	108	ALA	2.5
1	C	99	SER	2.5
1	C	912	PRO	2.4
1	A	328	VAL	2.4
1	A	154	ILE	2.4
1	C	583	ALA	2.4
2	D	605	PRO	2.4
1	A	609	VAL	2.4
2	D	475	GLU	2.4
1	A	214	TRP	2.4
2	B	580	LYS	2.4
1	C	818	ILE	2.4
2	D	531	TYR	2.4
1	C	21	PHE	2.4
2	D	132	GLN	2.4
1	A	267	VAL	2.4
1	C	37	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	357	GLY	2.4
1	C	51	GLY	2.4
2	D	69	LEU	2.4
2	D	375	LEU	2.4
1	A	793	THR	2.4
1	A	137	SER	2.4
1	A	472	SER	2.4
1	A	323	ALA	2.4
1	C	141	ALA	2.4
2	B	505	GLN	2.4
2	D	15	GLN	2.4
1	A	419	PHE	2.4
1	A	43	LEU	2.4
2	B	138	LEU	2.4
2	D	548	LEU	2.4
2	B	562	THR	2.4
2	B	278	ASP	2.4
1	A	741	PRO	2.4
1	A	930	PHE	2.4
1	C	52	GLY	2.4
2	B	223	PHE	2.4
2	D	279	ASN	2.4
1	C	193	GLY	2.4
2	B	658	LYS	2.4
2	D	181	LYS	2.4
1	A	181	LEU	2.4
1	C	55	LEU	2.4
2	D	196	LEU	2.4
2	B	449	ASN	2.3
1	A	146	CYS	2.3
1	A	836	LYS	2.3
2	B	468	GLY	2.3
2	B	421	PHE	2.3
1	C	611	GLN	2.3
2	B	310	VAL	2.3
2	D	145	LEU	2.3
1	C	144	SER	2.3
1	A	249	ASN	2.3
2	D	463	GLY	2.3
1	A	70	PHE	2.3
2	D	594	TYR	2.3
2	B	549	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	716	SER	2.3
2	D	266	VAL	2.3
1	A	927	HIS	2.3
1	C	198	ALA	2.3
1	C	469	ALA	2.3
1	C	363	LEU	2.3
2	B	573	LEU	2.3
2	D	562	THR	2.3
1	A	587[A]	HIS	2.3
1	C	787	HIS	2.3
1	A	185	ALA	2.3
1	A	383	PRO	2.3
1	C	203	ILE	2.3
2	B	256	ILE	2.3
2	B	472	GLU	2.3
2	D	151	ILE	2.3
2	D	512	ASP	2.3
1	C	191	PHE	2.3
1	C	736	VAL	2.3
2	B	450	ASN	2.3
1	C	943	SER	2.3
1	A	892	LEU	2.3
1	A	50	THR	2.3
1	C	20	GLY	2.3
1	C	756	PRO	2.3
1	A	377	ALA	2.3
1	A	744	ALA	2.3
1	A	335	ARG	2.3
2	B	660	GLU	2.3
1	A	129	SER	2.3
2	B	292	LEU	2.3
2	B	320	ASN	2.3
1	A	440	TYR	2.3
2	D	553	TRP	2.3
2	B	163	PRO	2.3
1	A	746	ALA	2.2
2	D	568	MET	2.2
2	B	408	GLN	2.2
1	C	131	PHE	2.2
2	B	192	HIS	2.2
1	C	181	LEU	2.2
1	C	187	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	881	ASP	2.2
2	D	540	GLY	2.2
1	C	189	TYR	2.2
2	D	603	THR	2.2
1	A	496	HIS	2.2
1	C	25	PHE	2.2
2	D	223	PHE	2.2
1	A	307	LEU	2.2
1	A	604	GLU	2.2
2	D	357	LEU	2.2
2	B	296	THR	2.2
1	A	255	VAL	2.2
2	D	289	TYR	2.2
2	B	290	PRO	2.2
1	C	375	ALA	2.2
2	B	24	ALA	2.2
2	D	227	MET	2.2
1	C	358	SER	2.2
2	D	255	HIS	2.2
2	D	476	GLU	2.2
1	C	576	THR	2.2
1	A	951	VAL	2.2
1	C	482	VAL	2.2
1	A	424	ALA	2.2
1	C	133	ALA	2.2
1	C	679	GLU	2.2
2	B	18	ALA	2.2
1	A	236	GLY	2.2
1	A	131	PHE	2.2
2	B	40	LEU	2.2
2	D	505	GLN	2.2
1	A	740	VAL	2.2
2	B	200	VAL	2.2
1	C	673	ILE	2.2
1	C	124	LYS	2.2
1	C	923	VAL	2.2
2	D	524	ASP	2.2
1	A	89	ALA	2.2
1	A	152	SER	2.2
1	A	287	SER	2.2
1	A	439	ALA	2.2
1	C	645	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	556	TYR	2.2
1	C	805	GLY	2.2
2	D	460	CYS	2.2
1	A	54	PHE	2.2
1	C	461	LEU	2.2
1	C	165	ARG	2.2
1	C	327	ARG	2.2
2	B	561	THR	2.2
1	A	311	PRO	2.2
1	C	40	PRO	2.2
1	A	309	GLY	2.1
1	C	714	GLY	2.1
2	B	189	GLY	2.1
2	D	1	GLY	2.1
1	C	655	GLN	2.1
2	B	153	PHE	2.1
2	B	341	LEU	2.1
2	B	512	ASP	2.1
1	A	175	VAL	2.1
1	A	282	GLY	2.1
1	C	36	VAL	2.1
2	B	465	GLY	2.1
2	D	372	ALA	2.1
2	B	295	MET	2.1
2	D	520	TYR	2.1
1	A	946	ARG	2.1
1	A	21	PHE	2.1
1	A	132	LEU	2.1
1	A	935	LEU	2.1
1	C	19	PHE	2.1
1	C	69	LEU	2.1
1	C	347	LEU	2.1
2	B	370	PHE	2.1
1	C	680	ASN	2.1
2	D	294	LEU	2.1
2	D	449	ASN	2.1
1	A	364	GLY	2.1
1	A	805	GLY	2.1
1	C	718	SER	2.1
1	A	763	ALA	2.1
1	A	888	VAL	2.1
2	B	62	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	497	ASN	2.1
1	A	787	HIS	2.1
2	D	509	HIS	2.1
2	B	433	CYS	2.1
2	D	588	CYS	2.1
1	C	437	VAL	2.1
1	C	742	VAL	2.1
2	B	187	MET	2.1
2	D	96	ASP	2.1
1	C	436	ILE	2.1
1	A	821	GLN	2.1
2	D	268	PRO	2.1
1	A	358	SER	2.1
1	A	79	VAL	2.1
1	A	932	VAL	2.1
1	C	24	ASP	2.1
1	C	323	ALA	2.1
2	D	231	VAL	2.1
2	D	450	ASN	2.1
1	C	329	TYR	2.1
1	C	487	ILE	2.1
2	D	318	TYR	2.1
1	A	460	LEU	2.1
1	C	345	LEU	2.1
1	C	433	PRO	2.1
1	A	259	THR	2.1
1	A	22	SER	2.1
1	C	807	SER	2.1
1	A	196	ALA	2.1
1	A	257	ALA	2.1
2	B	263	ALA	2.1
1	A	18	GLN	2.1
1	A	825	GLN	2.1
2	B	589	ILE	2.1
1	A	265	GLY	2.1
1	A	326	GLY	2.1
1	A	329	TYR	2.1
1	C	168	GLU	2.1
1	C	393	LEU	2.1
1	C	623	LEU	2.1
2	D	317	LEU	2.1
1	C	22	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	621	SER	2.1
1	C	751	ARG	2.0
1	A	193	GLY	2.0
2	B	154	GLY	2.0
2	B	265	ILE	2.0
1	A	166	TYR	2.0
1	A	356	PHE	2.0
1	A	612	LEU	2.0
2	D	604	CYS	2.0
1	C	111	GLN	2.0
2	D	133	ASN	2.0
2	B	125	LYS	2.0
1	A	742	VAL	2.0
2	D	340	VAL	2.0
2	B	325	ILE	2.0
2	D	265	ILE	2.0
2	D	290	PRO	2.0
2	B	609	THR	2.0
2	D	397	PHE	2.0
1	A	56	CYS	2.0
1	A	130	CYS	2.0
2	B	89	ALA	2.0
1	C	6	VAL	2.0
1	C	625	VAL	2.0
1	C	717	VAL	2.0
2	B	359	VAL	2.0
2	D	34	GLY	2.0
1	A	327	ARG	2.0
1	A	577	GLU	2.0
1	C	542	SER	2.0
2	D	92	LEU	2.0
1	A	313	TYR	2.0
1	C	125	THR	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
9	NAG	B	3371	14/15	0.94	0.28	1.50	51,54,57,62	0
7	NAG	D	3371	14/15	0.94	0.31	1.34	55,56,59,60	0
8	NAG	B	3320	14/15	0.85	0.20	-0.99	61,65,69,74	0
7	NAG	D	3320	14/15	0.92	0.12	-3.81	55,57,60,63	0
7	NAG	D	3560	14/15	0.84	0.29	-	75,76,78,78	0
10	NAG	B	3559	14/15	0.87	0.24	-	68,69,72,75	0
7	NAG	C	3250	14/15	0.87	0.34	-	66,69,69,69	0
7	NAG	B	3100	14/15	0.87	0.48	-	77,78,78,79	0
7	NAG	B	3099	14/15	0.84	0.43	-	71,73,75,76	0
10	MAN	B	3562	11/12	0.72	0.31	-	94,94,95,95	0
9	MAN	B	3373	11/12	0.70	0.53	-	73,74,75,75	0
10	MAN	B	3561	11/12	0.53	0.27	-	87,88,90,92	0
7	NAG	D	3559	14/15	0.89	0.29	-	69,72,74,75	0
9	NAG	B	3372	14/15	0.82	0.34	-	66,69,70,72	0
8	MAN	B	3323	11/12	0.79	0.35	-	92,93,94,94	0
10	NAG	B	3560	14/15	0.77	0.32	-	79,80,83,85	0
8	MAN	B	3322	11/12	0.56	0.31	-	89,90,91,92	0
7	NAG	D	3452	14/15	0.84	0.39	-	83,86,87,89	0
7	NAG	D	3321	14/15	0.94	0.14	-	66,69,69,69	0
7	NAG	C	3249	14/15	0.89	0.26	-	51,56,58,62	0
8	NAG	B	3321	14/15	0.80	0.27	-	77,79,83,86	0
7	NAG	D	3372	14/15	0.83	0.38	-	61,62,63,64	0
7	NAG	D	3453	14/15	0.73	0.42	-	90,91,92,92	0
7	NAG	B	3453	14/15	0.66	0.41	-	88,89,90,90	0
10	MAN	B	3563	11/12	0.59	0.36	-	94,95,96,96	0
7	NAG	B	3452	14/15	0.88	0.35	-	81,82,84,86	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, 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	NAG	C	3570	14/15	0.84	0.37	6.88	45,48,49,50	0
4	NAG	A	3570	14/15	0.85	0.26	3.00	35,38,39,39	14
3	CA	D	2003	1/1	0.98	0.23	-0.34	26,26,26,26	0
3	CA	A	2007	1/1	0.91	0.16	-0.45	20,20,20,20	0
3	CA	C	2007	1/1	0.95	0.17	-0.75	23,23,23,23	0
3	CA	C	2006	1/1	0.89	0.17	-1.05	29,29,29,29	0
5	IMD	C	5001	5/5	0.92	0.19	-1.47	52,52,52,52	0
3	CA	C	2004	1/1	0.96	0.13	-1.86	29,29,29,29	0
3	CA	C	2005	1/1	0.89	0.16	-1.88	41,41,41,41	0
3	CA	B	2003	1/1	0.94	0.15	-2.05	37,37,37,37	0
3	CA	A	2004	1/1	0.89	0.09	-2.10	25,25,25,25	0
3	CA	A	2008	1/1	0.98	0.06	-2.21	23,23,23,23	0
3	CA	D	2002	1/1	0.92	0.10	-2.32	42,42,42,42	0
5	IMD	C	5002	5/5	0.97	0.13	-2.33	21,21,21,22	0
3	CA	C	2008	1/1	0.93	0.08	-2.33	14,14,14,14	0
5	IMD	C	960	5/5	0.97	0.18	-2.47	33,33,34,34	0
5	IMD	C	5003	5/5	0.95	0.16	-2.64	28,29,29,29	0
3	CA	B	2002	1/1	0.85	0.11	-2.74	34,34,34,34	0
3	CA	A	2005	1/1	0.94	0.11	-2.82	17,17,17,17	0
6	MG	B	2001	1/1	0.88	0.10	-2.95	23,23,23,23	0
3	CA	A	2006	1/1	0.88	0.10	-2.96	29,29,29,29	0
5	IMD	A	5001	5/5	0.96	0.08	-3.03	37,37,37,38	0
6	MG	D	2001	1/1	0.85	0.07	-3.93	23,23,23,23	0
4	NAG	A	3015	14/15	0.87	0.26	-	52,55,57,58	0
4	NAG	D	3099	14/15	0.71	0.43	-	71,73,74,74	0
4	NAG	C	3015	14/15	0.88	0.26	-	51,55,55,56	0
5	IMD	C	5004	5/5	0.97	0.26	-	47,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.