



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:56 PM GMT

PDB ID : 1MQ8  
Title : Crystal structure of alphaL I domain in complex with ICAM-1  
Authors : Shimaoka, M.; Xiao, T.; Liu, J.-H.; Yang, Y.; Dong, Y.; Jun, C.-D.; McCormack, A.; Zhang, R.; Joachimiak, A.; Takagi, J.; Wang, J.-H.; Springer, T.A.  
Deposited on : 2002-09-15  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

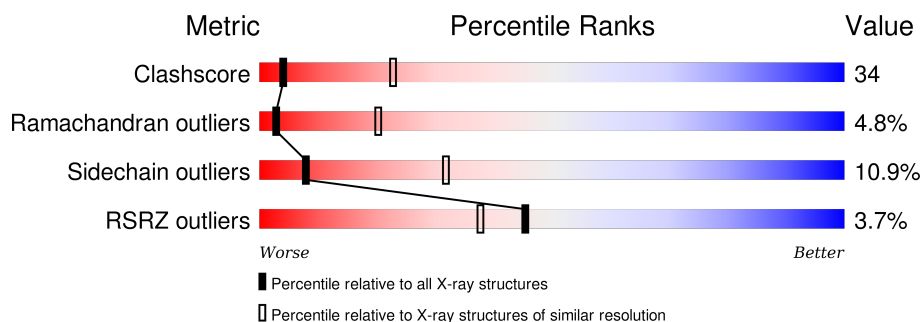
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	291	
1	C	291	
2	B	177	
2	D	177	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	410	-	-	-	X
4	NAG	A	402	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5854 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 intercellular adhesion molecule-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1421	889	250	275	7			
1	C	184	Total	C	N	O	S	0	0	0
			1421	889	250	275	7			

- Molecule 2 is a protein called Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1419	914	228	271	6			
2	D	177	Total	C	N	O	S	0	0	0
			1419	914	228	271	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	161	CYS	LEU	ENGINEERED	UNP P20701
B	299	CYS	PHE	ENGINEERED	UNP P20701
D	161	CYS	LEU	ENGINEERED	UNP P20701
D	299	CYS	PHE	ENGINEERED	UNP P20701

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		

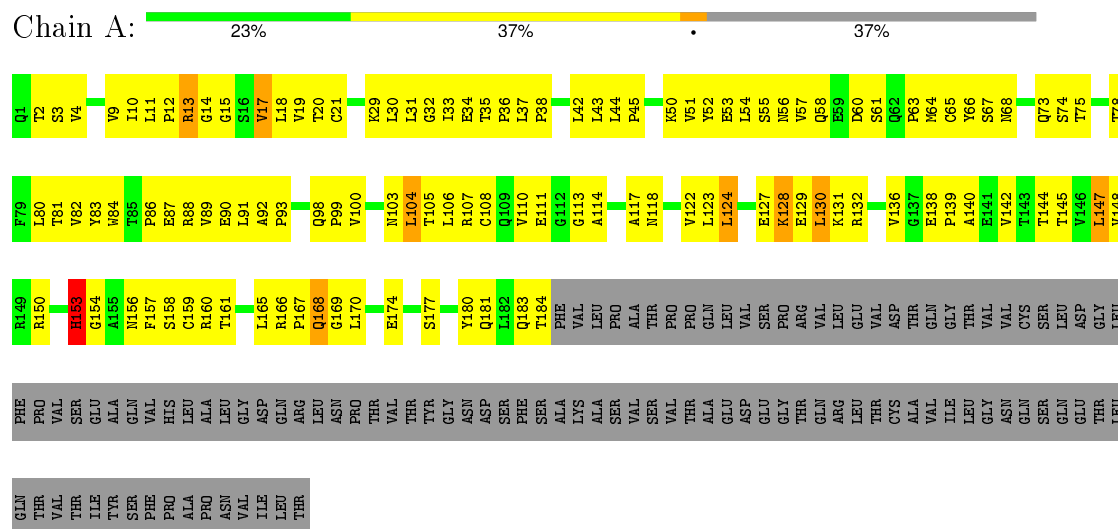
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	O	0	0
			2	2		
6	D	2	Total	O	0	0
			2	2		

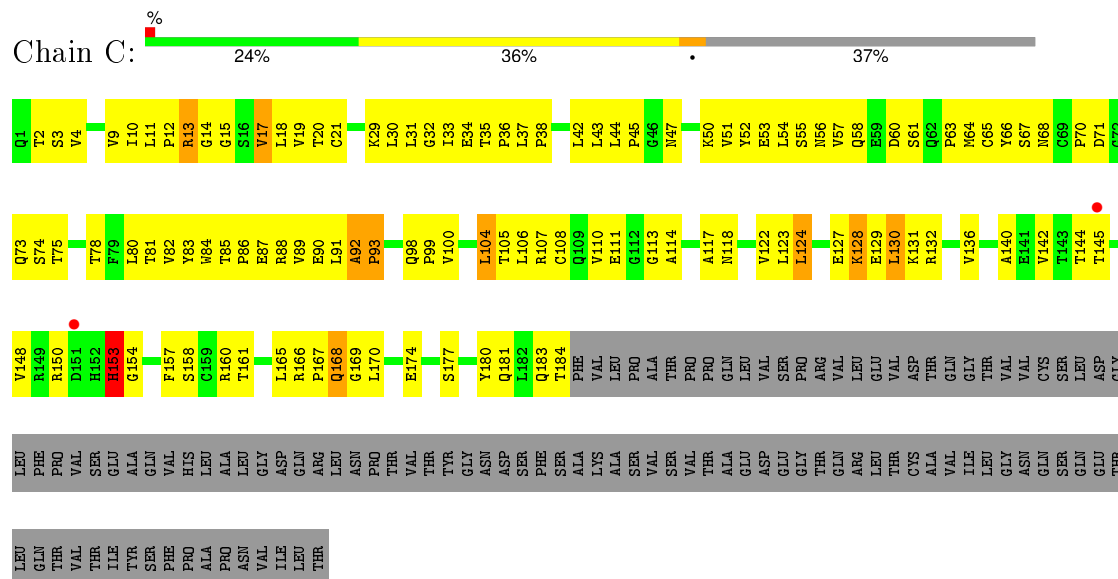
### 3 Residue-property plots

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.

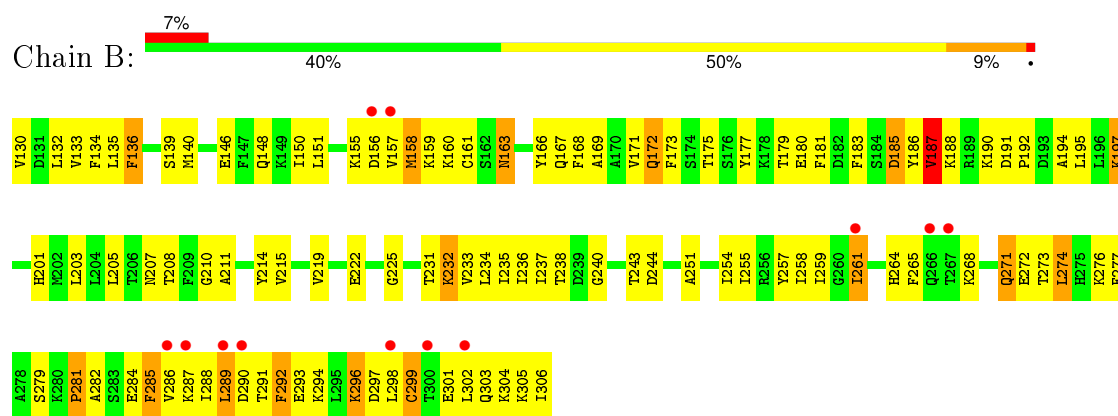
#### • Molecule 1: intercellular adhesion molecule-1



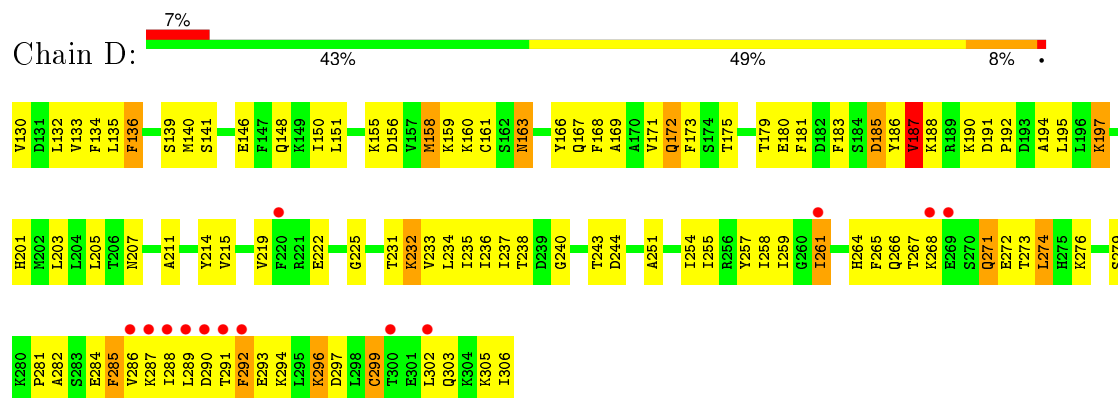
#### • Molecule 1: intercellular adhesion molecule-1



#### • Molecule 2: Integrin alpha-L



• Molecule 2: Integrin alpha-L





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.56 Å 62.87 Å 81.52 Å 95.39° 106.67° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 34.56 – 3.28	Depositor EDS
% Data completeness (in resolution range)	86.4 (50.00-3.30) 84.1 (34.56-3.28)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.20 (at 3.25 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.264 , 0.313 0.255 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 73.3	EDS
Estimated twinning fraction	0.418 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 12338 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	5854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: MG, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	0/1450	0.79	0/1977
1	C	0.53	0/1450	0.80	1/1977 (0.1%)
2	B	0.46	0/1445	0.70	0/1943
2	D	0.45	0/1445	0.69	0/1943
All	All	0.49	0/5790	0.74	1/7840 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ALA	C-N-CD	-7.28	104.59	120.60

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	1421	0	1426	86	0
1	C	1421	0	1426	87	0
2	B	1419	0	1425	117	0
2	D	1419	0	1425	106	0
3	A	28	0	26	1	0
3	C	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	56	0	50	8	0
4	C	56	0	50	7	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
All	All	5854	0	5854	398	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 34.

All (398) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LEU:HB3	2:B:302:LEU:HG	1.42	0.99
4:A:402:NAG:H61	4:A:403:NAG:O5	1.63	0.97
1:C:2:THR:HG22	1:C:3:SER:H	1.33	0.94
1:A:2:THR:HG22	1:A:3:SER:H	1.34	0.92
1:A:42:LEU:HD13	1:C:42:LEU:HD13	1.49	0.91
1:C:92:ALA:HB1	1:C:93:PRO:HB3	1.56	0.88
4:C:408:NAG:H61	4:C:409:NAG:O5	1.74	0.87
2:D:133:VAL:HG22	2:D:169:ALA:HB3	1.58	0.86
2:B:130:VAL:HG22	2:B:231:THR:HB	1.58	0.86
2:B:133:VAL:HG22	2:B:169:ALA:HB3	1.58	0.86
2:D:130:VAL:HG22	2:D:231:THR:HB	1.58	0.86
1:A:110:VAL:HG22	1:A:140:ALA:HB3	1.59	0.85
1:C:110:VAL:HG22	1:C:140:ALA:HB3	1.60	0.84
2:D:150:ILE:HA	2:D:292:PHE:CZ	2.15	0.82
2:B:271:GLN:HE21	2:B:271:GLN:HA	1.44	0.82
2:D:271:GLN:HA	2:D:271:GLN:HE21	1.44	0.82
1:C:11:LEU:O	1:C:82:VAL:HA	1.79	0.81
2:B:163:ASN:ND2	2:B:163:ASN:H	1.78	0.80
2:D:163:ASN:H	2:D:163:ASN:ND2	1.78	0.80
2:B:150:ILE:HA	2:B:292:PHE:CZ	2.18	0.79
1:A:11:LEU:O	1:A:82:VAL:HA	1.82	0.79
1:A:167:PRO:HG2	1:A:168:GLN:OE1	1.83	0.78
1:C:167:PRO:HG2	1:C:168:GLN:OE1	1.83	0.78
1:C:87:GLU:HB2	1:C:111:GLU:HG3	1.67	0.77
1:A:105:THR:HG22	1:A:145:THR:HG22	1.67	0.77
1:C:105:THR:HG22	1:C:145:THR:HG22	1.67	0.77
2:D:150:ILE:HA	2:D:292:PHE:HZ	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:PHE:HZ	2:B:180:GLU:HG3	1.51	0.76
2:D:136:PHE:HZ	2:D:180:GLU:HG3	1.51	0.76
1:A:68:ASN:HD21	2:B:244:ASP:HA	1.51	0.76
1:C:68:ASN:HD21	2:D:244:ASP:HA	1.51	0.76
4:C:408:NAG:O3	4:C:409:NAG:H83	1.87	0.74
1:C:68:ASN:ND2	2:D:244:ASP:HA	2.02	0.74
2:D:240:GLY:HA3	2:D:274:LEU:HD23	1.67	0.74
2:B:240:GLY:HA3	2:B:274:LEU:HD23	1.69	0.73
1:A:68:ASN:ND2	2:B:244:ASP:HA	2.04	0.73
2:B:150:ILE:HA	2:B:292:PHE:HZ	1.55	0.71
2:B:298:LEU:HB3	2:B:302:LEU:CG	2.17	0.71
4:A:402:NAG:C6	4:A:403:NAG:O5	2.37	0.71
1:A:87:GLU:HB2	1:A:111:GLU:HG3	1.74	0.70
1:C:67:SER:O	1:C:73:GLN:HA	1.92	0.70
1:A:67:SER:O	1:A:73:GLN:HA	1.92	0.70
2:B:136:PHE:CZ	2:B:180:GLU:HG3	2.27	0.70
2:D:136:PHE:CZ	2:D:180:GLU:HG3	2.27	0.69
2:D:237:ILE:HG12	2:D:259:ILE:HD11	1.73	0.69
2:B:237:ILE:HG12	2:B:259:ILE:HD11	1.73	0.69
2:B:303:GLN:HA	2:B:306:ILE:HG12	1.73	0.69
2:B:161:CYS:HA	2:B:163:ASN:HD21	1.58	0.69
2:D:161:CYS:HA	2:D:163:ASN:HD21	1.58	0.69
2:B:298:LEU:HD13	2:B:302:LEU:HD21	1.75	0.68
2:D:159:LYS:HD3	2:D:192:PRO:HD2	1.76	0.68
2:B:237:ILE:HG23	2:B:259:ILE:HG13	1.76	0.68
2:B:159:LYS:HD3	2:B:192:PRO:HD2	1.76	0.68
1:C:2:THR:HG22	1:C:3:SER:N	2.08	0.68
1:C:35:THR:HG22	1:C:63:PRO:HA	1.76	0.67
1:A:37:LEU:HD11	1:A:61:SER:OG	1.94	0.67
1:A:2:THR:HG22	1:A:3:SER:N	2.09	0.67
2:D:237:ILE:HG23	2:D:259:ILE:HG13	1.77	0.67
2:B:279:SER:H	2:B:285:PHE:HE1	1.42	0.67
1:C:37:LEU:HD11	1:C:61:SER:OG	1.95	0.67
2:D:235:ILE:HD13	2:D:257:TYR:HB3	1.75	0.66
2:D:136:PHE:HD1	2:D:136:PHE:H	1.41	0.66
2:B:136:PHE:H	2:B:136:PHE:HD1	1.42	0.66
2:B:235:ILE:HD13	2:B:257:TYR:HB3	1.75	0.66
1:A:35:THR:HG22	1:A:63:PRO:HA	1.77	0.66
4:A:402:NAG:O3	4:A:403:NAG:H83	1.96	0.66
4:C:408:NAG:C6	4:C:409:NAG:O5	2.44	0.66
2:B:185:ASP:HA	2:B:188:LYS:HZ2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:236:ILE:O	2:D:258:ILE:HA	1.97	0.65
2:B:236:ILE:O	2:B:258:ILE:HA	1.97	0.65
1:A:31:LEU:HG	1:A:50:LYS:HE2	1.78	0.65
2:D:185:ASP:HA	2:D:188:LYS:HZ2	1.61	0.65
2:B:261:ILE:HD12	2:B:290:ASP:O	1.97	0.64
2:B:271:GLN:NE2	2:B:271:GLN:HA	2.11	0.64
2:D:271:GLN:HA	2:D:271:GLN:NE2	2.11	0.64
2:B:268:LYS:O	2:B:272:GLU:HG3	1.98	0.64
1:C:118:ASN:HA	4:C:408:NAG:O7	1.98	0.63
1:C:89:VAL:HG13	1:C:177:SER:HB3	1.80	0.63
1:C:157:PHE:HB2	1:C:180:TYR:HB3	1.81	0.63
2:B:197:LYS:HD3	2:B:197:LYS:H	1.62	0.63
2:D:197:LYS:H	2:D:197:LYS:HD3	1.62	0.63
1:A:157:PHE:HB2	1:A:180:TYR:HB3	1.81	0.63
2:D:303:GLN:HA	2:D:306:ILE:HG12	1.80	0.62
1:C:31:LEU:HG	1:C:50:LYS:HE2	1.81	0.62
1:A:103:ASN:HA	1:A:147:LEU:CD1	2.29	0.62
2:B:299:CYS:O	2:B:303:GLN:HG2	2.00	0.62
1:C:122:VAL:HA	1:C:131:LYS:O	2.00	0.61
2:D:261:ILE:HD12	2:D:290:ASP:O	2.00	0.61
2:B:157:VAL:HG11	2:B:302:LEU:HD12	1.83	0.61
2:D:136:PHE:CZ	2:D:172:GLN:HB2	2.36	0.61
2:D:268:LYS:O	2:D:272:GLU:HG3	2.01	0.61
2:B:251:ALA:HB1	2:B:254:ILE:HD12	1.83	0.60
2:B:136:PHE:CZ	2:B:172:GLN:HB2	2.36	0.60
1:A:122:VAL:HA	1:A:131:LYS:O	2.01	0.60
1:C:100:VAL:HA	1:C:148:VAL:HB	1.83	0.60
1:A:91:LEU:HD23	1:A:91:LEU:H	1.67	0.60
2:D:299:CYS:O	2:D:303:GLN:HG2	2.01	0.60
1:C:91:LEU:HB2	1:C:107:ARG:O	2.01	0.60
1:A:20:THR:HG22	1:A:51:VAL:HG22	1.83	0.60
2:D:251:ALA:HB1	2:D:254:ILE:HD12	1.84	0.59
2:D:288:ILE:O	2:D:288:ILE:HG22	2.01	0.59
2:D:185:ASP:HA	2:D:188:LYS:NZ	2.18	0.59
1:C:166:ARG:N	1:C:167:PRO:HD2	2.18	0.59
1:A:37:LEU:HD22	1:A:54:LEU:HB3	1.85	0.59
1:A:100:VAL:HA	1:A:148:VAL:HB	1.84	0.59
2:B:185:ASP:HA	2:B:188:LYS:NZ	2.18	0.59
2:B:215:VAL:O	2:B:219:VAL:HB	2.03	0.59
2:B:136:PHE:HB3	2:B:237:ILE:HD12	1.83	0.58
1:C:92:ALA:HB1	1:C:93:PRO:CB	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:PHE:HB3	2:D:237:ILE:HD12	1.83	0.58
2:D:215:VAL:O	2:D:219:VAL:HB	2.03	0.58
2:B:291:THR:HG22	2:B:293:GLU:HB3	1.84	0.58
1:A:124:LEU:HA	1:A:130:LEU:HB2	1.85	0.58
2:D:279:SER:H	2:D:285:PHE:HE1	1.50	0.58
1:C:124:LEU:HA	1:C:130:LEU:HB2	1.85	0.58
1:A:166:ARG:N	1:A:167:PRO:HD2	2.19	0.58
1:C:37:LEU:HD22	1:C:54:LEU:HB3	1.86	0.57
2:D:271:GLN:CA	2:D:271:GLN:HE21	2.11	0.57
2:D:291:THR:HG22	2:D:293:GLU:HB3	1.87	0.57
2:B:132:LEU:HB3	2:B:168:PHE:CD1	2.39	0.57
2:B:279:SER:N	2:B:285:PHE:CE1	2.72	0.57
1:A:13:ARG:HG3	1:A:58:GLN:HA	1.87	0.57
2:D:132:LEU:HB3	2:D:168:PHE:CD1	2.39	0.57
2:B:303:GLN:HA	2:B:306:ILE:CG1	2.35	0.57
1:C:13:ARG:HG3	1:C:58:GLN:HA	1.87	0.56
1:A:91:LEU:HB2	1:A:107:ARG:O	2.05	0.56
1:C:84:TRP:O	1:C:113:GLY:HA2	2.06	0.56
1:C:20:THR:HG22	1:C:51:VAL:HG22	1.87	0.56
1:C:183:GLN:O	1:C:184:THR:HB	2.04	0.56
1:A:84:TRP:O	1:A:113:GLY:HA2	2.06	0.56
2:B:132:LEU:O	2:B:168:PHE:HA	2.06	0.56
2:B:271:GLN:HE21	2:B:271:GLN:CA	2.12	0.56
2:D:132:LEU:O	2:D:168:PHE:HA	2.06	0.56
1:A:183:GLN:O	1:A:184:THR:HB	2.04	0.56
2:B:279:SER:N	2:B:285:PHE:HE1	2.04	0.56
1:A:2:THR:CG2	1:A:3:SER:H	2.15	0.56
2:D:132:LEU:HB3	2:D:168:PHE:HD1	1.71	0.56
2:B:132:LEU:HB3	2:B:168:PHE:HD1	1.71	0.55
1:C:124:LEU:HB2	1:C:128:LYS:O	2.06	0.55
2:B:298:LEU:CB	2:B:302:LEU:HG	2.26	0.55
2:B:288:ILE:O	2:B:290:ASP:N	2.39	0.55
2:B:156:ASP:O	2:B:160:LYS:HD2	2.05	0.55
1:A:103:ASN:HA	1:A:147:LEU:HD12	1.88	0.55
1:A:124:LEU:HD23	1:A:158:SER:O	2.07	0.55
2:B:276:LYS:HB3	2:B:276:LYS:NZ	2.22	0.55
2:D:156:ASP:O	2:D:160:LYS:HD2	2.05	0.55
1:A:36:PRO:HG3	2:B:140:MET:O	2.06	0.55
2:D:303:GLN:HA	2:D:306:ILE:CG1	2.37	0.55
1:C:124:LEU:HD23	1:C:158:SER:O	2.07	0.55
1:A:124:LEU:HB2	1:A:128:LYS:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LEU:HD11	1:C:61:SER:CB	2.38	0.54
1:C:33:ILE:HG22	1:C:52:TYR:CE1	2.42	0.54
2:B:132:LEU:HD23	2:B:133:VAL:N	2.22	0.54
2:D:132:LEU:HD23	2:D:133:VAL:N	2.22	0.54
1:A:33:ILE:HG22	1:A:52:TYR:CE1	2.42	0.54
2:B:264:HIS:O	2:B:271:GLN:HG3	2.08	0.54
1:C:117:ALA:C	1:C:118:ASN:HD22	2.11	0.54
1:A:37:LEU:HD11	1:A:61:SER:CB	2.38	0.54
1:C:91:LEU:HD23	1:C:91:LEU:H	1.73	0.54
2:B:232:LYS:HG3	2:B:254:ILE:HG12	1.88	0.53
1:A:18:LEU:HD23	1:C:18:LEU:HD23	1.89	0.53
2:D:232:LYS:HG3	2:D:254:ILE:HG12	1.89	0.53
1:C:21:CYS:HB3	1:C:31:LEU:HD11	1.91	0.52
2:D:133:VAL:HG11	2:D:215:VAL:HG13	1.91	0.52
1:C:85:THR:HG21	4:C:411:NAG:H5	1.90	0.52
2:D:235:ILE:HD13	2:D:257:TYR:CB	2.40	0.52
2:D:163:ASN:N	2:D:163:ASN:ND2	2.53	0.52
1:A:21:CYS:HB3	1:A:31:LEU:HD11	1.91	0.52
1:A:106:LEU:HD11	1:A:157:PHE:CD1	2.44	0.52
2:B:235:ILE:HD13	2:B:257:TYR:CB	2.40	0.52
2:B:133:VAL:HG11	2:B:215:VAL:HG13	1.91	0.52
1:C:106:LEU:HD11	1:C:157:PHE:CD1	2.45	0.52
2:B:284:GLU:HA	2:B:287:LYS:HE3	1.92	0.52
1:C:88:ARG:HH21	1:C:90:GLU:HB3	1.75	0.52
2:B:163:ASN:ND2	2:B:163:ASN:N	2.53	0.51
2:D:134:PHE:HD1	2:D:235:ILE:HB	1.76	0.51
2:D:136:PHE:HA	2:D:237:ILE:HB	1.93	0.51
1:C:63:PRO:HD2	1:C:78:THR:HG23	1.93	0.51
2:D:135:LEU:HD23	2:D:236:ILE:HG12	1.93	0.51
2:B:175:THR:HA	2:B:207:ASN:ND2	2.26	0.51
2:B:298:LEU:HB3	2:B:302:LEU:CD1	2.40	0.51
2:B:298:LEU:HD13	2:B:302:LEU:HD11	1.92	0.51
1:A:118:ASN:HA	4:A:402:NAG:O7	2.10	0.51
2:B:134:PHE:HD1	2:B:235:ILE:HB	1.76	0.51
1:A:11:LEU:HB2	1:A:12:PRO:HD2	1.92	0.51
2:B:136:PHE:HA	2:B:237:ILE:HB	1.93	0.51
1:C:38:PRO:HD2	1:C:55:SER:O	2.12	0.50
1:C:43:LEU:HB3	1:C:45:PRO:HD2	1.92	0.50
2:B:135:LEU:HD23	2:B:236:ILE:HG12	1.93	0.50
2:D:179:THR:HG23	2:D:214:TYR:HE1	1.76	0.50
2:B:291:THR:HB	2:B:294:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:THR:HG23	2:B:214:TYR:HE1	1.76	0.50
1:C:36:PRO:HG3	2:D:140:MET:O	2.11	0.50
2:B:167:GLN:HA	2:B:186:TYR:HE1	1.75	0.50
2:D:264:HIS:O	2:D:271:GLN:HG3	2.12	0.50
1:A:63:PRO:HD2	1:A:78:THR:HG23	1.94	0.50
2:D:289:LEU:C	2:D:291:THR:H	2.13	0.50
2:D:175:THR:HA	2:D:207:ASN:ND2	2.27	0.50
2:B:296:LYS:HG3	2:B:297:ASP:N	2.27	0.50
1:A:117:ALA:C	1:A:118:ASN:HD22	2.16	0.49
2:D:167:GLN:HA	2:D:186:TYR:HE1	1.75	0.49
2:D:284:GLU:HA	2:D:287:LYS:HE3	1.95	0.49
1:A:14:GLY:HA2	1:A:56:ASN:HA	1.94	0.49
1:C:108:CYS:HB2	1:C:123:LEU:HD21	1.95	0.49
1:A:38:PRO:HD2	1:A:55:SER:O	2.13	0.49
2:D:291:THR:HB	2:D:294:LYS:HE3	1.95	0.49
1:A:108:CYS:HB2	1:A:123:LEU:HD21	1.95	0.49
1:C:11:LEU:HB2	1:C:12:PRO:HD2	1.94	0.48
2:D:195:LEU:HA	2:D:197:LYS:NZ	2.28	0.48
2:B:289:LEU:C	2:B:291:THR:H	2.14	0.48
1:C:63:PRO:HB2	1:C:78:THR:CG2	2.44	0.48
1:A:4:VAL:CG2	1:A:65:CYS:SG	3.01	0.48
1:A:89:VAL:HG13	1:A:177:SER:HB3	1.95	0.48
1:A:63:PRO:HB2	1:A:78:THR:CG2	2.44	0.48
2:D:188:LYS:NZ	2:D:188:LYS:HB2	2.27	0.48
2:D:130:VAL:HG13	2:D:231:THR:O	2.13	0.48
2:D:167:GLN:HB3	2:D:183:PHE:CE1	2.48	0.48
1:C:14:GLY:HA2	1:C:56:ASN:HA	1.95	0.48
2:B:167:GLN:HB3	2:B:183:PHE:CE1	2.48	0.48
2:B:195:LEU:HA	2:B:197:LYS:NZ	2.29	0.48
2:D:183:PHE:O	2:D:186:TYR:HB3	2.14	0.48
2:B:183:PHE:O	2:B:186:TYR:HB3	2.14	0.48
1:A:43:LEU:HB3	1:A:45:PRO:HD2	1.95	0.48
1:C:4:VAL:CG2	1:C:65:CYS:SG	3.02	0.48
2:B:130:VAL:HG13	2:B:231:THR:O	2.13	0.48
2:D:297:ASP:OD2	2:D:299:CYS:HB2	2.14	0.48
2:D:205:LEU:HB3	2:D:243:THR:HG21	1.95	0.48
2:B:157:VAL:HG11	2:B:302:LEU:CD1	2.44	0.48
2:D:279:SER:N	2:D:285:PHE:CE1	2.78	0.48
2:B:205:LEU:HB3	2:B:243:THR:HG21	1.96	0.48
2:B:232:LYS:O	2:B:254:ILE:HG23	2.13	0.47
2:D:234:LEU:HB2	2:D:254:ILE:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:LYS:NZ	2:B:188:LYS:HB2	2.28	0.47
1:A:159:CYS:H	1:A:177:SER:HG	1.63	0.47
1:C:44:LEU:N	1:C:45:PRO:CD	2.78	0.47
2:B:234:LEU:HB2	2:B:254:ILE:CG2	2.45	0.47
2:D:240:GLY:HA3	2:D:274:LEU:CD2	2.39	0.47
1:C:9:VAL:HG11	1:C:17:VAL:HG11	1.96	0.47
1:C:42:LEU:HD12	1:C:51:VAL:CG1	2.45	0.47
2:B:261:ILE:HA	2:B:290:ASP:O	2.14	0.47
1:A:90:GLU:HG2	1:A:91:LEU:N	2.30	0.47
1:C:10:ILE:HA	1:C:81:THR:HB	1.97	0.47
1:A:9:VAL:HG11	1:A:17:VAL:HG11	1.96	0.47
1:A:44:LEU:N	1:A:45:PRO:CD	2.78	0.47
4:A:402:NAG:H61	4:A:403:NAG:O6	2.14	0.46
1:A:106:LEU:HD11	1:A:157:PHE:HD1	1.81	0.46
2:B:186:TYR:CD1	2:B:187:VAL:HG22	2.50	0.46
2:D:296:LYS:HG3	2:D:297:ASP:N	2.31	0.46
1:C:122:VAL:HB	1:C:132:ARG:HG2	1.96	0.46
2:D:186:TYR:CD1	2:D:187:VAL:HG22	2.50	0.46
1:C:47:ASN:OD1	1:C:47:ASN:N	2.48	0.46
2:B:298:LEU:O	2:B:302:LEU:HB2	2.16	0.46
2:D:133:VAL:HG11	2:D:215:VAL:CG1	2.45	0.46
2:B:240:GLY:O	2:B:271:GLN:NE2	2.48	0.46
2:D:232:LYS:O	2:D:254:ILE:HG23	2.15	0.46
1:C:123:LEU:HD13	1:C:144:THR:HG22	1.97	0.46
1:A:83:TYR:HA	1:A:114:ALA:O	2.16	0.46
1:C:83:TYR:HA	1:C:114:ALA:O	2.16	0.46
2:D:148:GLN:HA	2:D:151:LEU:HG	1.98	0.46
1:A:122:VAL:HB	1:A:132:ARG:HG2	1.97	0.46
1:A:123:LEU:HD13	1:A:144:THR:HG22	1.97	0.46
1:C:2:THR:CG2	1:C:3:SER:H	2.15	0.46
2:B:233:VAL:HG22	2:B:255:ILE:HD12	1.98	0.46
2:D:233:VAL:HG22	2:D:255:ILE:HD12	1.98	0.46
1:C:110:VAL:HG22	1:C:140:ALA:CB	2.41	0.46
2:D:240:GLY:O	2:D:271:GLN:NE2	2.48	0.46
2:D:276:LYS:NZ	2:D:276:LYS:HB3	2.31	0.46
1:C:166:ARG:N	1:C:167:PRO:CD	2.80	0.45
2:D:302:LEU:O	2:D:302:LEU:HD23	2.15	0.45
2:D:292:PHE:N	2:D:292:PHE:CD1	2.83	0.45
2:B:298:LEU:HD22	2:B:302:LEU:HG	1.98	0.45
1:C:106:LEU:HD11	1:C:157:PHE:HD1	1.81	0.45
2:B:133:VAL:HG11	2:B:215:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:CG	1:A:161:THR:N	2.80	0.45
2:B:157:VAL:CG1	2:B:302:LEU:HD12	2.45	0.45
2:B:130:VAL:HG21	2:B:306:ILE:HD12	1.98	0.45
2:D:267:THR:O	2:D:271:GLN:HB2	2.17	0.45
1:A:153:HIS:ND1	1:A:153:HIS:N	2.65	0.45
2:D:130:VAL:HG22	2:D:231:THR:CB	2.39	0.45
1:A:17:VAL:O	1:A:53:GLU:HA	2.17	0.45
1:C:34:GLU:HB3	1:C:64:MET:HB3	1.99	0.45
2:B:130:VAL:HG22	2:B:231:THR:CB	2.39	0.45
2:B:148:GLN:HA	2:B:151:LEU:HG	1.99	0.45
1:C:160:ARG:CG	1:C:161:THR:N	2.80	0.45
2:D:150:ILE:HG12	2:D:292:PHE:CZ	2.52	0.45
2:D:264:HIS:O	2:D:266:GLN:N	2.48	0.45
1:A:34:GLU:HB3	1:A:64:MET:HB3	1.99	0.45
2:B:234:LEU:O	2:B:257:TYR:HB2	2.17	0.45
1:C:136:VAL:O	1:C:140:ALA:HA	2.17	0.45
2:B:240:GLY:HA3	2:B:274:LEU:CD2	2.41	0.45
2:B:155:LYS:HE2	2:B:192:PRO:O	2.16	0.45
2:D:288:ILE:O	2:D:288:ILE:CG2	2.65	0.45
1:C:153:HIS:ND1	1:C:153:HIS:N	2.65	0.45
2:D:234:LEU:O	2:D:257:TYR:HB2	2.17	0.44
2:D:155:LYS:HE2	2:D:192:PRO:O	2.16	0.44
1:C:10:ILE:HG12	1:C:81:THR:HB	1.99	0.44
1:A:166:ARG:N	1:A:167:PRO:CD	2.81	0.44
1:A:10:ILE:HG12	1:A:81:THR:HB	1.99	0.44
1:A:10:ILE:HA	1:A:81:THR:HB	1.99	0.44
1:A:136:VAL:O	1:A:140:ALA:HA	2.18	0.44
1:C:32:GLY:HA2	1:C:52:TYR:OH	2.18	0.44
1:A:32:GLY:HA2	1:A:52:TYR:OH	2.18	0.44
2:D:136:PHE:N	2:D:136:PHE:CD1	2.76	0.44
1:C:17:VAL:HG21	1:C:80:LEU:HD13	2.00	0.44
1:C:17:VAL:O	1:C:53:GLU:HA	2.18	0.44
2:D:130:VAL:HG21	2:D:306:ILE:HD12	1.99	0.44
1:A:167:PRO:O	1:C:167:PRO:O	2.36	0.44
2:B:136:PHE:CD1	2:B:136:PHE:N	2.77	0.44
2:B:140:MET:HB2	2:B:203:LEU:O	2.18	0.44
1:A:42:LEU:HD12	1:A:51:VAL:CG1	2.48	0.43
1:C:118:ASN:N	1:C:118:ASN:HD22	2.16	0.43
1:C:37:LEU:CD2	1:C:57:VAL:HB	2.48	0.43
1:C:165:LEU:HD13	1:C:170:LEU:HD12	1.98	0.43
2:B:167:GLN:HA	2:B:186:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:LEU:N	2:D:151:LEU:HD23	2.33	0.43
2:B:292:PHE:CD1	2:B:292:PHE:N	2.85	0.43
2:D:167:GLN:HA	2:D:186:TYR:CE1	2.53	0.43
2:D:172:GLN:HB3	2:D:172:GLN:HE21	1.53	0.43
1:A:50:LYS:HD2	1:A:52:TYR:OH	2.19	0.43
2:D:194:ALA:O	2:D:197:LYS:HD2	2.19	0.43
2:B:150:ILE:HG12	2:B:292:PHE:CZ	2.54	0.43
2:B:194:ALA:O	2:B:197:LYS:HD2	2.19	0.43
2:D:140:MET:HB2	2:D:203:LEU:O	2.19	0.43
1:A:165:LEU:HD13	1:A:170:LEU:HD12	1.98	0.43
1:A:42:LEU:HD23	1:C:43:LEU:HD12	2.01	0.43
1:C:157:PHE:O	1:C:180:TYR:N	2.52	0.43
1:A:104:LEU:O	1:A:104:LEU:HD23	2.19	0.43
1:A:66:TYR:CD1	1:A:66:TYR:C	2.92	0.43
1:C:50:LYS:HD2	1:C:52:TYR:OH	2.19	0.43
1:C:64:MET:HG2	1:C:75:THR:CG2	2.49	0.43
1:C:104:LEU:HD23	1:C:104:LEU:O	2.19	0.43
1:C:66:TYR:C	1:C:66:TYR:CD1	2.92	0.43
2:D:158:MET:HG3	2:D:168:PHE:CD2	2.54	0.42
2:D:279:SER:N	2:D:285:PHE:HE1	2.13	0.42
1:A:13:ARG:C	1:A:15:GLY:H	2.22	0.42
2:D:183:PHE:HA	2:D:186:TYR:HB3	2.00	0.42
2:B:273:THR:O	2:B:273:THR:HG22	2.19	0.42
2:B:158:MET:HG3	2:B:168:PHE:CD2	2.54	0.42
1:A:88:ARG:HH21	1:A:90:GLU:HB3	1.85	0.42
2:B:183:PHE:HA	2:B:186:TYR:HB3	2.00	0.42
1:A:4:VAL:HG21	1:A:65:CYS:SG	2.59	0.42
1:A:64:MET:HG2	1:A:75:THR:CG2	2.50	0.42
2:B:208:THR:HG21	2:B:277:PHE:CE1	2.55	0.42
1:A:89:VAL:HG22	1:A:89:VAL:O	2.19	0.42
2:B:301:GLU:O	2:B:304:LYS:HE3	2.20	0.42
2:D:132:LEU:HD21	2:D:235:ILE:HG13	2.01	0.42
1:C:13:ARG:C	1:C:15:GLY:H	2.22	0.42
1:A:17:VAL:HG21	1:A:80:LEU:HD13	2.01	0.42
2:B:172:GLN:HE21	2:B:172:GLN:HB3	1.53	0.42
2:B:274:LEU:HD12	2:B:286:VAL:HG22	2.02	0.42
1:A:98:GLN:HA	1:A:99:PRO:HD3	1.81	0.42
2:D:274:LEU:HD12	2:D:286:VAL:HG22	2.02	0.42
2:B:155:LYS:HG2	2:B:192:PRO:HB2	2.00	0.42
1:A:157:PHE:O	1:A:180:TYR:N	2.53	0.42
4:A:402:NAG:O4	4:A:403:NAG:C8	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:LYS:HG2	2:D:192:PRO:HB2	2.00	0.42
2:D:135:LEU:HD23	2:D:236:ILE:HG23	2.01	0.42
2:B:151:LEU:N	2:B:151:LEU:HD23	2.35	0.42
1:A:37:LEU:CD2	1:A:57:VAL:HB	2.50	0.42
1:C:88:ARG:NH2	1:C:90:GLU:HB3	2.33	0.42
2:B:132:LEU:HD21	2:B:235:ILE:HG13	2.02	0.41
2:B:305:LYS:C	2:B:306:ILE:HD13	2.40	0.41
1:C:91:LEU:HA	1:C:108:CYS:HA	2.02	0.41
2:D:273:THR:HG22	2:D:273:THR:O	2.20	0.41
4:A:402:NAG:H61	4:A:403:NAG:C6	2.50	0.41
2:D:288:ILE:O	2:D:290:ASP:N	2.50	0.41
1:A:92:ALA:HA	1:A:93:PRO:HD2	1.82	0.41
2:B:158:MET:HE1	2:B:181:PHE:HZ	1.85	0.41
2:D:135:LEU:HD11	2:D:211:ALA:HB1	2.02	0.41
1:C:4:VAL:HG21	1:C:65:CYS:SG	2.60	0.41
2:D:235:ILE:HG22	2:D:235:ILE:O	2.20	0.41
1:C:37:LEU:HD23	1:C:57:VAL:HB	2.03	0.41
2:B:135:LEU:HD11	2:B:211:ALA:HB1	2.02	0.41
2:B:288:ILE:O	2:B:288:ILE:HG22	2.20	0.41
2:D:284:GLU:HG2	2:D:287:LYS:HE3	2.03	0.41
4:C:409:NAG:H2	4:C:409:NAG:H82	1.91	0.41
2:D:158:MET:HE1	2:D:181:PHE:HZ	1.86	0.41
2:B:173:PHE:HZ	2:B:238:THR:HB	1.85	0.41
2:D:173:PHE:HZ	2:D:238:THR:HB	1.85	0.41
1:A:156:ASN:ND2	3:A:404:NAG:H83	2.36	0.41
2:B:235:ILE:O	2:B:235:ILE:HG22	2.21	0.41
2:B:139:SER:CB	2:B:205:LEU:O	2.69	0.41
1:C:161:THR:O	1:C:174:GLU:HA	2.21	0.41
1:A:138:GLU:HA	1:A:139:PRO:HA	1.95	0.41
1:C:70:PRO:HG2	1:C:71:ASP:H	1.85	0.41
2:B:251:ALA:HB1	2:B:254:ILE:CD1	2.51	0.40
2:B:163:ASN:HD22	2:B:163:ASN:H	1.64	0.40
4:C:408:NAG:H61	4:C:409:NAG:O6	2.20	0.40
2:B:130:VAL:HG13	2:B:233:VAL:HG23	2.04	0.40
2:D:163:ASN:H	2:D:163:ASN:HD22	1.63	0.40
1:A:44:LEU:HB3	1:A:45:PRO:HD3	2.03	0.40
2:B:177:TYR:OH	2:B:210:GLY:HA3	2.21	0.40
1:A:161:THR:O	1:A:174:GLU:HA	2.21	0.40
1:C:98:GLN:HA	1:C:99:PRO:HD3	1.81	0.40
2:D:130:VAL:HG13	2:D:233:VAL:HG23	2.04	0.40
2:B:135:LEU:HD23	2:B:236:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:SER:CB	2:D:205:LEU:O	2.70	0.40
4:A:406:NAG:O3	4:A:406:NAG:C7	2.69	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	182/291 (62%)	157 (86%)	19 (10%)	6 (3%)	5	30
1	C	182/291 (62%)	155 (85%)	20 (11%)	7 (4%)	4	26
2	B	175/177 (99%)	128 (73%)	37 (21%)	10 (6%)	2	16
2	D	175/177 (99%)	127 (73%)	37 (21%)	11 (6%)	2	13
All	All	714/936 (76%)	567 (79%)	113 (16%)	34 (5%)	3	20

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	289	LEU
1	C	93	PRO
1	A	127	GLU
1	A	154	GLY
2	B	261	ILE
2	B	282	ALA
1	C	127	GLU
1	C	154	GLY
2	D	261	ILE
2	D	265	PHE
2	D	282	ALA
1	A	60	ASP
2	B	190	LYS

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Mol	Chain	Res	Type
1	C	60	ASP
2	D	190	LYS
2	B	225	GLY
2	D	141	SER
2	D	225	GLY
2	D	305	LYS
2	B	146	GLU
1	C	86	PRO
2	D	146	GLU
1	A	153	HIS
2	B	158	MET
2	B	281	PRO
1	C	153	HIS
2	D	158	MET
1	A	86	PRO
2	B	187	VAL
2	B	191	ASP
1	C	169	GLY
2	D	187	VAL
2	D	191	ASP
1	A	169	GLY

### 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	164/257 (64%)	147 (90%)	17 (10%)	9	34
1	C	164/257 (64%)	148 (90%)	16 (10%)	10	37
2	B	158/158 (100%)	139 (88%)	19 (12%)	6	27
2	D	158/158 (100%)	140 (89%)	18 (11%)	7	29
All	All	644/830 (78%)	574 (89%)	70 (11%)	8	32

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	17	VAL
1	A	19	VAL
1	A	29	LYS
1	A	30	LEU
1	A	74	SER
1	A	104	LEU
1	A	124	LEU
1	A	128	LYS
1	A	129	GLU
1	A	130	LEU
1	A	142	VAL
1	A	147	LEU
1	A	150	ARG
1	A	153	HIS
1	A	168	GLN
1	A	181	GLN
2	B	136	PHE
2	B	163	ASN
2	B	166	TYR
2	B	171	VAL
2	B	172	GLN
2	B	185	ASP
2	B	187	VAL
2	B	197	LYS
2	B	201	HIS
2	B	222	GLU
2	B	232	LYS
2	B	265	PHE
2	B	271	GLN
2	B	274	LEU
2	B	281	PRO
2	B	285	PHE
2	B	292	PHE
2	B	296	LYS
2	B	299	CYS
1	C	13	ARG
1	C	17	VAL
1	C	19	VAL
1	C	29	LYS
1	C	30	LEU
1	C	74	SER
1	C	104	LEU

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Mol	Chain	Res	Type
1	C	124	LEU
1	C	128	LYS
1	C	129	GLU
1	C	130	LEU
1	C	142	VAL
1	C	150	ARG
1	C	153	HIS
1	C	168	GLN
1	C	181	GLN
2	D	136	PHE
2	D	163	ASN
2	D	166	TYR
2	D	171	VAL
2	D	172	GLN
2	D	185	ASP
2	D	187	VAL
2	D	197	LYS
2	D	201	HIS
2	D	222	GLU
2	D	232	LYS
2	D	271	GLN
2	D	274	LEU
2	D	281	PRO
2	D	285	PHE
2	D	292	PHE
2	D	296	LYS
2	D	299	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
2	B	148	GLN
2	B	163	ASN
2	B	207	ASN
2	B	271	GLN
1	C	1	GLN
1	C	181	GLN
2	D	148	GLN
2	D	163	ASN
2	D	207	ASN
2	D	271	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 ⓘ

8 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	A	402	1,4	14,14,15	0.65	0	15,19,21	2.50	4 (26%)
4	NAG	A	403	4	14,14,15	0.55	0	15,19,21	0.69	0
4	NAG	A	405	1,4	14,14,15	0.55	0	15,19,21	0.84	0
4	NAG	A	406	4	14,14,15	0.76	1 (7%)	15,19,21	0.81	0
4	NAG	C	408	1,4	14,14,15	0.89	0	15,19,21	1.07	1 (6%)
4	NAG	C	409	4	14,14,15	0.51	0	15,19,21	0.73	0
4	NAG	C	411	1,4	14,14,15	0.69	0	15,19,21	1.07	2 (13%)
4	NAG	C	412	4	14,14,15	1.00	1 (7%)	15,19,21	0.64	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	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	403	4	-	0/6/23/26	0/1/1/1
4	NAG	A	405	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	406	4	-	0/6/23/26	0/1/1/1
4	NAG	C	408	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	409	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	411	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	412	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	406	NAG	C1-C2	2.15	1.55	1.52
4	C	412	NAG	C1-C2	2.75	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	NAG	C4-C3-C2	-7.23	99.99	111.23
4	A	402	NAG	C2-N2-C7	-3.79	118.17	123.04
4	C	408	NAG	C2-N2-C7	-3.18	118.95	123.04
4	C	411	NAG	C2-N2-C7	-2.09	120.36	123.04
4	C	411	NAG	C4-C3-C2	2.03	114.39	111.23
4	A	402	NAG	O4-C4-C5	2.67	116.33	109.24
4	A	402	NAG	C1-O5-C5	3.33	116.48	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	NAG	7	0
4	A	403	NAG	6	0
4	A	406	NAG	1	0
4	C	408	NAG	5	0
4	C	409	NAG	5	0
4	C	411	NAG	1	0

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
3	NAG	A	401	1	14,14,15	0.57	0	15,19,21	0.77	0
3	NAG	A	404	1	14,14,15	0.67	1 (7%)	15,19,21	0.55	0
3	NAG	C	407	1	14,14,15	0.55	0	15,19,21	0.90	1 (6%)
3	NAG	C	410	1	14,14,15	0.59	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
3	NAG	A	401	1	-	1/6/23/26	0/1/1/1
3	NAG	A	404	1	-	0/6/23/26	0/1/1/1
3	NAG	C	407	1	-	1/6/23/26	0/1/1/1
3	NAG	C	410	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	NAG	C1-C2	2.03	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	407	NAG	C2-N2-C7	-2.31	120.07	123.04
3	C	410	NAG	C2-N2-C7	-2.10	120.35	123.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	407	NAG	O7-C7-N2-C2
3	A	401	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	184/291 (63%)	-0.26	0 100 100	11, 53, 97, 99	0
1	C	184/291 (63%)	-0.29	2 (1%) 82 78	11, 53, 97, 99	0
2	B	177/177 (100%)	0.28	12 (6%) 20 17	19, 85, 102, 104	6 (3%)
2	D	177/177 (100%)	0.33	13 (7%) 18 15	19, 85, 102, 104	7 (3%)
All	All	722/936 (77%)	0.01	27 (3%) 45 38	11, 69, 99, 104	13 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	290	ASP	9.4
2	D	286	VAL	5.5
2	B	298	LEU	5.4
2	B	286	VAL	5.2
2	B	287	LYS	5.0
2	D	291	THR	4.8
2	D	289	LEU	4.8
2	D	287	LYS	4.1
2	B	290	ASP	2.9
2	D	288	ILE	2.9
2	D	292	PHE	2.7
1	C	151	ASP	2.7
2	D	261	ILE	2.7
2	B	300	THR	2.6
2	B	289	LEU	2.4
2	D	302	LEU	2.3
2	D	268	LYS	2.3
2	B	266	GLN	2.2
2	D	220	PHE	2.2
2	B	261	ILE	2.2
2	B	302	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	145	THR	2.2
2	B	156	ASP	2.1
2	D	269	GLU	2.1
2	D	300	THR	2.0
2	B	267	THR	2.0
2	B	157	VAL	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	C	408	14/15	0.94	0.14	-0.90	59,59,59,59	0
4	NAG	C	411	14/15	0.92	0.17	-1.28	30,30,30,30	0
4	NAG	A	402	14/15	0.94	0.14	-1.34	72,72,72,72	0
4	NAG	A	405	14/15	0.96	0.13	-1.45	36,36,36,36	0
4	NAG	A	406	14/15	0.85	0.19	-	96,96,96,96	0
4	NAG	C	412	14/15	0.78	0.24	-	96,96,96,96	0
4	NAG	C	409	14/15	0.87	0.16	-	78,78,78,78	0
4	NAG	A	403	14/15	0.81	0.21	-	81,81,81,81	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	C	410	14/15	0.83	0.23	2.17	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	404	14/15	0.85	0.21	0.75	95,95,95,95	0
5	MG	B	901	1/1	0.96	0.10	-1.40	95,95,95,95	0
5	MG	D	902	1/1	0.90	0.12	-1.60	95,95,95,95	0
3	NAG	A	401	14/15	0.81	0.20	-	96,96,96,96	0
3	NAG	C	407	14/15	0.75	0.24	-	96,96,96,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.