



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:07 AM GMT

PDB ID : 1ZTM  
Title : Structure of the Uncleaved Paramyxovirus (hPIV3) Fusion Protein  
Authors : Yin, H.S.; Paterson, R.G.; Wen, X.; Lamb, R.A.; Jardetzky, T.S.  
Deposited on : 2005-05-27  
Resolution : 3.05 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

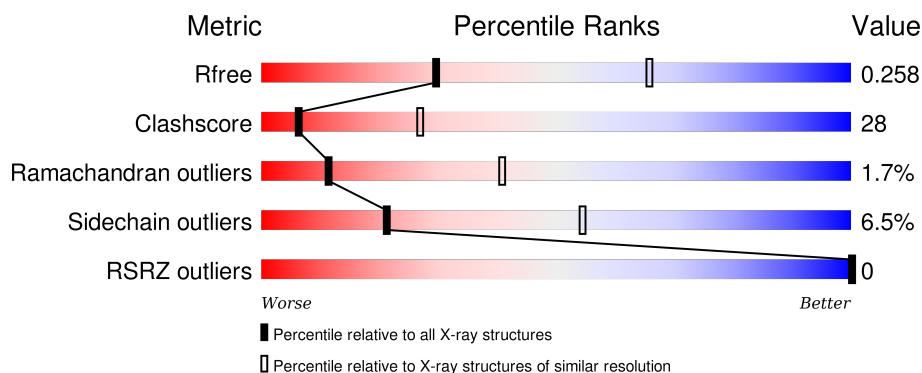
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	490	<div> <div>50%</div> <div>32%</div> <div>•</div> <div>15%</div> </div>
1	B	490	<div> <div>50%</div> <div>32%</div> <div>•</div> <div>15%</div> </div>
1	C	490	<div> <div>50%</div> <div>33%</div> <div>•</div> <div>13%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9432 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 Fusion glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3137	1983	522	618	14			
1	B	418	Total	C	N	O	S	0	0	0
			3117	1970	516	617	14			
1	C	424	Total	C	N	O	S	0	0	0
			3149	1986	526	623	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	SER	ARG	ENGINEERED	UNP P06828
B	106	SER	ARG	ENGINEERED	UNP P06828
C	106	SER	ARG	ENGINEERED	UNP P06828
A	494	GLY	-	CLONING ARTIFACT	UNP P06828
B	494	GLY	-	CLONING ARTIFACT	UNP P06828
C	494	GLY	-	CLONING ARTIFACT	UNP P06828
A	495	GLY	-	CLONING ARTIFACT	UNP P06828
B	495	GLY	-	CLONING ARTIFACT	UNP P06828
C	495	GLY	-	CLONING ARTIFACT	UNP P06828
A	496	PRO	-	CLONING ARTIFACT	UNP P06828
B	496	PRO	-	CLONING ARTIFACT	UNP P06828
C	496	PRO	-	CLONING ARTIFACT	UNP P06828
A	497	LEU	-	CLONING ARTIFACT	UNP P06828
B	497	LEU	-	CLONING ARTIFACT	UNP P06828
C	497	LEU	-	CLONING ARTIFACT	UNP P06828
A	498	VAL	-	CLONING ARTIFACT	UNP P06828
B	498	VAL	-	CLONING ARTIFACT	UNP P06828
C	498	VAL	-	CLONING ARTIFACT	UNP P06828
A	499	PRO	-	CLONING ARTIFACT	UNP P06828
B	499	PRO	-	CLONING ARTIFACT	UNP P06828
C	499	PRO	-	CLONING ARTIFACT	UNP P06828
A	500	ARG	-	CLONING ARTIFACT	UNP P06828
B	500	ARG	-	CLONING ARTIFACT	UNP P06828

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Chain	Residue	Modelled	Actual	Comment	Reference
C	500	ARG	-	CLONING ARTIFACT	UNP P06828
A	501	GLY	-	CLONING ARTIFACT	UNP P06828
B	501	GLY	-	CLONING ARTIFACT	UNP P06828
C	501	GLY	-	CLONING ARTIFACT	UNP P06828
A	502	SER	-	CLONING ARTIFACT	UNP P06828
B	502	SER	-	CLONING ARTIFACT	UNP P06828
C	502	SER	-	CLONING ARTIFACT	UNP P06828
A	503	HIS	-	EXPRESSION TAG	UNP P06828
B	503	HIS	-	EXPRESSION TAG	UNP P06828
C	503	HIS	-	EXPRESSION TAG	UNP P06828
A	504	HIS	-	EXPRESSION TAG	UNP P06828
B	504	HIS	-	EXPRESSION TAG	UNP P06828
C	504	HIS	-	EXPRESSION TAG	UNP P06828
A	505	HIS	-	EXPRESSION TAG	UNP P06828
B	505	HIS	-	EXPRESSION TAG	UNP P06828
C	505	HIS	-	EXPRESSION TAG	UNP P06828
A	506	HIS	-	EXPRESSION TAG	UNP P06828
B	506	HIS	-	EXPRESSION TAG	UNP P06828
C	506	HIS	-	EXPRESSION TAG	UNP P06828
A	507	HIS	-	EXPRESSION TAG	UNP P06828
B	507	HIS	-	EXPRESSION TAG	UNP P06828
C	507	HIS	-	EXPRESSION TAG	UNP P06828
A	508	HIS	-	EXPRESSION TAG	UNP P06828
B	508	HIS	-	EXPRESSION TAG	UNP P06828
C	508	HIS	-	EXPRESSION TAG	UNP P06828

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

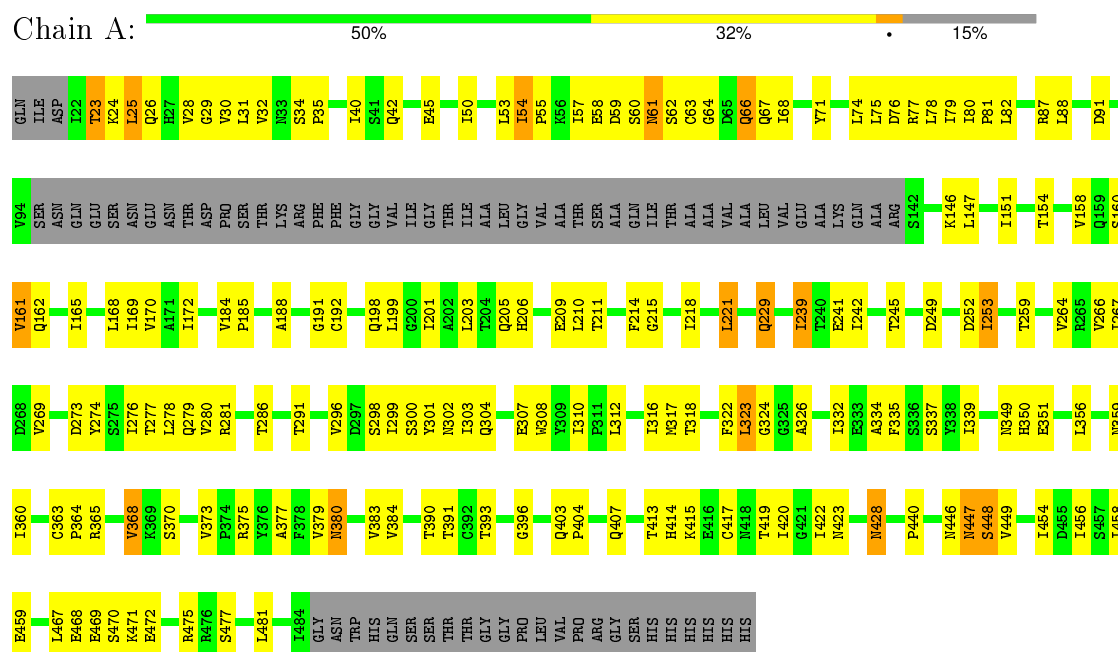
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		

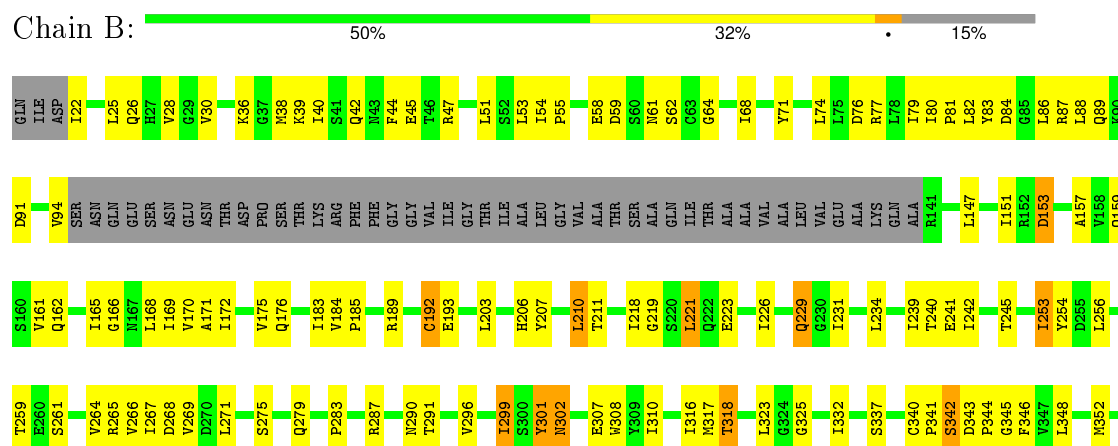
### 3 Residue-property plots

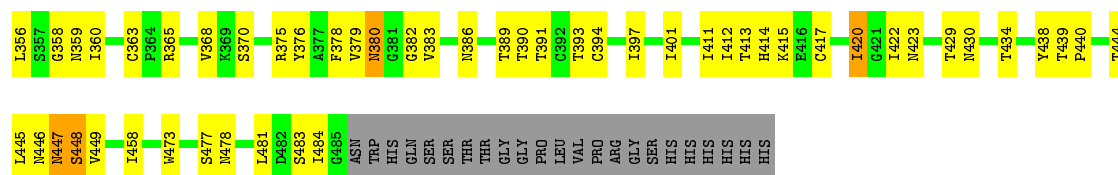
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Fusion glycoprotein

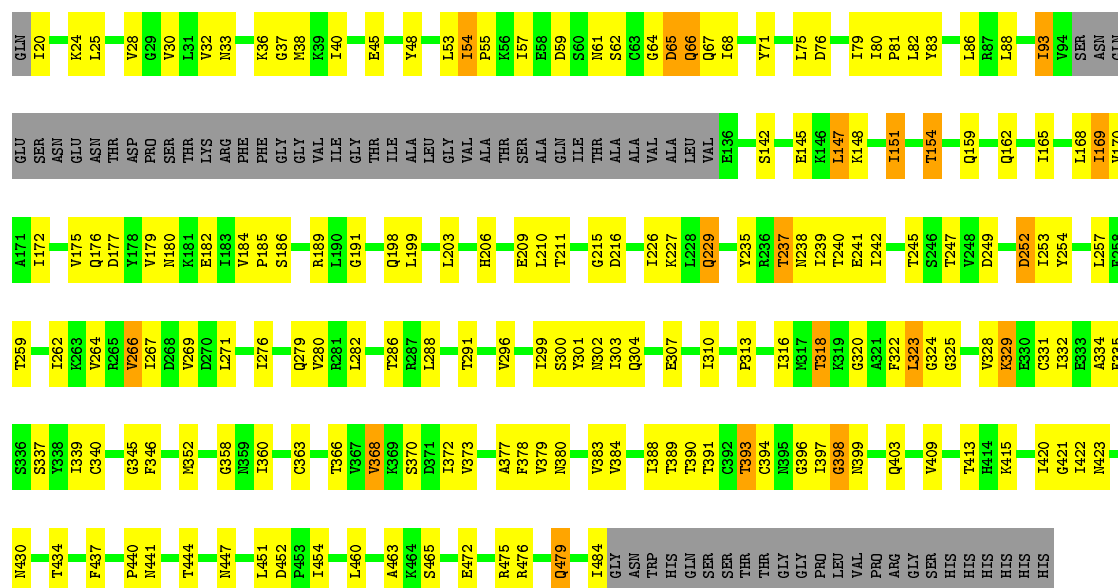


- Molecule 1: Fusion glycoprotein





• Molecule 1: Fusion glycoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.56Å 122.17Å 195.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 3.05 30.02 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.02-3.05) 99.6 (30.02-3.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.40 (at 3.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.217 , 0.264 0.213 , 0.258	Depositor DCC
$R_{free}$ test set	2365 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 64.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 48676 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: 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	0.37	0/3183	0.69	1/4337 (0.0%)
1	B	0.37	0/3163	0.68	0/4318
1	C	0.37	0/3193	0.67	1/4356 (0.0%)
All	All	0.37	0/9539	0.68	2/13011 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	LYS	N-CA-C	-5.71	95.59	111.00
1	A	35	PRO	N-CA-CB	5.26	109.61	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3137	0	3062	185	0
1	B	3117	0	3006	206	0
1	C	3149	0	3034	205	0
2	A	14	0	13	2	0
2	B	14	0	13	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9432	0	9128	516	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 28.

All (516) 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:413:THR:HG22	1:C:415:LYS:H	1.13	1.11
1:C:259:THR:HG23	1:C:332:ILE:HG21	1.46	0.96
1:C:264:VAL:HG12	1:C:280:VAL:HA	1.49	0.94
1:B:168:LEU:HD21	1:C:169:ILE:HG22	1.50	0.94
1:A:417:CYS:HB2	1:A:420:ILE:HG22	1.52	0.92
1:B:383:VAL:HG11	1:B:422:ILE:HD11	1.53	0.89
1:A:413:THR:HG22	1:A:415:LYS:H	1.35	0.88
1:B:296:VAL:HG11	1:B:316:ILE:HD12	1.54	0.88
1:C:299:ILE:HD11	1:C:377:ALA:HB2	1.56	0.88
1:A:383:VAL:HG11	1:A:422:ILE:HD11	1.58	0.85
1:B:391:THR:H	1:B:423:ASN:ND2	1.77	0.82
1:A:299:ILE:HD11	1:A:377:ALA:HB2	1.61	0.81
1:A:25:LEU:N	1:A:25:LEU:HD23	1.97	0.80
1:C:239:ILE:O	1:C:242:ILE:HG12	1.82	0.80
1:B:391:THR:H	1:B:423:ASN:HD21	1.28	0.79
1:A:64:GLY:O	1:A:68:ILE:HG12	1.83	0.79
1:C:80:ILE:HB	1:C:81:PRO:HD3	1.65	0.78
1:A:168:LEU:HD21	1:B:169:ILE:HG22	1.63	0.78
1:B:64:GLY:O	1:B:68:ILE:HG13	1.83	0.78
1:B:80:ILE:HB	1:B:81:PRO:HD3	1.64	0.78
1:A:165:ILE:HD11	1:B:165:ILE:HD12	1.66	0.77
1:B:267:ILE:CD1	1:B:279:GLN:HB2	2.14	0.77
1:C:368:VAL:HB	1:C:373:VAL:HG21	1.64	0.77
1:B:449:VAL:HG11	1:C:189:ARG:NH2	1.99	0.77
1:A:45:GLU:OE1	1:A:245:THR:HB	1.86	0.75
1:C:413:THR:HG22	1:C:415:LYS:N	1.97	0.75
1:B:259:THR:HG23	1:B:332:ILE:HG21	1.66	0.75
1:A:25:LEU:HD12	1:A:30:VAL:HG21	1.69	0.75
1:B:55:PRO:HB3	1:C:440:PRO:HG2	1.68	0.73
1:A:82:LEU:HD22	1:A:218:ILE:HG23	1.70	0.72
1:A:24:LYS:O	1:A:24:LYS:HG3	1.88	0.72
1:A:307:GLU:HG2	1:A:368:VAL:CG1	2.20	0.72
1:A:259:THR:HG23	1:A:332:ILE:HG21	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ILE:HD11	1:C:320:GLY:O	1.89	0.71
1:A:456:ILE:HG21	1:B:171:ALA:HB1	1.71	0.71
1:C:68:ILE:HD11	1:C:199:LEU:HD21	1.71	0.71
1:C:79:ILE:HG23	1:C:269:VAL:HG11	1.72	0.71
1:C:82:LEU:HD11	1:C:266:VAL:HG21	1.73	0.71
1:C:45:GLU:OE1	1:C:245:THR:HB	1.89	0.70
1:B:267:ILE:HD12	1:B:279:GLN:HB2	1.72	0.70
1:C:38:MET:CE	1:C:288:LEU:HD12	2.21	0.70
1:C:235:TYR:HD2	1:C:242:ILE:HD11	1.57	0.69
1:C:28:VAL:HG12	1:C:28:VAL:O	1.92	0.69
1:A:239:ILE:O	1:A:242:ILE:HG13	1.91	0.69
1:C:36:LYS:HE2	1:C:335:PHE:O	1.91	0.69
1:C:168:LEU:O	1:C:172:ILE:HG12	1.93	0.68
1:C:370:SER:OG	1:C:372:ILE:HG12	1.92	0.68
1:B:221:LEU:HD21	1:C:257:LEU:HB3	1.75	0.68
1:A:165:ILE:CD1	1:C:165:ILE:HD11	2.24	0.68
1:A:253:ILE:HD11	1:C:88:LEU:CD2	2.24	0.68
1:A:169:ILE:HG13	1:A:170:VAL:N	2.09	0.68
1:C:393:THR:HG23	1:C:421:GLY:HA3	1.75	0.68
1:C:32:VAL:O	1:C:32:VAL:HG23	1.93	0.67
1:A:191:GLY:C	1:B:448:SER:HB3	2.14	0.67
1:A:68:ILE:HD11	1:A:199:LEU:HD21	1.75	0.67
1:A:370:SER:HA	1:C:322:PHE:CE2	2.29	0.67
1:C:310:ILE:HD13	1:C:363:CYS:HB3	1.77	0.67
1:A:31:LEU:HD11	1:A:384:VAL:HG11	1.76	0.67
1:A:449:VAL:HB	1:B:189:ARG:NH2	2.08	0.67
1:B:207:TYR:O	1:B:211:THR:HG23	1.94	0.67
1:A:221:LEU:H	1:A:221:LEU:CD2	2.07	0.67
1:C:299:ILE:HG22	1:C:300:SER:N	2.10	0.66
1:B:45:GLU:OE1	1:B:245:THR:HB	1.96	0.66
1:B:219:GLY:HA2	1:C:229:GLN:OE1	1.97	0.65
1:A:53:LEU:HD11	1:A:79:ILE:HD11	1.78	0.65
1:A:79:ILE:HG23	1:A:269:VAL:HG11	1.79	0.65
1:A:158:VAL:O	1:A:162:GLN:HG3	1.97	0.65
1:B:310:ILE:HD13	1:B:363:CYS:HB3	1.79	0.65
1:A:25:LEU:H	1:A:25:LEU:HD23	1.62	0.64
1:B:383:VAL:HB	1:B:420:ILE:HD13	1.78	0.64
1:A:146:LYS:CB	1:C:484:ILE:HD11	2.27	0.64
1:C:28:VAL:HG13	1:C:301:TYR:CZ	2.32	0.64
1:A:55:PRO:HB3	1:B:440:PRO:HG2	1.80	0.64
1:B:391:THR:HG22	1:B:423:ASN:ND2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:O	1:C:151:ILE:HG23	1.98	0.63
1:A:413:THR:HG22	1:A:415:LYS:N	2.11	0.63
1:A:307:GLU:HG2	1:A:368:VAL:HG11	1.79	0.63
1:A:481:LEU:HD13	1:C:151:ILE:HD11	1.80	0.63
1:A:68:ILE:CD1	1:A:199:LEU:HD21	2.29	0.63
1:B:39:LYS:HG2	1:B:287:ARG:HD3	1.81	0.63
1:A:301:TYR:CE2	1:A:308:TRP:HB2	2.34	0.62
1:B:147:LEU:O	1:B:151:ILE:HG13	2.00	0.62
1:B:253:ILE:HD12	1:B:253:ILE:C	2.20	0.62
1:C:179:VAL:HG13	1:C:180:ASN:N	2.15	0.62
1:C:62:SER:HB2	1:C:65:ASP:OD2	2.00	0.62
1:C:403:GLN:HE22	1:C:409:VAL:HA	1.65	0.62
1:C:168:LEU:C	1:C:170:VAL:H	2.03	0.62
1:A:50:ILE:HD13	1:A:277:THR:HG23	1.81	0.61
1:B:25:LEU:HB2	1:B:30:VAL:HG22	1.82	0.61
1:B:323:LEU:C	1:B:323:LEU:HD12	2.21	0.61
1:C:76:ASP:O	1:C:80:ILE:HG12	2.01	0.61
1:C:302:ASN:HD21	1:C:389:THR:HG23	1.65	0.61
1:B:221:LEU:HD23	1:B:221:LEU:H	1.66	0.61
1:C:296:VAL:HG11	1:C:316:ILE:HD12	1.81	0.61
1:B:317:MET:CE	1:B:345:GLY:HA3	2.31	0.60
1:A:192:CYS:N	1:B:448:SER:HB3	2.16	0.60
1:A:169:ILE:HG13	1:A:170:VAL:H	1.65	0.60
1:B:59:ASP:OD2	1:B:62:SER:HA	2.00	0.60
1:C:323:LEU:C	1:C:323:LEU:HD12	2.22	0.60
1:A:310:ILE:HD13	1:A:363:CYS:HB3	1.83	0.60
1:C:226:ILE:HD11	1:C:264:VAL:HG21	1.83	0.60
1:A:391:THR:H	1:A:423:ASN:HD21	1.49	0.60
1:B:53:LEU:HD11	1:B:79:ILE:HD11	1.83	0.60
1:C:38:MET:HE1	1:C:288:LEU:HD12	1.84	0.60
1:A:23:THR:HG22	1:A:24:LYS:H	1.67	0.60
1:A:165:ILE:HD11	1:C:165:ILE:HD11	1.83	0.59
1:A:448:SER:HB3	1:C:191:GLY:C	2.22	0.59
1:C:57:ILE:HD12	1:C:68:ILE:HD12	1.83	0.59
1:A:454:ILE:HG22	1:C:180:ASN:OD1	2.02	0.59
1:B:394:CYS:CB	1:B:401:ILE:HD11	2.31	0.59
1:A:76:ASP:O	1:A:80:ILE:HG12	2.03	0.59
1:C:80:ILE:HD13	1:C:271:LEU:HD22	1.85	0.59
1:A:467:LEU:O	1:A:470:SER:HB3	2.03	0.59
1:C:313:PRO:HD2	1:C:352:MET:CE	2.32	0.59
1:C:259:THR:CG2	1:C:332:ILE:HG21	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HD13	1:A:55:PRO:O	2.02	0.59
1:A:79:ILE:HG23	1:A:269:VAL:CG1	2.33	0.59
1:A:88:LEU:HD13	1:B:253:ILE:HD11	1.86	0.58
1:C:379:VAL:O	1:C:380:ASN:HB3	2.02	0.58
1:B:38:MET:SD	1:B:344:PRO:HD2	2.43	0.58
1:C:182:GLU:O	1:C:186:SER:HB2	2.02	0.58
1:C:53:LEU:HD22	1:C:210:LEU:HD21	1.86	0.58
1:C:318:THR:O	1:C:318:THR:HG22	2.03	0.58
1:B:348:LEU:HB3	1:B:352:MET:HE2	1.84	0.58
1:B:358:GLY:O	1:B:360:ILE:N	2.36	0.58
1:C:37:GLY:O	1:C:337:SER:HB2	2.04	0.58
1:A:359:ASN:CG	2:A:1359:NAG:H82	2.23	0.58
1:B:79:ILE:HG23	1:B:269:VAL:HG11	1.86	0.58
1:A:471:LYS:HG2	1:C:162:GLN:NE2	2.18	0.57
1:A:267:ILE:HD12	1:A:279:GLN:HB2	1.85	0.57
1:C:226:ILE:HG22	1:C:227:LYS:O	2.05	0.57
1:B:25:LEU:CB	1:B:30:VAL:HG22	2.34	0.57
1:A:312:LEU:HD13	1:A:356:LEU:HD21	1.87	0.57
1:B:82:LEU:HG	1:B:269:VAL:HG21	1.85	0.57
1:A:239:ILE:HG22	1:A:242:ILE:HD11	1.86	0.57
1:B:301:TYR:CE2	1:B:308:TRP:HB2	2.39	0.57
1:B:47:ARG:NH1	1:B:234:LEU:HB3	2.20	0.57
1:B:267:ILE:HD11	1:B:279:GLN:HB2	1.84	0.57
1:B:348:LEU:HB3	1:B:352:MET:CE	2.35	0.57
1:B:477:SER:OG	1:C:154:THR:HG22	2.05	0.56
1:A:448:SER:HB3	1:C:191:GLY:HA3	1.86	0.56
1:B:299:ILE:HD12	1:B:376:TYR:N	2.21	0.56
1:C:249:ASP:HB2	1:C:252:ASP:HB2	1.87	0.56
1:A:32:VAL:HG12	1:A:296:VAL:HG12	1.87	0.56
1:A:253:ILE:HD11	1:C:88:LEU:HD22	1.88	0.56
1:A:370:SER:HA	1:C:322:PHE:CD2	2.41	0.56
1:C:239:ILE:O	1:C:239:ILE:HG22	2.04	0.56
1:A:307:GLU:HG2	1:A:368:VAL:HG13	1.85	0.56
1:B:296:VAL:HG11	1:B:316:ILE:CD1	2.33	0.56
1:B:166:GLY:HA2	1:B:169:ILE:HG12	1.88	0.56
1:B:166:GLY:O	1:B:169:ILE:HG12	2.06	0.56
1:A:308:TRP:CE3	1:A:365:ARG:HD2	2.41	0.56
1:C:403:GLN:HE22	1:C:409:VAL:CA	2.19	0.56
1:B:375:ARG:NH1	1:B:389:THR:HB	2.21	0.56
1:A:25:LEU:CD1	1:A:30:VAL:HG21	2.36	0.55
1:A:23:THR:CG2	1:A:24:LYS:H	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLN:HG3	1:A:67:GLN:N	2.22	0.55
1:B:449:VAL:HG11	1:C:189:ARG:HH22	1.67	0.55
1:B:323:LEU:O	1:B:323:LEU:HD12	2.05	0.55
1:B:176:GLN:HG3	1:C:454:ILE:HG23	1.88	0.55
1:C:383:VAL:HG12	1:C:384:VAL:N	2.22	0.55
1:C:176:GLN:HG2	1:C:176:GLN:O	2.05	0.55
1:B:89:GLN:HG3	1:C:254:TYR:CE1	2.42	0.55
1:B:307:GLU:HG2	1:B:368:VAL:HG13	1.88	0.55
1:A:383:VAL:CG2	1:A:420:ILE:HD11	2.37	0.55
1:A:477:SER:HB2	1:B:153:ASP:HB3	1.88	0.55
1:A:267:ILE:CD1	1:A:279:GLN:HB2	2.36	0.55
1:A:165:ILE:HD12	1:C:165:ILE:HD11	1.88	0.54
1:B:161:VAL:O	1:B:165:ILE:HG12	2.07	0.54
1:B:394:CYS:HB2	1:B:401:ILE:HD11	1.86	0.54
1:A:53:LEU:HD22	1:A:210:LEU:HD21	1.89	0.54
1:C:313:PRO:HD2	1:C:352:MET:HE1	1.90	0.54
1:C:40:ILE:CG1	1:C:286:THR:HB	2.38	0.54
1:B:383:VAL:HB	1:B:420:ILE:CD1	2.37	0.54
1:B:358:GLY:O	1:B:360:ILE:HG13	2.07	0.54
1:C:53:LEU:HD22	1:C:210:LEU:CD2	2.38	0.54
1:B:168:LEU:O	1:B:172:ILE:HG13	2.08	0.54
1:C:323:LEU:HD12	1:C:324:GLY:N	2.23	0.54
1:A:391:THR:H	1:A:423:ASN:ND2	2.05	0.54
1:A:74:LEU:HA	1:A:77:ARG:NH1	2.22	0.54
1:B:240:THR:C	1:B:242:ILE:H	2.11	0.54
1:A:448:SER:HB3	1:C:191:GLY:CA	2.38	0.53
1:A:296:VAL:HG11	1:A:316:ILE:CD1	2.38	0.53
1:C:53:LEU:HD11	1:C:79:ILE:HD11	1.89	0.53
1:C:291:THR:HA	1:C:318:THR:O	2.09	0.53
1:A:88:LEU:CD1	1:B:253:ILE:HD11	2.38	0.53
1:A:88:LEU:HD21	1:B:254:TYR:HB2	1.91	0.53
1:B:390:THR:HG23	1:B:423:ASN:ND2	2.24	0.53
1:C:240:THR:C	1:C:242:ILE:H	2.10	0.53
1:C:328:VAL:O	1:C:328:VAL:HG12	2.09	0.53
1:C:307:GLU:CD	1:C:389:THR:HG21	2.29	0.53
1:A:253:ILE:HD12	1:A:253:ILE:C	2.29	0.53
1:C:40:ILE:HG13	1:C:286:THR:HB	1.91	0.53
1:A:165:ILE:HD12	1:C:165:ILE:CD1	2.39	0.52
1:B:42:GLN:HG3	1:C:378:PHE:CE2	2.45	0.52
1:A:184:VAL:HB	1:A:185:PRO:HD3	1.90	0.52
1:B:449:VAL:CG1	1:C:189:ARG:HH22	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:VAL:HG23	1:A:420:ILE:HD11	1.92	0.52
1:B:44:PHE:HB2	1:C:430:ASN:OD1	2.09	0.52
1:B:55:PRO:HB3	1:C:440:PRO:CG	2.38	0.52
1:A:71:TYR:CE2	1:A:75:LEU:HD11	2.44	0.52
1:A:481:LEU:O	1:C:148:LYS:HE3	2.10	0.52
1:A:403:GLN:O	1:A:403:GLN:HG3	2.08	0.52
1:C:303:ILE:O	1:C:304:GLN:HB2	2.09	0.52
1:B:325:GLY:HA3	1:B:346:PHE:CZ	2.45	0.52
1:B:291:THR:HA	1:B:318:THR:O	2.10	0.52
1:B:36:LYS:HB3	1:B:337:SER:HA	1.90	0.52
1:B:447:ASN:O	1:B:448:SER:O	2.27	0.52
1:B:77:ARG:NH1	1:B:77:ARG:CB	2.73	0.52
1:B:184:VAL:HB	1:B:185:PRO:HD3	1.92	0.52
1:C:79:ILE:HG23	1:C:269:VAL:CG1	2.39	0.52
1:B:299:ILE:HD12	1:B:375:ARG:C	2.29	0.52
1:B:61:ASN:HD22	1:C:447:ASN:CB	2.23	0.51
1:B:429:THR:HG22	1:B:430:ASN:N	2.25	0.51
1:B:307:GLU:HG2	1:B:368:VAL:CG1	2.40	0.51
1:A:58:GLU:O	1:B:444:THR:HG23	2.09	0.51
1:C:334:ALA:HB3	1:C:337:SER:O	2.11	0.51
1:B:307:GLU:O	1:B:368:VAL:HG13	2.10	0.51
1:A:61:ASN:ND2	1:B:447:ASN:CB	2.73	0.51
1:C:249:ASP:HB2	1:C:252:ASP:H	1.74	0.51
1:A:323:LEU:HD12	1:A:323:LEU:C	2.31	0.51
1:B:307:GLU:CD	1:B:389:THR:HG21	2.31	0.51
1:B:375:ARG:HH11	1:B:389:THR:HB	1.75	0.51
1:B:226:ILE:HD12	1:B:264:VAL:HG11	1.92	0.51
1:C:64:GLY:O	1:C:68:ILE:HG12	2.10	0.51
1:C:28:VAL:CG1	1:C:310:ILE:HD11	2.40	0.51
1:C:20:ILE:O	1:C:20:ILE:HG22	2.10	0.50
1:A:172:ILE:HD11	1:C:172:ILE:HD12	1.93	0.50
1:A:40:ILE:HG13	1:A:286:THR:HB	1.93	0.50
1:A:291:THR:HA	1:A:318:THR:O	2.12	0.50
1:A:273:ASP:O	1:A:274:TYR:HB2	2.11	0.50
1:A:165:ILE:CD1	1:B:165:ILE:HD12	2.38	0.50
1:B:25:LEU:O	1:B:28:VAL:HG22	2.11	0.50
1:B:449:VAL:HG23	1:B:449:VAL:O	2.11	0.50
1:B:77:ARG:HB3	1:B:77:ARG:HH11	1.76	0.50
1:C:358:GLY:O	1:C:360:ILE:N	2.42	0.50
1:C:422:ILE:HG22	1:C:422:ILE:O	2.10	0.50
1:B:478:ASN:O	1:B:481:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:GLY:O	1:C:398:GLY:N	2.44	0.50
1:A:59:ASP:CB	1:B:445:LEU:HB2	2.41	0.50
1:C:299:ILE:HG22	1:C:300:SER:H	1.76	0.50
1:C:299:ILE:CG2	1:C:300:SER:N	2.74	0.50
1:C:325:GLY:O	1:C:345:GLY:HA2	2.11	0.50
1:B:348:LEU:HD13	1:B:352:MET:HE3	1.94	0.50
1:B:318:THR:O	1:B:318:THR:HG22	2.11	0.50
1:A:440:PRO:HG2	1:C:55:PRO:HB3	1.94	0.50
1:A:28:VAL:HG12	1:A:310:ILE:CD1	2.42	0.49
1:A:80:ILE:HB	1:A:81:PRO:HD3	1.93	0.49
1:B:259:THR:O	1:B:259:THR:HG22	2.12	0.49
1:A:54:ILE:C	1:A:54:ILE:HD13	2.32	0.49
1:C:259:THR:O	1:C:259:THR:HG22	2.13	0.49
1:B:391:THR:HG23	1:B:423:ASN:HA	1.93	0.49
1:B:317:MET:HE2	1:B:345:GLY:HA3	1.95	0.49
1:A:456:ILE:HD11	1:B:175:VAL:HG23	1.94	0.49
1:B:412:ILE:HG21	1:B:420:ILE:HB	1.93	0.49
1:C:79:ILE:HD11	1:C:276:ILE:HD11	1.95	0.49
1:B:89:GLN:HG3	1:C:254:TYR:CZ	2.47	0.49
1:C:235:TYR:CD2	1:C:242:ILE:HD11	2.44	0.49
1:B:449:VAL:HG11	1:C:189:ARG:CZ	2.43	0.49
1:A:82:LEU:CD2	1:A:218:ILE:HG23	2.38	0.49
1:C:240:THR:C	1:C:242:ILE:N	2.65	0.49
1:B:80:ILE:O	1:B:83:TYR:HB3	2.13	0.49
1:A:221:LEU:H	1:A:221:LEU:HD23	1.76	0.49
1:C:54:ILE:HD13	1:C:55:PRO:N	2.28	0.49
1:B:223:GLU:HG2	1:B:265:ARG:HB2	1.94	0.49
1:A:168:LEU:HD21	1:B:169:ILE:CG2	2.39	0.48
1:A:23:THR:HG22	1:A:24:LYS:N	2.27	0.48
1:C:175:VAL:O	1:C:179:VAL:HG12	2.12	0.48
1:B:38:MET:O	1:B:287:ARG:HD2	2.14	0.48
1:A:440:PRO:HB3	1:C:206:HIS:CE1	2.48	0.48
1:B:82:LEU:HD21	1:B:266:VAL:HG11	1.94	0.48
1:C:142:SER:OG	1:C:145:GLU:HG3	2.13	0.48
1:B:58:GLU:HB3	1:C:444:THR:OG1	2.14	0.48
1:B:210:LEU:C	1:B:210:LEU:HD12	2.34	0.48
1:B:88:LEU:HD22	1:C:253:ILE:HD11	1.95	0.48
1:A:221:LEU:H	1:A:221:LEU:HD22	1.76	0.48
1:C:302:ASN:HB2	1:C:388:ILE:HD12	1.94	0.48
1:C:383:VAL:HG23	1:C:420:ILE:HD12	1.96	0.48
1:A:302:ASN:O	1:A:303:ILE:HD13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:CB	1:C:61:ASN:HD22	2.26	0.48
1:B:40:ILE:HA	1:B:340:CYS:O	2.13	0.48
1:B:391:THR:CG2	1:B:423:ASN:HA	2.44	0.47
1:C:238:ASN:C	1:C:240:THR:H	2.16	0.47
1:A:307:GLU:OE2	1:A:375:ARG:NH1	2.47	0.47
1:C:54:ILE:HD13	1:C:55:PRO:HD2	1.96	0.47
1:C:472:GLU:O	1:C:475:ARG:N	2.47	0.47
1:A:334:ALA:HB3	1:A:337:SER:O	2.13	0.47
1:B:414:HIS:HA	1:B:417:CYS:O	2.14	0.47
1:B:390:THR:HG21	1:B:422:ILE:HG23	1.95	0.47
1:B:166:GLY:HA2	1:B:169:ILE:CD1	2.45	0.47
1:C:57:ILE:HD12	1:C:68:ILE:CD1	2.44	0.47
1:B:299:ILE:HD11	1:B:376:TYR:C	2.35	0.47
1:B:22:ILE:HA	1:B:356:LEU:O	2.15	0.47
1:A:201:ILE:O	1:A:205:GLN:HG3	2.15	0.47
1:B:267:ILE:HG22	1:B:268:ASP:N	2.29	0.47
1:A:456:ILE:O	1:A:456:ILE:HG22	2.14	0.47
1:C:179:VAL:HG13	1:C:180:ASN:H	1.79	0.47
1:A:209:GLU:HG2	1:B:438:TYR:OH	2.14	0.47
1:A:71:TYR:CD1	1:A:203:LEU:HB3	2.50	0.47
1:C:328:VAL:HG13	1:C:331:CYS:HB3	1.96	0.47
1:C:262:ILE:HG23	1:C:282:LEU:HD23	1.97	0.47
1:B:239:ILE:O	1:B:242:ILE:HG12	2.15	0.47
1:C:451:LEU:O	1:C:452:ASP:C	2.51	0.47
1:C:264:VAL:HG11	1:C:280:VAL:HG22	1.97	0.47
1:A:28:VAL:HG12	1:A:310:ILE:HD11	1.97	0.47
1:A:447:ASN:O	1:A:448:SER:O	2.33	0.47
1:C:211:THR:O	1:C:215:GLY:HA3	2.15	0.47
1:B:316:ILE:HG22	1:B:317:MET:N	2.30	0.47
1:C:237:THR:HG23	1:C:241:GLU:OE1	2.15	0.47
1:C:238:ASN:O	1:C:241:GLU:HG3	2.14	0.47
1:B:446:ASN:O	1:B:447:ASN:O	2.33	0.47
1:C:328:VAL:O	1:C:329:LYS:C	2.53	0.47
1:C:54:ILE:HD13	1:C:55:PRO:CD	2.45	0.47
1:B:221:LEU:HD23	1:B:221:LEU:N	2.29	0.47
1:A:218:ILE:O	1:A:218:ILE:HG22	2.15	0.46
1:A:28:VAL:CG1	1:A:310:ILE:HD11	2.46	0.46
1:B:25:LEU:HB2	1:B:30:VAL:CG2	2.43	0.46
1:C:159:GLN:HA	1:C:162:GLN:HG2	1.96	0.46
1:B:86:LEU:CD1	1:B:269:VAL:HG23	2.45	0.46
1:A:161:VAL:O	1:A:165:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:HIS:CE1	1:C:440:PRO:HB3	2.50	0.46
1:B:77:ARG:HD2	1:C:209:GLU:OE2	2.15	0.46
1:C:296:VAL:HG22	1:C:313:PRO:O	2.16	0.46
1:B:299:ILE:CD1	1:B:376:TYR:N	2.79	0.46
1:B:88:LEU:O	1:B:88:LEU:HG	2.13	0.46
1:B:79:ILE:O	1:B:80:ILE:C	2.54	0.46
1:A:221:LEU:CD2	1:A:221:LEU:N	2.75	0.46
1:C:380:ASN:ND2	1:C:380:ASN:O	2.48	0.46
1:C:37:GLY:O	1:C:337:SER:CB	2.63	0.46
1:B:412:ILE:CD1	1:B:420:ILE:HD12	2.45	0.46
1:B:234:LEU:HB2	1:B:242:ILE:CD1	2.45	0.46
1:C:48:TYR:HE2	1:C:267:ILE:HD12	1.81	0.46
1:A:185:PRO:O	1:A:188:ALA:HB3	2.15	0.46
1:B:379:VAL:O	1:B:380:ASN:C	2.53	0.46
1:C:226:ILE:HD11	1:C:264:VAL:HG11	1.98	0.46
1:B:77:ARG:NH1	1:B:77:ARG:HB2	2.31	0.46
1:A:31:LEU:CD1	1:A:384:VAL:HG11	2.45	0.46
1:C:302:ASN:ND2	1:C:388:ILE:HB	2.31	0.46
1:A:446:ASN:O	1:A:447:ASN:O	2.34	0.46
1:B:77:ARG:HH11	1:B:77:ARG:CB	2.29	0.46
1:B:53:LEU:CD1	1:B:79:ILE:HD11	2.46	0.46
1:A:59:ASP:OD2	1:A:63:CYS:N	2.49	0.46
1:C:80:ILE:HD13	1:C:271:LEU:CD2	2.46	0.45
1:A:467:LEU:HD13	1:C:165:ILE:HG21	1.98	0.45
1:A:477:SER:O	1:A:481:LEU:HB2	2.16	0.45
1:C:179:VAL:CG1	1:C:180:ASN:N	2.79	0.45
1:B:168:LEU:CD2	1:C:169:ILE:HG22	2.34	0.45
1:A:71:TYR:O	1:A:75:LEU:HG	2.16	0.45
1:B:239:ILE:O	1:B:239:ILE:HG22	2.15	0.45
1:C:267:ILE:CD1	1:C:279:GLN:HB2	2.46	0.45
1:A:28:VAL:HA	1:A:301:TYR:CD1	2.52	0.45
1:A:296:VAL:HG11	1:A:316:ILE:HD12	1.98	0.45
1:A:211:THR:O	1:A:215:GLY:HA3	2.16	0.45
1:A:214:PHE:O	1:A:218:ILE:HG13	2.16	0.45
1:B:439:THR:HG23	1:B:440:PRO:HD2	1.97	0.45
1:A:165:ILE:HD11	1:B:165:ILE:CD1	2.43	0.45
1:A:404:PRO:HG2	1:A:407:GLN:OE1	2.16	0.45
1:A:264:VAL:HG11	1:A:278:LEU:HD13	1.98	0.45
1:B:412:ILE:HD13	1:B:420:ILE:HD12	1.99	0.45
1:A:25:LEU:O	1:A:30:VAL:HG22	2.15	0.45
1:A:79:ILE:CD1	1:A:276:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLU:OE1	1:A:375:ARG:NH1	2.50	0.45
1:C:82:LEU:HG	1:C:269:VAL:HG21	1.98	0.45
1:C:86:LEU:CD1	1:C:269:VAL:HG23	2.47	0.45
1:B:301:TYR:CZ	1:B:308:TRP:HB2	2.52	0.45
1:A:32:VAL:HG23	1:A:32:VAL:O	2.17	0.45
1:C:168:LEU:C	1:C:170:VAL:N	2.70	0.45
1:A:472:GLU:O	1:A:475:ARG:HB3	2.17	0.45
1:C:151:ILE:HA	1:C:154:THR:HG23	1.98	0.45
1:C:302:ASN:HD22	1:C:388:ILE:HB	1.82	0.45
1:B:87:ARG:O	1:B:91:ASP:HB2	2.17	0.45
1:A:317:MET:HB2	1:A:326:ALA:HB2	1.97	0.45
1:A:349:ASN:O	1:A:351:GLU:N	2.50	0.45
1:A:147:LEU:O	1:A:151:ILE:HG12	2.18	0.44
1:A:481:LEU:HD13	1:C:151:ILE:CD1	2.45	0.44
1:B:256:LEU:HD22	1:B:283:PRO:HG2	1.98	0.44
1:B:391:THR:HG22	1:B:423:ASN:HD22	1.79	0.44
1:A:363:CYS:HA	1:A:364:PRO:HD3	1.66	0.44
1:C:184:VAL:HG12	1:C:185:PRO:N	2.32	0.44
1:A:360:ILE:O	1:A:360:ILE:HG22	2.17	0.44
1:B:157:ALA:O	1:B:161:VAL:HG23	2.17	0.44
1:C:226:ILE:HG12	1:C:264:VAL:HG13	2.00	0.44
1:A:414:HIS:HA	1:A:417:CYS:O	2.17	0.44
1:C:238:ASN:C	1:C:240:THR:N	2.71	0.44
1:C:28:VAL:CG1	1:C:28:VAL:O	2.64	0.44
1:A:448:SER:CB	1:C:191:GLY:HA3	2.47	0.44
1:B:307:GLU:OE2	1:B:389:THR:HG21	2.18	0.44
1:A:456:ILE:CG2	1:B:171:ALA:HB1	2.42	0.44
1:B:58:GLU:O	1:C:444:THR:HG23	2.18	0.44
1:B:159:GLN:HA	1:B:162:GLN:OE1	2.17	0.44
1:C:299:ILE:HD11	1:C:377:ALA:CB	2.39	0.44
1:B:83:TYR:O	1:B:84:ASP:C	2.56	0.44
1:A:259:THR:HG22	1:A:259:THR:O	2.17	0.44
1:A:373:VAL:O	1:A:373:VAL:HG23	2.18	0.44
1:B:28:VAL:HG23	1:B:30:VAL:HG13	1.99	0.44
1:C:325:GLY:HA3	1:C:346:PHE:CZ	2.52	0.44
1:A:57:ILE:HD13	1:A:199:LEU:HD11	1.98	0.44
1:B:394:CYS:HB3	1:B:401:ILE:HD11	2.00	0.44
1:C:235:TYR:HB3	1:C:242:ILE:HD13	2.00	0.43
1:C:240:THR:O	1:C:242:ILE:N	2.51	0.43
1:B:166:GLY:O	1:B:169:ILE:CG1	2.65	0.43
1:C:32:VAL:O	1:C:32:VAL:CG2	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:O	1:A:380:ASN:C	2.57	0.43
1:A:459:GLU:HG2	1:B:170:VAL:HG12	2.00	0.43
1:B:317:MET:HE1	1:B:345:GLY:HA3	2.00	0.43
1:A:59:ASP:HB2	1:B:445:LEU:HB2	1.99	0.43
1:C:229:GLN:HB3	1:C:229:GLN:HE21	1.62	0.43
1:C:242:ILE:HD13	1:C:242:ILE:HA	1.82	0.43
1:B:183:ILE:O	1:B:184:VAL:C	2.56	0.43
1:A:393:THR:HB	1:A:396:GLY:O	2.18	0.43
1:C:168:LEU:O	1:C:170:VAL:N	2.51	0.43
1:C:296:VAL:HG23	1:C:296:VAL:O	2.19	0.43
1:B:397:ILE:O	1:B:397:ILE:HG22	2.17	0.43
1:A:322:PHE:CE2	1:B:370:SER:HA	2.53	0.43
1:A:390:THR:HG21	1:A:422:ILE:HG23	2.00	0.43
1:B:386:ASN:O	1:B:390:THR:HB	2.19	0.43
1:B:170:VAL:HG12	1:B:171:ALA:N	2.33	0.43
1:B:360:ILE:O	1:B:360:ILE:CG2	2.66	0.43
1:B:302:ASN:HB2	1:B:386:ASN:HD21	1.83	0.43
1:C:299:ILE:CG2	1:C:300:SER:H	2.32	0.43
1:A:57:ILE:HD11	1:A:203:LEU:HD11	2.01	0.43
1:C:307:GLU:CD	1:C:368:VAL:HG21	2.39	0.43
1:B:71:TYR:HE1	1:B:207:TYR:HB2	1.84	0.43
1:B:429:THR:CG2	1:B:430:ASN:N	2.82	0.43
1:A:59:ASP:OD2	1:A:62:SER:HA	2.19	0.43
1:C:38:MET:HE2	1:C:288:LEU:HD12	2.01	0.42
1:A:359:ASN:ND2	2:A:1359:NAG:C7	2.82	0.42
1:B:210:LEU:O	1:B:210:LEU:HD12	2.19	0.42
1:A:307:GLU:CD	1:A:375:ARG:NH1	2.72	0.42
1:A:29:GLY:O	1:A:298:SER:HA	2.19	0.42
1:B:316:ILE:CG2	1:B:317:MET:N	2.82	0.42
1:C:378:PHE:N	1:C:378:PHE:CD1	2.86	0.42
1:A:471:LYS:HG2	1:C:162:GLN:HE22	1.81	0.42
1:B:375:ARG:HH11	1:B:389:THR:CB	2.31	0.42
1:B:74:LEU:HA	1:B:77:ARG:HH12	1.83	0.42
1:A:151:ILE:CG2	1:B:481:LEU:HD11	2.49	0.42
1:C:422:ILE:O	1:C:423:ASN:HB2	2.19	0.42
1:A:368:VAL:CG2	1:A:373:VAL:HG21	2.49	0.42
1:A:26:GLN:C	1:A:28:VAL:H	2.22	0.42
1:A:87:ARG:O	1:A:91:ASP:HB2	2.19	0.42
1:C:71:TYR:HB2	1:C:203:LEU:HD23	2.01	0.42
1:A:151:ILE:HA	1:A:154:THR:HG22	2.02	0.42
1:A:32:VAL:CG2	1:A:32:VAL:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:THR:N	1:B:423:ASN:HD21	2.07	0.42
1:B:71:TYR:O	1:B:74:LEU:HB3	2.19	0.42
1:C:378:PHE:O	1:C:379:VAL:CG2	2.68	0.42
1:C:45:GLU:CD	1:C:245:THR:HB	2.41	0.42
1:A:323:LEU:HD12	1:A:324:GLY:N	2.35	0.42
1:B:341:PRO:O	1:B:342:SER:HB3	2.20	0.42
1:B:481:LEU:C	1:B:483:SER:H	2.23	0.42
1:B:42:GLN:HG3	1:C:378:PHE:CD2	2.55	0.42
1:C:472:GLU:OE2	1:C:475:ARG:NH1	2.53	0.42
1:C:476:ARG:HA	1:C:479:GLN:HB2	2.02	0.42
1:A:419:THR:HG23	1:A:428:ASN:OD1	2.20	0.42
1:B:391:THR:HG23	1:B:391:THR:O	2.19	0.41
1:A:75:LEU:O	1:A:78:LEU:HB3	2.20	0.41
1:C:307:GLU:OE1	1:C:368:VAL:HG21	2.20	0.41
1:C:296:VAL:HG11	1:C:316:ILE:CD1	2.49	0.41
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.81	0.41
1:C:253:ILE:C	1:C:253:ILE:HD12	2.41	0.41
1:B:259:THR:CG2	1:B:261:SER:OG	2.68	0.41
1:A:79:ILE:HD11	1:A:276:ILE:HD11	2.03	0.41
1:A:82:LEU:HG	1:A:269:VAL:HG21	2.02	0.41
1:C:288:LEU:HD23	1:C:288:LEU:HA	1.82	0.41
1:C:331:CYS:SG	1:C:339:ILE:O	2.78	0.41
1:B:51:LEU:O	1:B:275:SER:HA	2.21	0.41
1:B:413:THR:HG22	1:B:415:LYS:H	1.86	0.41
1:A:299:ILE:HG22	1:A:300:SER:N	2.35	0.41
1:C:86:LEU:HD12	1:C:269:VAL:HG23	2.03	0.41
1:C:40:ILE:HA	1:C:340:CYS:O	2.21	0.41
1:B:192:CYS:O	1:B:193:GLU:C	2.58	0.41
1:A:229:GLN:HE21	1:A:229:GLN:HB3	1.63	0.41
1:C:59:ASP:O	1:C:59:ASP:CG	2.59	0.41
1:C:437:PHE:N	1:C:437:PHE:CD1	2.88	0.41
1:B:363:CYS:O	1:B:365:ARG:N	2.51	0.41
1:A:26:GLN:C	1:A:28:VAL:N	2.73	0.41
1:B:299:ILE:HA	1:B:299:ILE:HD13	1.83	0.41
1:A:25:LEU:HG	1:A:30:VAL:CG2	2.51	0.41
1:B:76:ASP:O	1:B:80:ILE:HG12	2.20	0.41
1:C:159:GLN:HA	1:C:162:GLN:CG	2.51	0.41
1:B:231:ILE:HG23	1:B:242:ILE:HD11	2.01	0.41
1:B:242:ILE:HA	1:B:242:ILE:HD13	1.77	0.41
1:B:473:TRP:HA	1:B:473:TRP:CE3	2.55	0.41
1:B:79:ILE:HG21	1:B:271:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLN:HG3	1:C:378:PHE:CZ	2.56	0.41
1:C:267:ILE:HD11	1:C:279:GLN:HB2	2.03	0.41
1:B:379:VAL:O	1:B:382:GLY:N	2.53	0.41
1:A:468:GLU:O	1:A:469:GLU:C	2.58	0.41
1:A:42:GLN:HG3	1:B:378:PHE:CZ	2.56	0.41
1:B:229:GLN:HB3	1:B:229:GLN:HE21	1.54	0.41
1:A:206:HIS:CE1	1:B:440:PRO:HB3	2.56	0.41
1:A:151:ILE:HG21	1:B:481:LEU:HD11	2.03	0.41
1:C:147:LEU:O	1:C:148:LYS:C	2.59	0.41
1:C:66:GLN:HG3	1:C:67:GLN:N	2.35	0.41
1:C:460:LEU:O	1:C:463:ALA:HB3	2.21	0.41
1:B:26:GLN:OE1	1:B:411:ILE:HD11	2.21	0.41
1:A:335:PHE:CE1	1:C:93:ILE:HD12	2.56	0.41
1:B:481:LEU:O	1:B:484:ILE:HG12	2.21	0.40
1:B:38:MET:HE1	1:B:343:ASP:HA	2.03	0.40
1:B:299:ILE:HD11	1:B:376:TYR:O	2.21	0.40
1:A:184:VAL:CB	1:A:185:PRO:HD3	2.52	0.40
1:B:166:GLY:HA2	1:B:169:ILE:CG1	2.50	0.40
1:A:456:ILE:HB	1:C:176:GLN:OE1	2.21	0.40
1:A:151:ILE:HD11	1:B:151:ILE:CD1	2.51	0.40
1:B:147:LEU:CD1	1:C:147:LEU:HB3	2.52	0.40
1:B:360:ILE:HG22	1:B:360:ILE:O	2.21	0.40
1:C:71:TYR:CE2	1:C:75:LEU:HD11	2.57	0.40
1:A:25:LEU:HG	1:A:30:VAL:HG23	2.03	0.40
1:C:80:ILE:O	1:C:83:TYR:HB3	2.21	0.40
1:C:378:PHE:C	1:C:379:VAL:HG23	2.42	0.40
1:B:218:ILE:O	1:B:218:ILE:HG22	2.21	0.40
1:A:160:SER:C	1:A:162:GLN:N	2.73	0.40
1:B:477:SER:CB	1:C:154:THR:HG22	2.51	0.40
1:C:328:VAL:CG1	1:C:328:VAL:O	2.69	0.40
1:B:28:VAL:HA	1:B:301:TYR:CD1	2.57	0.40
1:C:296:VAL:CG2	1:C:313:PRO:O	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/490 (84%)	364 (88%)	41 (10%)	7 (2%)	11	41
1	B	414/490 (84%)	371 (90%)	36 (9%)	7 (2%)	11	41
1	C	420/490 (86%)	367 (87%)	46 (11%)	7 (2%)	11	41
All	All	1246/1470 (85%)	1102 (88%)	123 (10%)	21 (2%)	11	41

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	ASN
1	A	448	SER
1	B	359	ASN
1	B	380	ASN
1	B	447	ASN
1	B	448	SER
1	C	33	ASN
1	C	394	CYS
1	A	350	HIS
1	A	380	ASN
1	C	169	ILE
1	C	329	LYS
1	C	397	ILE
1	A	241	GLU
1	B	290	ASN
1	A	34	SER
1	A	304	GLN
1	B	241	GLU
1	B	342	SER
1	C	398	GLY
1	C	93	ILE

### 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	346/433 (80%)	324 (94%)	22 (6%)	22	55
1	B	340/433 (78%)	323 (95%)	17 (5%)	30	66
1	C	339/433 (78%)	311 (92%)	28 (8%)	14	44
All	All	1025/1299 (79%)	958 (94%)	67 (6%)	21	54

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	25	LEU
1	A	54	ILE
1	A	60	SER
1	A	61	ASN
1	A	66	GLN
1	A	161	VAL
1	A	198	GLN
1	A	221	LEU
1	A	229	GLN
1	A	239	ILE
1	A	249	ASP
1	A	252	ASP
1	A	253	ILE
1	A	266	VAL
1	A	280	VAL
1	A	281	ARG
1	A	323	LEU
1	A	339	ILE
1	A	368	VAL
1	A	428	ASN
1	A	458	ILE
1	B	54	ILE
1	B	94	VAL
1	B	153	ASP
1	B	192	CYS
1	B	203	LEU
1	B	210	LEU
1	B	221	LEU
1	B	229	GLN
1	B	253	ILE
1	B	299	ILE
1	B	301	TYR
1	B	302	ASN

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Mol	Chain	Res	Type
1	B	318	THR
1	B	393	THR
1	B	420	ILE
1	B	434	THR
1	B	458	ILE
1	C	25	LEU
1	C	30	VAL
1	C	54	ILE
1	C	65	ASP
1	C	66	GLN
1	C	147	LEU
1	C	151	ILE
1	C	154	THR
1	C	177	ASP
1	C	198	GLN
1	C	216	ASP
1	C	229	GLN
1	C	237	THR
1	C	247	THR
1	C	252	ASP
1	C	266	VAL
1	C	318	THR
1	C	323	LEU
1	C	366	THR
1	C	368	VAL
1	C	390	THR
1	C	391	THR
1	C	393	THR
1	C	399	ASN
1	C	434	THR
1	C	441	ASN
1	C	465	SER
1	C	479	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	61	ASN
1	A	162	GLN
1	A	206	HIS
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	229	GLN
1	A	279	GLN
1	A	399	ASN
1	A	423	ASN
1	B	61	ASN
1	B	66	GLN
1	B	206	HIS
1	B	222	GLN
1	B	229	GLN
1	B	272	ASN
1	B	279	GLN
1	B	302	ASN
1	B	315	HIS
1	B	414	HIS
1	B	423	ASN
1	B	441	ASN
1	C	61	ASN
1	C	70	GLN
1	C	155	ASN
1	C	198	GLN
1	C	272	ASN
1	C	302	ASN
1	C	380	ASN
1	C	403	GLN
1	C	414	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	1359	1	14,14,15	0.74	0	15,19,21	1.16	2 (13%)
2	NAG	B	1359	1	14,14,15	1.24	1 (7%)	15,19,21	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1359	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1359	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)
2	B	1359	NAG	C1-C2	3.78	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1359	NAG	C2-N2-C7	-2.52	119.81	123.04
2	A	1359	NAG	C4-C3-C2	-2.19	107.82	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1359	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	416/490 (84%)	-0.68	0 100 100	26, 53, 89, 123	0
1	B	418/490 (85%)	-0.72	0 100 100	23, 52, 87, 116	0
1	C	424/490 (86%)	-0.70	0 100 100	24, 56, 91, 117	0
All	All	1258/1470 (85%)	-0.70	0 100 100	23, 54, 90, 123	0

There are no RSRZ outliers to report.

### 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](#)

There are no carbohydrates in this entry.

### 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
2	NAG	A	1359	14/15	0.79	0.18	-	65,84,97,98	0
2	NAG	B	1359	14/15	0.73	0.21	-	49,99,105,105	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.