



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:20 AM GMT

PDB ID : 3OPM  
Title : Crystal Structure of Human DPP4 Bound to TAK-294  
Authors : Yano, J.K.; Aertgeerts, K.  
Deposited on : 2010-09-01  
Resolution : 2.72 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

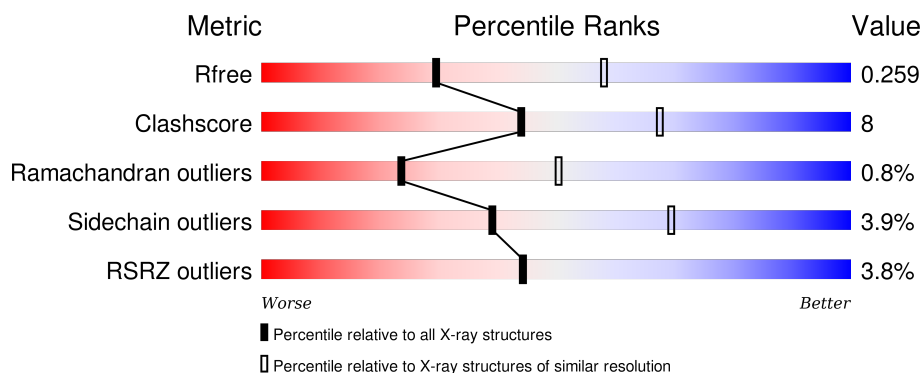
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	740	<div> <div>3%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	B	740	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
1	C	740	<div> <div>5%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	D	740	<div> <div>5%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>

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	A	3211	-	-	-	X
3	NAG	B	3211	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24713 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5950	3821	977	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	725	Total	C	N	O	S	0	0	0
			5937	3810	979	1122	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 48 discrepancies between the modelled and reference sequences:

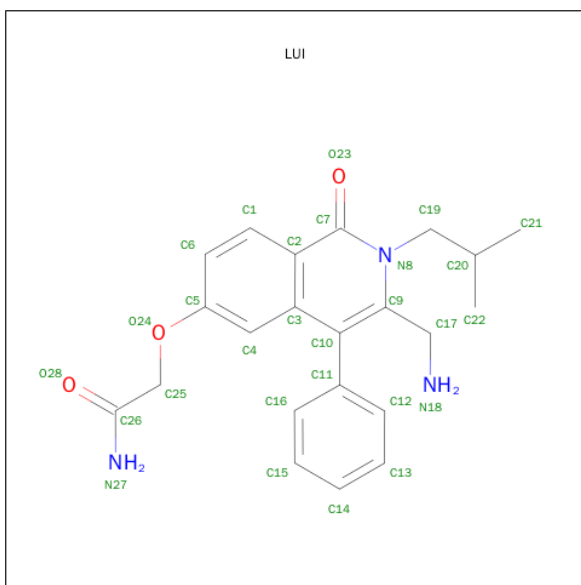
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
A	34	HIS	-	EXPRESSION TAG	UNP P27487
A	35	HIS	-	EXPRESSION TAG	UNP P27487
A	36	HIS	-	EXPRESSION TAG	UNP P27487
A	37	HIS	-	EXPRESSION TAG	UNP P27487
A	38	HIS	-	EXPRESSION TAG	UNP P27487
B	27	ALA	-	EXPRESSION TAG	UNP P27487
B	28	ASP	-	EXPRESSION TAG	UNP P27487
B	29	PRO	-	EXPRESSION TAG	UNP P27487
B	30	GLY	-	EXPRESSION TAG	UNP P27487
B	31	GLY	-	EXPRESSION TAG	UNP P27487
B	32	SER	-	EXPRESSION TAG	UNP P27487
B	33	HIS	-	EXPRESSION TAG	UNP P27487
B	34	HIS	-	EXPRESSION TAG	UNP P27487
B	35	HIS	-	EXPRESSION TAG	UNP P27487

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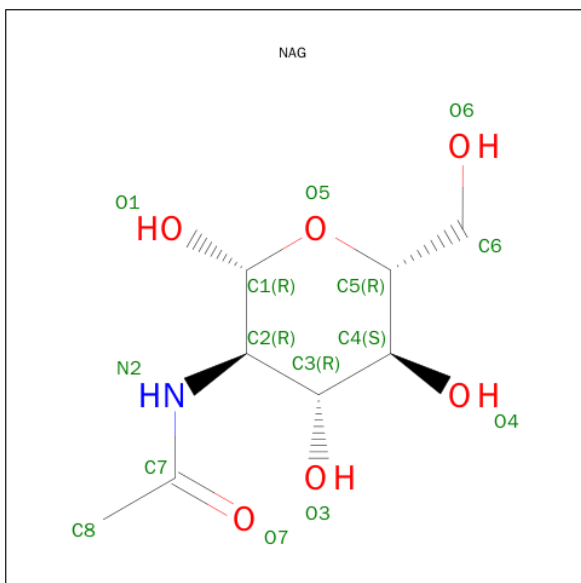
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
C	31	GLY	-	EXPRESSION TAG	UNP P27487
C	32	SER	-	EXPRESSION TAG	UNP P27487
C	33	HIS	-	EXPRESSION TAG	UNP P27487
C	34	HIS	-	EXPRESSION TAG	UNP P27487
C	35	HIS	-	EXPRESSION TAG	UNP P27487
C	36	HIS	-	EXPRESSION TAG	UNP P27487
C	37	HIS	-	EXPRESSION TAG	UNP P27487
C	38	HIS	-	EXPRESSION TAG	UNP P27487
D	27	ALA	-	EXPRESSION TAG	UNP P27487
D	28	ASP	-	EXPRESSION TAG	UNP P27487
D	29	PRO	-	EXPRESSION TAG	UNP P27487
D	30	GLY	-	EXPRESSION TAG	UNP P27487
D	31	GLY	-	EXPRESSION TAG	UNP P27487
D	32	SER	-	EXPRESSION TAG	UNP P27487
D	33	HIS	-	EXPRESSION TAG	UNP P27487
D	34	HIS	-	EXPRESSION TAG	UNP P27487
D	35	HIS	-	EXPRESSION TAG	UNP P27487
D	36	HIS	-	EXPRESSION TAG	UNP P27487
D	37	HIS	-	EXPRESSION TAG	UNP P27487
D	38	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is 2-{[3-(AMINOMETHYL)-2-(2-METHYLPROPYL)-1-OXO-4-PHENYL-1,2-DIHYDROISOQUINOLIN-6-YL]OXY}ACETAMIDE (three-letter code: LUI) (formula: C<sub>22</sub>H<sub>25</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 28	C 22	N 3	O 3	0	0
2	B	1	Total 28	C 22	N 3	O 3	0	0
2	C	1	Total 28	C 22	N 3	O 3	0	0
2	D	1	Total 28	C 22	N 3	O 3	0	0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	128	Total O 128 128	0	0
4	A	152	Total O 152 152	0	0
4	B	142	Total O 142 142	0	0

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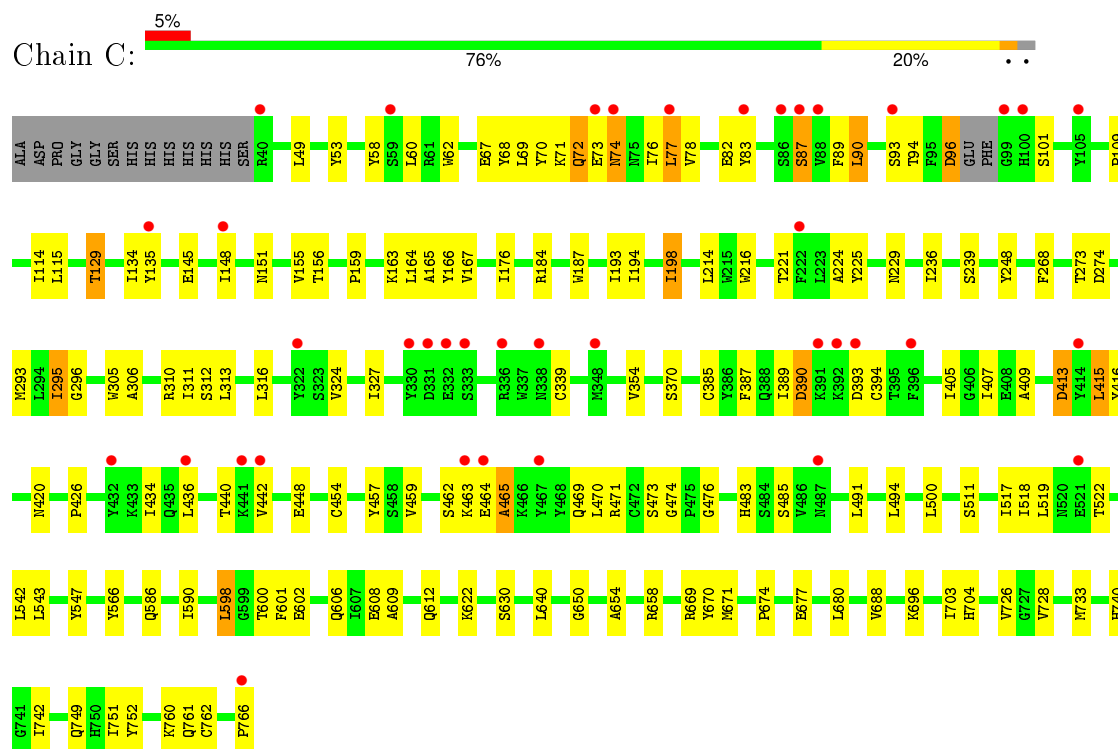
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	84	Total	O	0	0
			84	84		

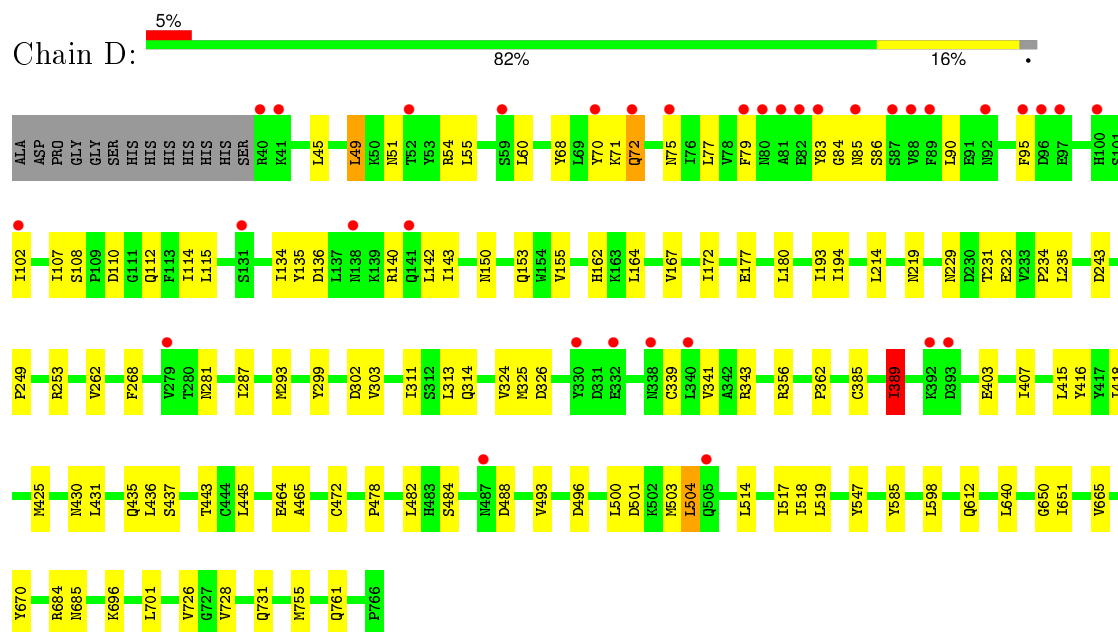




• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.77Å 122.56Å 144.74Å 90.00° 115.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.72 34.68 – 2.72	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.00-2.72) 97.5 (34.68-2.72)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.195 , 0.254 0.199 , 0.259	Depositor DCC
$R_{free}$ test set	5038 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.5	EDS
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 100685 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: LUI, 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	0.52	0/6122	0.63	0/8327
1	B	0.50	0/6190	0.61	0/8419
1	C	0.46	0/6107	0.58	0/8305
1	D	0.49	0/6129	0.62	1/8336 (0.0%)
All	All	0.49	0/24548	0.61	1/33387 (0.0%)

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
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	356	ARG	NE-CZ-NH1	5.34	122.97	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	96	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5950	0	5664	84	0
1	B	6013	0	5718	95	0
1	C	5937	0	5664	100	0
1	D	5957	0	5679	81	0
2	A	28	0	25	0	0
2	B	28	0	25	0	0
2	C	28	0	25	3	0
2	D	28	0	25	0	0
3	A	84	0	78	9	0
3	B	70	0	65	10	0
3	C	28	0	26	5	0
3	D	56	0	52	9	0
4	A	152	0	0	1	0
4	B	142	0	0	4	0
4	C	84	0	0	2	0
4	D	128	0	0	3	0
All	All	24713	0	23046	365	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 8.

All (365) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:HD21	3:B:1501:NAG:C1	1.09	1.57
1:C:229:ASN:HD21	3:C:2291:NAG:C1	1.07	1.55
1:B:229:ASN:HD21	3:B:2291:NAG:C1	0.94	1.54
1:B:281:ASN:HD21	3:B:2811:NAG:C1	1.16	1.51
1:D:229:ASN:HD21	3:D:2291:NAG:C1	1.15	1.51
1:A:281:ASN:HD21	3:A:2811:NAG:C1	0.89	1.50
1:D:281:ASN:HD21	3:D:2811:NAG:C1	1.29	1.42
1:D:219:ASN:HD21	3:D:2191:NAG:C1	1.44	1.27
1:B:150:ASN:HD21	3:B:1501:NAG:C2	1.72	1.02
1:D:193:ILE:HG22	1:D:194:ILE:HD12	1.45	0.99
3:A:2291:NAG:O4	3:A:2292:NAG:C1	2.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:THR:HG23	1:B:351:THR:HG23	1.54	0.88
1:A:82:GLU:OE2	1:A:467:TYR:OH	1.93	0.87
1:C:268:PHE:CD2	1:C:313:LEU:HD21	2.11	0.85
3:C:2291:NAG:HO4	3:C:2292:NAG:C1	1.92	0.82
1:C:193:ILE:HG22	1:C:194:ILE:HD12	1.62	0.81
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.62	0.80
1:C:470:LEU:HD12	1:C:483:HIS:NE2	1.98	0.79
1:B:327:ILE:HD13	1:B:389:ILE:CD1	2.12	0.79
1:A:63:ILE:HD11	1:A:69:LEU:HD12	1.63	0.79
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.64	0.78
1:C:72:GLN:HB2	1:C:77:LEU:HD11	1.66	0.77
1:C:630:SER:OG	1:C:740:HIS:NE2	2.19	0.75
1:A:347:GLU:OE1	1:A:373:LYS:NZ	2.18	0.74
1:B:327:ILE:HD13	1:B:389:ILE:HD11	1.70	0.74
1:B:327:ILE:HG21	1:B:389:ILE:HD11	1.69	0.73
1:A:321:ASN:CG	3:A:3211:NAG:C1	2.56	0.73
1:B:229:ASN:CG	3:B:2291:NAG:C1	2.58	0.72
1:D:193:ILE:HG22	1:D:194:ILE:CD1	2.19	0.72
1:C:407:ILE:HG23	1:C:415:LEU:HD21	1.73	0.70
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.72	0.70
1:C:71:LYS:HA	1:C:76:ILE:HD13	1.73	0.70
1:C:115:LEU:HD21	1:C:155:VAL:HG11	1.74	0.70
1:D:45:LEU:HG	1:D:49:LEU:HD22	1.72	0.69
1:D:107:ILE:HG22	1:D:108:SER:O	1.92	0.69
1:C:156:THR:HG23	1:C:216:TRP:HE1	1.57	0.69
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.75	0.68
1:A:115:LEU:HD21	1:A:155:VAL:HG21	1.76	0.68
3:A:2291:NAG:HO4	3:A:2292:NAG:C1	2.06	0.68
1:A:407:ILE:HG23	1:A:415:LEU:HD21	1.76	0.67
1:D:95:PHE:O	1:D:102:ILE:HD11	1.94	0.67
1:C:434:ILE:HG13	1:C:442:VAL:HG22	1.76	0.67
1:B:152:THR:HG21	1:B:155:VAL:HG22	1.75	0.67
1:D:517:ILE:HD12	1:D:612:GLN:HG3	1.77	0.67
1:B:517:ILE:HD12	1:B:612:GLN:HG3	1.77	0.67
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.76	0.67
1:D:407:ILE:HG23	1:D:415:LEU:HD21	1.77	0.66
1:C:511:SER:HB3	4:C:816:HOH:O	1.96	0.66
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.31	0.65
1:C:94:THR:HA	1:C:101:SER:HA	1.78	0.65
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.79	0.65
1:C:415:LEU:O	1:C:434:ILE:HG22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ASN:CG	3:D:2191:NAG:C1	2.64	0.65
1:C:114:ILE:HG22	1:C:135:TYR:HB2	1.77	0.65
1:C:518:ILE:O	1:C:519:LEU:HD23	1.97	0.64
1:B:407:ILE:HG23	1:B:415:LEU:HD21	1.79	0.64
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.80	0.64
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.27	0.64
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.79	0.64
1:A:194:ILE:HD12	3:A:2291:NAG:H82	1.81	0.63
1:C:542:LEU:HD23	1:C:543:LEU:N	2.13	0.63
1:C:464:GLU:O	1:C:465:ALA:CB	2.47	0.63
1:D:60:LEU:HD12	1:D:60:LEU:C	2.19	0.62
1:A:157:TRP:CE3	1:A:164:LEU:HD13	2.34	0.62
1:B:327:ILE:HD13	1:B:389:ILE:HD12	1.81	0.62
1:A:546:VAL:HG12	1:A:627:TRP:O	1.99	0.62
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.82	0.62
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.81	0.62
1:C:726:VAL:HG23	1:C:728:VAL:HG23	1.82	0.62
2:C:800:LUI:C16	2:C:800:LUI:HN18	2.12	0.62
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.83	0.61
1:B:281:ASN:ND2	4:B:891:HOH:O	2.35	0.60
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.36	0.60
1:C:94:THR:HG22	4:C:809:HOH:O	2.00	0.60
1:C:167:VAL:HG11	1:C:198:ILE:HD13	1.83	0.60
1:B:635:VAL:O	1:B:639:VAL:HG23	2.02	0.60
1:C:517:ILE:HD12	1:C:612:GLN:HG3	1.83	0.60
1:B:152:THR:HG21	1:B:155:VAL:CG2	2.31	0.60
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.82	0.60
1:C:464:GLU:O	1:C:465:ALA:HB2	2.02	0.60
1:D:268:PHE:CD2	1:D:313:LEU:HD11	2.37	0.60
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.84	0.60
1:A:512:LYS:HE2	1:A:556:ASP:O	2.02	0.60
2:C:800:LUI:C11	2:C:800:LUI:HN18	2.15	0.59
1:D:84:GLY:O	1:D:86:SER:N	2.35	0.59
1:B:208:PHE:O	1:B:209:SER:C	2.42	0.59
1:C:193:ILE:HG22	1:C:194:ILE:CD1	2.30	0.58
1:D:299:TYR:CE1	1:D:665:VAL:HG22	2.38	0.58
1:B:95:PHE:CZ	1:B:116:LEU:HD11	2.38	0.58
1:C:71:LYS:HZ2	1:C:74:ASN:HA	1.68	0.58
1:D:518:ILE:O	1:D:519:LEU:HD23	2.03	0.58
1:C:229:ASN:CG	3:C:2291:NAG:C1	2.69	0.58
1:D:60:LEU:HB2	1:D:68:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:ASP:OD1	1:C:390:ASP:N	2.35	0.58
1:C:96:ASP:N	1:C:96:ASP:OD2	2.36	0.58
1:D:55:LEU:HD12	1:D:500:LEU:CD2	2.34	0.58
1:C:306:ALA:HB3	1:C:310:ARG:HB3	1.85	0.58
1:B:150:ASN:CG	3:B:1501:NAG:C1	2.68	0.57
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.87	0.57
1:B:279:VAL:HG23	1:B:280:THR:HG23	1.86	0.57
1:B:471:ARG:HG2	1:B:480:TYR:CE1	2.39	0.57
1:B:85:ASN:CG	3:B:901:NAG:C1	2.64	0.57
1:C:53:TYR:HB3	1:C:500:LEU:HD11	1.86	0.57
3:C:2291:NAG:C4	3:C:2292:NAG:C1	2.83	0.57
1:A:517:ILE:HD12	1:A:612:GLN:HG3	1.88	0.56
1:B:542:LEU:HD23	1:B:542:LEU:C	2.26	0.56
1:A:174:VAL:HG23	1:A:185:ILE:HD11	1.86	0.56
1:C:608:GLU:O	1:C:612:GLN:HG2	2.06	0.56
1:B:190:LYS:HD3	1:B:193:ILE:HD12	1.88	0.56
1:A:486:VAL:HG13	1:A:487:ASN:H	1.71	0.56
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.88	0.56
3:A:2291:NAG:C4	3:A:2292:NAG:C1	2.84	0.56
1:C:459:VAL:HG23	1:C:469:GLN:O	2.05	0.56
1:D:229:ASN:CG	3:D:2291:NAG:C1	2.70	0.55
1:B:202:VAL:HG22	1:B:665:VAL:HG13	1.89	0.55
1:D:136:ASP:HB2	1:D:143:ILE:HD11	1.88	0.55
1:D:75:ASN:O	1:D:77:LEU:HD12	2.07	0.55
1:A:325:MET:CE	1:A:327:ILE:HD11	2.36	0.55
3:D:1501:NAG:H81	4:D:835:HOH:O	2.08	0.54
1:B:397:ILE:HG22	1:B:439:TYR:CE2	2.43	0.54
3:A:2811:NAG:H2	4:A:866:HOH:O	2.08	0.54
1:D:281:ASN:HD21	3:D:2811:NAG:C2	2.12	0.54
1:B:202:VAL:HG22	1:B:665:VAL:CG1	2.38	0.54
1:D:79:PHE:HA	1:D:86:SER:HB3	1.89	0.54
1:B:242:SER:OG	1:B:243:ASP:N	2.40	0.53
1:B:425:MET:CE	1:B:514:LEU:HD13	2.38	0.53
1:C:71:LYS:NZ	1:C:74:ASN:HA	2.24	0.53
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.44	0.53
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.43	0.53
1:A:55:LEU:HD23	1:A:500:LEU:HD23	1.88	0.53
1:A:500:LEU:HA	1:A:503:MET:HE3	1.89	0.53
1:D:435:GLN:HE21	1:D:437:SER:HG	1.57	0.53
1:A:415:LEU:HD23	1:A:416:TYR:N	2.24	0.53
1:A:69:LEU:HD22	1:A:76:ILE:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:LEU:HD22	1:C:76:ILE:CG2	2.39	0.52
1:B:316:LEU:HD13	1:B:320:GLN:HG2	1.91	0.52
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.44	0.52
1:C:70:TYR:O	1:C:77:LEU:HD12	2.10	0.52
1:D:500:LEU:HG	1:D:504:LEU:HD22	1.92	0.52
1:A:54:ARG:O	1:A:500:LEU:HD22	2.09	0.52
1:D:303:VAL:HG22	1:D:313:LEU:HD22	1.92	0.52
1:D:325:MET:HE1	1:D:362:PRO:HB3	1.91	0.52
2:C:800:LUI:N18	2:C:800:LUI:C11	2.72	0.52
1:C:293:MET:CE	1:C:324:VAL:HG23	2.40	0.52
1:C:78:VAL:HG13	1:C:78:VAL:O	2.10	0.52
1:D:232:GLU:CB	1:D:262:VAL:HG11	2.40	0.51
1:C:184:ARG:HD2	1:C:187:TRP:CZ2	2.45	0.51
1:A:720:SER:O	1:A:724:VAL:HG23	2.11	0.51
1:B:546:VAL:HG12	1:B:606:GLN:OE1	2.10	0.51
1:B:723:LEU:HD22	1:B:728:VAL:HG11	1.93	0.51
1:A:71:LYS:O	1:A:73:GLU:N	2.44	0.51
1:C:60:LEU:HD22	1:C:68:TYR:CG	2.45	0.51
1:B:81:ALA:HB1	1:B:482:LEU:HD11	1.93	0.51
1:C:229:ASN:ND2	3:C:2291:NAG:O5	2.43	0.50
1:C:518:ILE:HA	1:C:522:THR:O	2.11	0.50
1:D:153:GLN:OE1	1:D:167:VAL:HG12	2.10	0.50
1:B:658:ARG:HB2	1:B:689:MET:HE1	1.93	0.50
1:B:752:TYR:CD2	1:B:755:MET:HE3	2.46	0.50
1:A:620:ASP:C	1:A:620:ASP:OD2	2.49	0.50
1:D:235:LEU:HD13	1:D:253:ARG:HB3	1.93	0.50
1:C:312:SER:C	1:C:313:LEU:HD12	2.32	0.50
1:C:60:LEU:C	1:C:60:LEU:HD12	2.32	0.50
1:B:92:ASN:ND2	4:B:854:HOH:O	2.44	0.50
1:D:232:GLU:HB2	1:D:262:VAL:HG11	1.93	0.49
1:D:425:MET:HE3	1:D:514:LEU:HD12	1.94	0.49
1:A:107:ILE:HD11	1:A:114:ILE:HD12	1.94	0.49
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.94	0.49
1:A:321:ASN:ND2	3:A:3211:NAG:C2	2.64	0.49
1:A:598:LEU:O	1:A:682:HIS:NE2	2.44	0.49
1:D:194:ILE:HG12	3:D:2291:NAG:H82	1.94	0.49
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.93	0.49
1:A:562:ASN:OD1	1:A:564:ALA:HB3	2.12	0.49
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.41	0.49
1:B:107:ILE:HD12	1:B:107:ILE:N	2.27	0.49
1:D:343:ARG:HD2	1:D:389:ILE:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLN:HG3	1:D:77:LEU:HD13	1.95	0.49
1:A:477:LEU:HD12	1:A:477:LEU:H	1.77	0.49
1:A:69:LEU:HD22	1:A:76:ILE:CG2	2.43	0.48
1:B:107:ILE:HG22	1:B:108:SER:O	2.13	0.48
1:B:470:LEU:HD12	1:B:483:HIS:NE2	2.28	0.48
1:A:185:ILE:HD12	1:A:185:ILE:N	2.28	0.48
1:D:172:ILE:HD13	1:D:214:LEU:HD21	1.95	0.48
1:C:387:PHE:CD1	1:C:394:CYS:HB3	2.47	0.48
1:A:107:ILE:HG22	1:A:108:SER:O	2.13	0.48
1:C:248:TYR:OH	1:D:234:PRO:HG2	2.14	0.48
1:C:465:ALA:O	1:C:485:SER:OG	2.20	0.48
1:C:163:LYS:HE2	1:C:176:ILE:HD12	1.96	0.48
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.79	0.48
1:C:216:TRP:CZ3	1:C:273:THR:HG21	2.49	0.48
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.96	0.48
1:C:696:LYS:HG3	1:C:728:VAL:HG22	1.96	0.47
1:A:484:SER:O	1:A:488:ASP:HA	2.14	0.47
1:C:760:LYS:NZ	1:C:766:PRO:O	2.46	0.47
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.45	0.47
1:D:303:VAL:CG1	1:D:311:ILE:HD11	2.45	0.47
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.95	0.47
1:C:586:GLN:HB3	1:C:590:ILE:HD12	1.97	0.47
1:A:425:MET:CE	1:A:514:LEU:HD23	2.44	0.47
1:C:78:VAL:HG12	1:C:87:SER:O	2.13	0.47
1:B:640:LEU:HB3	1:B:698:VAL:HG21	1.96	0.47
1:A:242:SER:HB3	1:A:246:LEU:HD23	1.97	0.47
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.49	0.47
1:B:150:ASN:ND2	3:B:1501:NAG:C2	2.54	0.47
1:C:293:MET:HE2	1:C:324:VAL:HG23	1.97	0.47
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.96	0.47
1:D:472:CYS:O	1:D:478:PRO:HA	2.15	0.47
1:B:165:ALA:HB2	1:B:216:TRP:CZ2	2.50	0.47
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.95	0.47
1:C:295:ILE:HG13	1:C:296:GLY:N	2.30	0.47
1:B:85:ASN:ND2	3:B:901:NAG:O5	2.41	0.47
1:B:409:ALA:HB3	1:B:416:TYR:HB2	1.97	0.47
1:C:327:ILE:HD13	1:C:389:ILE:CD1	2.45	0.46
1:C:474:GLY:HA2	1:C:476:GLY:O	2.15	0.46
1:C:248:TYR:CZ	1:D:234:PRO:HG2	2.50	0.46
1:B:81:ALA:CB	1:B:482:LEU:HD11	2.45	0.46
1:B:600:THR:OG1	1:B:601:PHE:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:HD11	1:C:148:ILE:HD11	1.96	0.46
1:D:701:LEU:HD13	1:D:731:GLN:HB2	1.97	0.46
1:D:484:SER:O	1:D:488:ASP:HA	2.15	0.46
1:A:75:ASN:ND2	1:A:88:VAL:HG13	2.30	0.46
1:A:327:ILE:HD13	1:A:389:ILE:HD12	1.96	0.46
1:C:214:LEU:HD23	1:C:225:TYR:HB3	1.97	0.46
1:D:162:HIS:NE2	1:D:177:GLU:OE1	2.43	0.46
1:A:281:ASN:CG	3:A:2811:NAG:C1	2.70	0.46
1:C:268:PHE:CE2	1:C:313:LEU:HD21	2.50	0.46
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.97	0.46
1:C:115:LEU:HD21	1:C:155:VAL:CG1	2.42	0.46
1:B:723:LEU:HB3	1:B:728:VAL:HG13	1.98	0.46
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.51	0.46
1:D:110:ASP:OD2	1:D:112:GLN:NE2	2.49	0.46
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.42	0.46
1:C:89:PHE:O	1:C:90:LEU:CB	2.63	0.46
1:A:415:LEU:HB2	1:A:436:LEU:HD21	1.98	0.46
1:D:598:LEU:HD21	1:D:670:TYR:HB3	1.98	0.46
1:B:235:LEU:HD23	1:B:255:PRO:HA	1.97	0.46
1:C:602:GLU:OE2	1:C:602:GLU:N	2.44	0.46
1:C:600:THR:OG1	1:C:601:PHE:N	2.48	0.46
1:B:78:VAL:HG12	1:B:87:SER:O	2.16	0.46
1:D:268:PHE:CZ	1:D:313:LEU:HD21	2.51	0.45
1:B:542:LEU:HD23	1:B:543:LEU:N	2.31	0.45
1:D:155:VAL:HG12	1:D:164:LEU:HD22	1.99	0.45
1:D:415:LEU:HD23	1:D:416:TYR:N	2.32	0.45
1:B:81:ALA:HB1	1:B:482:LEU:CD1	2.47	0.45
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.99	0.45
1:A:519:LEU:O	1:A:520:ASN:C	2.54	0.45
1:A:327:ILE:HD12	1:A:343:ARG:O	2.17	0.45
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.51	0.45
1:A:63:ILE:CD1	1:A:69:LEU:HD12	2.42	0.45
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.98	0.45
1:D:431:LEU:CD2	1:D:445:LEU:HD12	2.47	0.45
1:D:403:GLU:OE2	1:D:585:TYR:HA	2.16	0.45
1:D:231:THR:HG23	4:D:861:HOH:O	2.17	0.45
1:B:281:ASN:HD21	3:B:2811:NAG:C2	2.10	0.45
1:A:486:VAL:HG13	1:A:487:ASN:N	2.31	0.45
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.47	0.45
1:B:614:SER:HA	1:B:619:VAL:HB	1.99	0.45
1:C:221:THR:HG23	1:C:274:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:LEU:HD22	1:A:671:MET:CG	2.45	0.45
1:D:418:ILE:HA	1:D:430:ASN:O	2.17	0.45
1:C:457:TYR:HA	1:C:471:ARG:O	2.18	0.44
1:D:299:TYR:CZ	1:D:665:VAL:HG22	2.53	0.44
1:B:658:ARG:NH1	4:B:817:HOH:O	2.43	0.44
1:D:293:MET:HE2	1:D:324:VAL:HG23	1.98	0.44
1:B:543:LEU:HD21	1:B:627:TRP:CD1	2.52	0.44
1:D:293:MET:CE	1:D:324:VAL:HG23	2.48	0.44
1:A:598:LEU:HB2	1:A:671:MET:SD	2.57	0.44
1:B:744:SER:HB2	1:B:747:ALA:HB3	1.98	0.44
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.99	0.44
1:B:680:LEU:HD11	1:B:684:ARG:CZ	2.48	0.44
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.44
1:C:313:LEU:HD12	1:C:313:LEU:N	2.33	0.44
1:D:115:LEU:HD12	1:D:134:ILE:HG12	1.98	0.44
1:C:409:ALA:HB3	1:C:416:TYR:HB2	2.00	0.44
1:B:631:TYR:O	1:B:634:TYR:HB3	2.17	0.44
1:A:69:LEU:HD23	1:A:77:LEU:O	2.18	0.44
1:B:388:GLN:HB2	1:B:391:LYS:HG2	2.00	0.44
1:C:654:ALA:HA	1:C:704:HIS:CE1	2.53	0.43
1:B:150:ASN:O	1:B:151:ASN:HB2	2.19	0.43
1:A:487:ASN:HD21	1:A:489:LYS:HD3	1.83	0.43
1:B:114:ILE:HG23	1:B:135:TYR:HB3	2.00	0.43
1:B:765:LEU:HD22	4:B:867:HOH:O	2.17	0.43
1:A:170:ASN:O	1:A:196:ASN:HB2	2.18	0.43
1:B:326:ASP:OD2	1:B:344:GLN:HG2	2.18	0.43
1:C:405:ILE:HG22	1:C:405:ILE:O	2.18	0.43
1:C:674:PRO:O	1:C:680:LEU:HD13	2.17	0.43
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.53	0.43
1:A:107:ILE:CD1	1:A:114:ILE:HD12	2.48	0.43
1:A:102:ILE:HG21	1:A:116:LEU:HD22	2.00	0.43
1:A:115:LEU:HD21	1:A:155:VAL:CG2	2.48	0.43
1:D:684:ARG:HG3	4:D:825:HOH:O	2.18	0.43
1:C:155:VAL:HG23	1:C:166:TYR:HB3	2.00	0.43
1:C:387:PHE:CZ	1:C:394:CYS:SG	3.12	0.43
1:A:674:PRO:O	1:A:680:LEU:HD13	2.19	0.43
1:A:136:ASP:HB2	1:A:143:ILE:HD11	2.01	0.43
1:D:281:ASN:CG	3:D:2811:NAG:C1	2.83	0.43
1:C:193:ILE:C	1:C:194:ILE:HD12	2.39	0.43
1:C:415:LEU:HB2	1:C:436:LEU:HD11	2.01	0.43
1:D:425:MET:CE	1:D:514:LEU:HD12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ALA:O	1:B:295:ILE:HG23	2.18	0.43
1:C:415:LEU:HD13	1:C:415:LEU:C	2.39	0.43
1:C:58:TYR:CD1	1:C:494:LEU:HD13	2.54	0.43
1:A:90:LEU:HD21	1:A:114:ILE:HD13	2.01	0.42
1:B:723:LEU:CD2	1:B:728:VAL:HG11	2.48	0.42
1:B:741:GLY:O	1:B:742:ILE:C	2.55	0.42
1:A:190:LYS:HE2	1:A:193:ILE:HD12	2.00	0.42
1:C:761:GLN:NE2	1:D:761:GLN:HE22	2.17	0.42
1:D:60:LEU:HD13	1:D:68:TYR:HB2	2.02	0.42
1:D:54:ARG:NH1	1:D:54:ARG:HB2	2.35	0.42
1:A:251:THR:OG1	1:B:237:GLU:OE2	2.25	0.42
1:A:499:ALA:O	1:A:503:MET:HE3	2.20	0.42
1:D:493:VAL:HG11	1:D:496:ASP:HB3	2.01	0.42
1:C:413:ASP:OD1	1:C:413:ASP:N	2.52	0.42
1:C:129:THR:HG23	1:C:151:ASN:HA	2.02	0.42
1:C:72:GLN:CB	1:C:77:LEU:HD11	2.43	0.42
1:B:148:ILE:HG23	1:B:149:PRO:HD2	2.02	0.42
1:D:415:LEU:C	1:D:415:LEU:HD23	2.40	0.42
1:C:236:ILE:HD12	1:D:249:PRO:HD2	2.00	0.42
1:A:513:LYS:O	1:A:527:GLN:HA	2.20	0.42
1:B:157:TRP:CZ3	1:B:164:LEU:HD13	2.54	0.42
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.55	0.42
1:B:295:ILE:HD11	1:B:317:ARG:NH1	2.35	0.42
1:C:751:ILE:HG23	1:C:752:TYR:N	2.35	0.42
1:B:213:ALA:HB1	1:B:226:ALA:HB3	2.01	0.42
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.84	0.41
1:B:471:ARG:CG	1:B:480:TYR:CE1	3.02	0.41
1:D:134:ILE:HD11	1:D:164:LEU:CD1	2.50	0.41
1:C:703:ILE:HA	1:C:733:MET:O	2.20	0.41
1:B:73:GLU:C	1:B:75:ASN:H	2.22	0.41
1:C:165:ALA:HB2	1:C:216:TRP:CZ2	2.55	0.41
1:A:438:ASP:OD2	1:A:440:THR:HB	2.20	0.41
1:A:236:ILE:HD13	1:A:712:HIS:ND1	2.35	0.41
1:C:606:GLN:O	1:C:609:ALA:HB3	2.21	0.41
1:B:76:ILE:HD12	1:B:90:LEU:CD2	2.50	0.41
1:A:72:GLN:O	1:A:74:ASN:N	2.52	0.41
1:D:651:ILE:HD13	1:D:755:MET:HG2	2.00	0.41
1:A:658:ARG:CB	1:A:687:THR:HG22	2.47	0.41
1:C:420:ASN:ND2	1:C:426:PRO:HA	2.35	0.41
1:B:109:PRO:HG3	1:B:158:SER:O	2.20	0.41
1:D:70:TYR:HB3	1:D:79:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ILE:HG22	1:B:439:TYR:CZ	2.56	0.41
1:B:65:ASP:OD2	1:B:464:GLU:N	2.47	0.41
1:C:62:TRP:CD2	1:C:462:SER:HA	2.56	0.41
1:D:79:PHE:HA	1:D:86:SER:CB	2.50	0.41
1:B:751:ILE:HG12	1:B:755:MET:HE2	2.01	0.41
1:B:331:ASP:HB3	1:B:334:SER:HB3	2.03	0.41
1:C:305:TRP:CZ2	1:C:311:ILE:HD12	2.55	0.41
1:D:287:ILE:CG2	1:D:339:CYS:SG	3.09	0.41
1:B:215:TRP:HB2	1:B:224:ALA:HB3	2.03	0.41
1:C:407:ILE:CG2	1:C:415:LEU:HD21	2.47	0.40
1:D:115:LEU:HD21	1:D:155:VAL:HG11	2.02	0.40
1:A:208:PHE:O	1:A:209:SER:C	2.59	0.40
1:B:308:GLN:OE1	1:B:308:GLN:HA	2.20	0.40
1:D:303:VAL:HG22	1:D:313:LEU:CD2	2.52	0.40
1:C:454:CYS:HB3	1:C:457:TYR:CZ	2.56	0.40
1:B:435:GLN:NE2	1:B:437:SER:OG	2.50	0.40
1:A:490:GLY:O	1:A:491:LEU:C	2.60	0.40
1:B:708:ASP:OD1	1:B:740:HIS:HA	2.21	0.40
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.56	0.40
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.89	0.40
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.56	0.40
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.56	0.40
1:B:509:MET:HE3	1:B:510:PRO:HD2	2.02	0.40
1:A:60:LEU:C	1:A:60:LEU:HD12	2.42	0.40
1:C:155:VAL:HG22	1:C:164:LEU:HD11	2.04	0.40
1:D:464:GLU:O	1:D:465:ALA:HB3	2.22	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	725/740 (98%)	677 (93%)	42 (6%)	6 (1%)	24	50
1	B	731/740 (99%)	691 (94%)	39 (5%)	1 (0%)	56	83
1	C	721/740 (97%)	673 (93%)	39 (5%)	9 (1%)	16	38
1	D	725/740 (98%)	674 (93%)	45 (6%)	6 (1%)	24	50
All	All	2902/2960 (98%)	2715 (94%)	165 (6%)	22 (1%)	24	50

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	73	GLU
1	C	90	LEU
1	C	93	SER
1	C	465	ALA
1	D	85	ASN
1	A	92	ASN
1	D	503	MET
1	A	491	LEU
1	C	393	ASP
1	D	51	ASN
1	D	72	GLN
1	A	714	GLN
1	B	96	ASP
1	C	73	GLU
1	C	463	LYS
1	D	389	ILE
1	C	82	GLU
1	D	150	ASN
1	C	109	PRO
1	A	88	VAL
1	C	742	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	651/662 (98%)	625 (96%)	26 (4%)	38	68
1	B	658/662 (99%)	631 (96%)	27 (4%)	37	67
1	C	650/662 (98%)	618 (95%)	32 (5%)	31	60
1	D	652/662 (98%)	634 (97%)	18 (3%)	51	80
All	All	2611/2648 (99%)	2508 (96%)	103 (4%)	39	69

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	75	ASN
1	A	87	SER
1	A	133	ASP
1	A	138	ASN
1	A	142	LEU
1	A	212	SER
1	A	283	THR
1	A	334	SER
1	A	340	LEU
1	A	360	SER
1	A	385	CYS
1	A	390	ASP
1	A	413	ASP
1	A	433	LYS
1	A	440	THR
1	A	443	THR
1	A	472	CYS
1	A	482	LEU
1	A	488	ASP
1	A	504	LEU
1	A	547	TYR
1	A	566	TYR
1	A	594	ILE
1	A	598	LEU
1	A	677	GLU
1	B	51	ASN
1	B	72	GLN
1	B	80	ASN
1	B	96	ASP
1	B	98	PHE
1	B	141	GLN
1	B	164	LEU

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Mol	Chain	Res	Type
1	B	316	LEU
1	B	354	VAL
1	B	358	ARG
1	B	385	CYS
1	B	436	LEU
1	B	452	GLU
1	B	472	CYS
1	B	482	LEU
1	B	514	LEU
1	B	521	GLU
1	B	547	TYR
1	B	554	LYS
1	B	589	LYS
1	B	594	ILE
1	B	627	TRP
1	B	630	SER
1	B	665	VAL
1	B	677	GLU
1	B	688	VAL
1	B	704	HIS
1	C	67	GLU
1	C	72	GLN
1	C	74	ASN
1	C	77	LEU
1	C	83	TYR
1	C	87	SER
1	C	96	ASP
1	C	129	THR
1	C	145	GLU
1	C	198	ILE
1	C	239	SER
1	C	295	ILE
1	C	316	LEU
1	C	339	CYS
1	C	354	VAL
1	C	370	SER
1	C	385	CYS
1	C	390	ASP
1	C	413	ASP
1	C	415	LEU
1	C	440	THR
1	C	448	GLU

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Mol	Chain	Res	Type
1	C	473	SER
1	C	491	LEU
1	C	547	TYR
1	C	566	TYR
1	C	598	LEU
1	C	622	LYS
1	C	658	ARG
1	C	677	GLU
1	C	688	VAL
1	C	762	CYS
1	D	49	LEU
1	D	71	LYS
1	D	83	TYR
1	D	140	ARG
1	D	142	LEU
1	D	180	LEU
1	D	243	ASP
1	D	326	ASP
1	D	341	VAL
1	D	385	CYS
1	D	389	ILE
1	D	436	LEU
1	D	443	THR
1	D	482	LEU
1	D	501	ASP
1	D	504	LEU
1	D	547	TYR
1	D	685	ASN

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

Mol	Chain	Res	Type
1	A	112	GLN
1	A	119	ASN
1	A	281	ASN
1	B	119	ASN
1	B	150	ASN
1	B	169	ASN
1	B	229	ASN
1	B	281	ASN
1	B	314	GLN
1	B	748	HIS

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Mol	Chain	Res	Type
1	C	72	GLN
1	C	74	ASN
1	C	229	ASN
1	C	314	GLN
1	C	344	GLN
1	C	508	GLN
1	C	592	HIS
1	C	612	GLN
1	D	92	ASN
1	D	112	GLN
1	D	229	ASN
1	D	281	ASN
1	D	369	ASN
1	D	748	HIS
1	D	761	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	1501	1	14,14,15	0.66	0	15,19,21	1.70	4 (26%)
3	NAG	A	2191	1	14,14,15	0.65	0	15,19,21	1.08	1 (6%)
3	NAG	A	2291	1	14,14,15	0.63	0	15,19,21	1.30	1 (6%)
3	NAG	A	2292	-	14,14,15	0.64	0	15,19,21	1.19	1 (6%)
3	NAG	A	2811	1	14,14,15	0.85	0	15,19,21	1.34	4 (26%)
3	NAG	A	3211	1	14,14,15	0.57	0	15,19,21	0.77	0
2	LUI	A	800	-	28,30,30	2.72	5 (17%)	30,42,42	1.77	3 (10%)
3	NAG	B	1501	1	14,14,15	0.56	0	15,19,21	1.35	1 (6%)
3	NAG	B	2291	1	14,14,15	0.49	0	15,19,21	1.14	1 (6%)
3	NAG	B	2811	1	14,14,15	0.50	0	15,19,21	0.90	0
3	NAG	B	3211	1	14,14,15	0.69	0	15,19,21	1.23	1 (6%)
2	LUI	B	800	-	28,30,30	2.62	5 (17%)	30,42,42	1.85	3 (10%)
3	NAG	B	901	1	14,14,15	0.75	0	15,19,21	2.23	4 (26%)
3	NAG	C	2291	1,3	14,14,15	0.44	0	15,19,21	1.21	1 (6%)
3	NAG	C	2292	3	14,14,15	0.55	0	15,19,21	1.35	2 (13%)
2	LUI	C	800	-	28,30,30	2.97	5 (17%)	30,42,42	1.74	3 (10%)
3	NAG	D	1501	1	14,14,15	0.83	0	15,19,21	1.52	3 (20%)
3	NAG	D	2191	1	14,14,15	0.58	0	15,19,21	0.94	1 (6%)
3	NAG	D	2291	1	14,14,15	0.50	0	15,19,21	2.25	2 (13%)
3	NAG	D	2811	1	14,14,15	0.84	0	15,19,21	1.31	2 (13%)
2	LUI	D	800	-	28,30,30	2.94	4 (14%)	30,42,42	1.89	3 (10%)

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	1501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2191	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2291	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2292	-	-	0/6/23/26	0/1/1/1
3	NAG	A	2811	1	-	0/6/23/26	0/1/1/1
3	NAG	A	3211	1	-	0/6/23/26	0/1/1/1
2	LUI	A	800	-	-	0/13/15/15	0/3/3/3
3	NAG	B	1501	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2291	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2811	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	3211	1	-	0/6/23/26	0/1/1/1
2	LUI	B	800	-	-	0/13/15/15	0/3/3/3
3	NAG	B	901	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2291	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2292	3	-	0/6/23/26	0/1/1/1
2	LUI	C	800	-	-	0/13/15/15	0/3/3/3
3	NAG	D	1501	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2191	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2291	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2811	1	-	0/6/23/26	0/1/1/1
2	LUI	D	800	-	-	0/13/15/15	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	LUI	C3-C2	-2.75	1.38	1.42
2	A	800	LUI	C7-N8	-2.55	1.34	1.38
2	B	800	LUI	C3-C2	-2.54	1.38	1.42
2	A	800	LUI	C3-C2	-2.37	1.38	1.42
2	D	800	LUI	C3-C2	-2.31	1.38	1.42
2	B	800	LUI	C7-N8	-2.17	1.35	1.38
2	C	800	LUI	C7-N8	-2.06	1.35	1.38
2	A	800	LUI	C10-C3	2.20	1.47	1.43
2	D	800	LUI	C10-C3	2.27	1.47	1.43
2	B	800	LUI	C10-C3	2.35	1.47	1.43
2	C	800	LUI	C10-C3	2.66	1.48	1.43
2	C	800	LUI	C7-C2	4.63	1.49	1.41
2	B	800	LUI	C7-C2	4.70	1.49	1.41
2	A	800	LUI	C7-C2	5.01	1.49	1.41
2	D	800	LUI	C7-C2	5.24	1.50	1.41
2	B	800	LUI	C10-C9	11.95	1.48	1.36
2	A	800	LUI	C10-C9	12.44	1.48	1.36
2	D	800	LUI	C10-C9	13.75	1.49	1.36
2	C	800	LUI	C10-C9	13.99	1.50	1.36

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	LUI	C12-C11-C10	-3.57	115.18	120.76
2	B	800	LUI	C12-C11-C10	-3.39	115.47	120.76
2	A	800	LUI	C12-C11-C10	-3.23	115.72	120.76
3	B	2291	NAG	C3-C2-N2	-3.00	103.38	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	NAG	C3-C2-N2	-2.95	103.49	110.56
3	A	1501	NAG	C4-C3-C2	-2.68	107.07	111.23
3	B	901	NAG	O7-C7-C8	-2.61	117.27	122.06
3	C	2291	NAG	O4-C4-C3	-2.26	105.25	110.34
2	C	800	LUI	O24-C5-C4	-2.25	116.35	123.89
2	A	800	LUI	C16-C11-C10	2.09	124.02	120.76
3	D	1501	NAG	O4-C4-C5	2.09	114.77	109.24
3	C	2292	NAG	O7-C7-N2	2.09	126.13	121.86
3	D	1501	NAG	O3-C3-C2	2.11	113.30	109.11
2	B	800	LUI	C16-C11-C10	2.14	124.10	120.76
3	A	2811	NAG	C3-C2-N2	2.14	115.69	110.56
3	A	2811	NAG	C4-C3-C2	2.14	114.56	111.23
3	D	2191	NAG	C2-N2-C7	2.21	125.88	123.04
3	A	2292	NAG	C3-C2-N2	2.29	116.04	110.56
3	D	2811	NAG	C2-N2-C7	2.31	126.01	123.04
3	A	2811	NAG	C1-O5-C5	2.33	115.21	112.25
3	A	1501	NAG	C3-C2-N2	2.46	116.44	110.56
3	C	2292	NAG	C3-C2-N2	2.47	116.48	110.56
3	D	2291	NAG	C3-C4-C5	2.52	114.59	110.20
3	A	2191	NAG	C3-C2-N2	2.59	116.75	110.56
2	D	800	LUI	C16-C11-C10	2.62	124.86	120.76
3	A	1501	NAG	C1-O5-C5	2.63	115.58	112.25
3	A	2811	NAG	C3-C4-C5	2.78	115.05	110.20
3	D	2811	NAG	C4-C3-C2	2.91	115.75	111.23
3	D	1501	NAG	C2-N2-C7	3.41	127.41	123.04
3	A	1501	NAG	C2-N2-C7	3.45	127.47	123.04
3	B	1501	NAG	C1-O5-C5	3.53	116.73	112.25
3	A	2291	NAG	C3-C4-C5	3.76	116.75	110.20
3	B	3211	NAG	C4-C3-C2	3.77	117.08	111.23
2	C	800	LUI	C25-O24-C5	4.23	125.62	117.62
3	B	901	NAG	C4-C3-C2	4.30	117.92	111.23
3	B	901	NAG	C1-O5-C5	4.63	118.13	112.25
2	C	800	LUI	C2-C7-N8	7.40	122.20	116.09
3	D	2291	NAG	C1-O5-C5	7.54	121.82	112.25
2	A	800	LUI	C2-C7-N8	7.62	122.38	116.09
2	D	800	LUI	C2-C7-N8	7.88	122.60	116.09
2	B	800	LUI	C2-C7-N8	7.90	122.62	116.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2291	NAG	4	0
3	A	2292	NAG	3	0
3	A	2811	NAG	3	0
3	A	3211	NAG	2	0
3	B	1501	NAG	4	0
3	B	2291	NAG	2	0
3	B	2811	NAG	2	0
3	B	901	NAG	2	0
3	C	2291	NAG	5	0
3	C	2292	NAG	2	0
2	C	800	LUI	3	0
3	D	1501	NAG	1	0
3	D	2191	NAG	2	0
3	D	2291	NAG	3	0
3	D	2811	NAG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	727/740 (98%)	-0.04	25 (3%) 49 49	21, 42, 79, 100	0
1	B	733/740 (99%)	-0.16	14 (1%) 70 71	24, 46, 69, 85	0
1	C	725/740 (97%)	0.19	39 (5%) 29 28	25, 61, 101, 122	0
1	D	727/740 (98%)	0.02	34 (4%) 35 34	24, 47, 91, 117	0
All	All	2912/2960 (98%)	0.00	112 (3%) 44 44	21, 48, 91, 122	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	SER	4.7
1	D	92	ASN	4.6
1	C	73	GLU	4.5
1	D	97	GLU	4.5
1	D	81	ALA	4.4
1	D	72	GLN	4.4
1	C	40	ARG	4.3
1	A	97	GLU	4.1
1	A	73	GLU	3.9
1	A	88	VAL	3.8
1	C	441	LYS	3.8
1	C	333	SER	3.8
1	D	89	PHE	3.8
1	C	330	TYR	3.7
1	A	87	SER	3.7
1	D	87	SER	3.6
1	C	464	GLU	3.6
1	D	100	HIS	3.5
1	C	100	HIS	3.4
1	D	82	GLU	3.4
1	B	72	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	81	ALA	3.3
1	D	83	TYR	3.2
1	A	95	PHE	3.2
1	D	279	VAL	3.2
1	C	77	LEU	3.1
1	D	79	PHE	3.1
1	B	70	TYR	3.1
1	C	467	TYR	3.0
1	A	98	PHE	3.0
1	B	81	ALA	2.9
1	D	41	LYS	2.9
1	A	140	ARG	2.9
1	C	766	PRO	2.9
1	A	72	GLN	2.9
1	C	393	ASP	2.9
1	C	442	VAL	2.8
1	C	332	GLU	2.8
1	D	85	ASN	2.8
1	D	392	LYS	2.8
1	A	766	PRO	2.8
1	D	95	PHE	2.8
1	B	34	HIS	2.7
1	A	279	VAL	2.7
1	C	105	TYR	2.7
1	D	40	ARG	2.7
1	B	88	VAL	2.7
1	C	432	TYR	2.7
1	C	88	VAL	2.7
1	C	87	SER	2.6
1	C	222	PHE	2.6
1	B	87	SER	2.6
1	C	86	SER	2.6
1	D	393	ASP	2.6
1	B	86	SER	2.6
1	A	144	THR	2.6
1	D	70	TYR	2.6
1	C	396	PHE	2.6
1	D	340	LEU	2.6
1	C	348	MET	2.5
1	A	332	GLU	2.5
1	C	391	LYS	2.5
1	D	102	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	78	VAL	2.5
1	C	74	ASN	2.5
1	C	331	ASP	2.5
1	C	487	ASN	2.5
1	A	86	SER	2.5
1	A	89	PHE	2.5
1	A	96	ASP	2.4
1	A	57	LEU	2.4
1	C	436	LEU	2.4
1	C	59	SER	2.4
1	D	52	THR	2.4
1	C	93	SER	2.4
1	D	131	SER	2.4
1	A	77	LEU	2.4
1	C	463	LYS	2.4
1	D	75	ASN	2.4
1	C	135	TYR	2.3
1	D	487	ASN	2.3
1	D	96	ASP	2.3
1	D	88	VAL	2.3
1	B	84	GLY	2.3
1	B	89	PHE	2.2
1	D	80	ASN	2.2
1	C	322	TYR	2.2
1	D	330	TYR	2.2
1	B	73	GLU	2.2
1	A	91	GLU	2.2
1	C	148	ILE	2.2
1	A	92	ASN	2.2
1	A	74	ASN	2.1
1	C	99	GLY	2.1
1	C	83	TYR	2.1
1	C	414	TYR	2.1
1	B	83	TYR	2.1
1	B	140	ARG	2.1
1	C	336	ARG	2.1
1	A	138	ASN	2.1
1	C	521	GLU	2.1
1	D	59	SER	2.1
1	D	338	ASN	2.1
1	D	141	GLN	2.1
1	D	505	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	392	LYS	2.1
1	C	338	ASN	2.1
1	A	392	LYS	2.1
1	D	332	GLU	2.1
1	B	71	LYS	2.0
1	A	101	SER	2.0
1	D	138	ASN	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](#)

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
3	NAG	B	3211	14/15	0.84	0.36	5.29	55,57,57,58	0
3	NAG	A	3211	14/15	0.93	0.26	4.54	49,52,54,55	0
3	NAG	D	2291	14/15	0.89	0.21	1.37	50,51,53,54	0
2	LUI	A	800	28/28	0.95	0.21	0.89	36,40,47,50	0
2	LUI	B	800	28/28	0.97	0.17	0.36	37,39,40,40	0
3	NAG	A	2291	14/15	0.93	0.19	0.33	45,48,50,51	0
2	LUI	D	800	28/28	0.96	0.15	0.31	35,38,42,43	0
2	LUI	C	800	28/28	0.95	0.16	-0.17	39,41,46,47	0
3	NAG	B	2291	14/15	0.91	0.14	-0.47	45,48,49,49	0
3	NAG	C	2291	14/15	0.94	0.13	-1.11	42,44,46,46	0
3	NAG	A	2191	14/15	0.81	0.33	-	53,56,59,60	0
3	NAG	D	1501	14/15	0.82	0.28	-	51,53,54,54	0
3	NAG	B	901	14/15	0.75	0.15	-	53,54,55,55	0
3	NAG	B	1501	14/15	0.89	0.27	-	50,51,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1501	14/15	0.80	0.32	-	53,55,57,59	0
3	NAG	D	2811	14/15	0.83	0.22	-	52,53,54,54	0
3	NAG	A	2292	14/15	0.86	0.24	-	50,51,52,52	0
3	NAG	A	2811	14/15	0.76	0.17	-	48,51,54,54	0
3	NAG	B	2811	14/15	0.87	0.13	-	51,52,55,55	0
3	NAG	D	2191	14/15	0.87	0.28	-	51,53,57,58	0
3	NAG	C	2292	14/15	0.82	0.24	-	55,55,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.