



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:26 AM GMT

PDB ID : 3ENH  
Title : Crystal structure of Cgi121/Bud32/Kae1 complex  
Authors : Neculai, D.  
Deposited on : 2008-09-25  
Resolution : 3.60 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

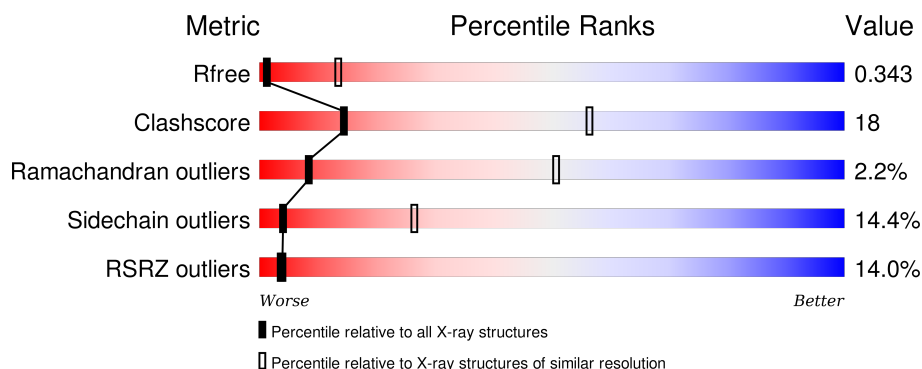
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	540	
1	B	540	
2	C	150	
2	D	150	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TBR	A	4769	-	-	-	X
3	TBR	A	5769	-	-	X	-
3	TBR	B	2769	-	-	-	X
3	TBR	B	7769	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10142 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 Putative O-sialoglycoprotein endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3926	2509	661	736	20			
1	B	485	Total	C	N	O	S	0	0	0
			3856	2466	643	726	21			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q58530
A	-3	ALA	-	EXPRESSION TAG	UNP Q58530
A	-2	MET	-	EXPRESSION TAG	UNP Q58530
A	-1	ASP	-	EXPRESSION TAG	UNP Q58530
A	0	PRO	-	EXPRESSION TAG	UNP Q58530
B	-4	GLY	-	EXPRESSION TAG	UNP Q58530
B	-3	ALA	-	EXPRESSION TAG	UNP Q58530
B	-2	MET	-	EXPRESSION TAG	UNP Q58530
B	-1	ASP	-	EXPRESSION TAG	UNP Q58530
B	0	PRO	-	EXPRESSION TAG	UNP Q58530

- Molecule 2 is a protein called Uncharacterized protein MJ0187.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	138	Total	C	N	O	S	0	0	0
			1108	708	196	200	4			
2	D	138	Total	C	N	O	S	0	0	0
			1108	708	196	200	4			

There are 10 discrepancies between the modelled and reference sequences:

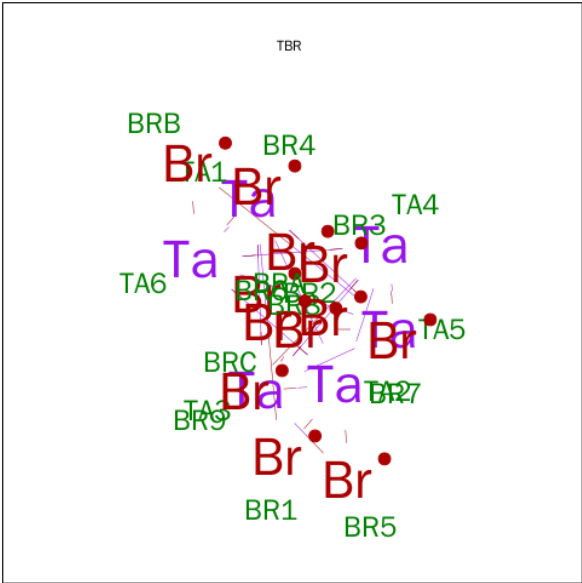
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLY	-	EXPRESSION TAG	UNP Q57646
C	2	ALA	-	EXPRESSION TAG	UNP Q57646

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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	MET	-	EXPRESSION TAG	UNP Q57646
C	4	ASP	-	EXPRESSION TAG	UNP Q57646
C	5	PRO	-	EXPRESSION TAG	UNP Q57646
D	1	GLY	-	EXPRESSION TAG	UNP Q57646
D	2	ALA	-	EXPRESSION TAG	UNP Q57646
D	3	MET	-	EXPRESSION TAG	UNP Q57646
D	4	ASP	-	EXPRESSION TAG	UNP Q57646
D	5	PRO	-	EXPRESSION TAG	UNP Q57646

- Molecule 3 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: Br<sub>12</sub>Ta<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	B	1	Total	Br	Ta	0	0
			18	12	6		
3	B	1	Total	Br	Ta	0	0
			18	12	6		
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	A	1	Total	Br	Ta	0	0
			18	12	6		
3	B	1	Total	Br	Ta	0	0
			18	12	6		

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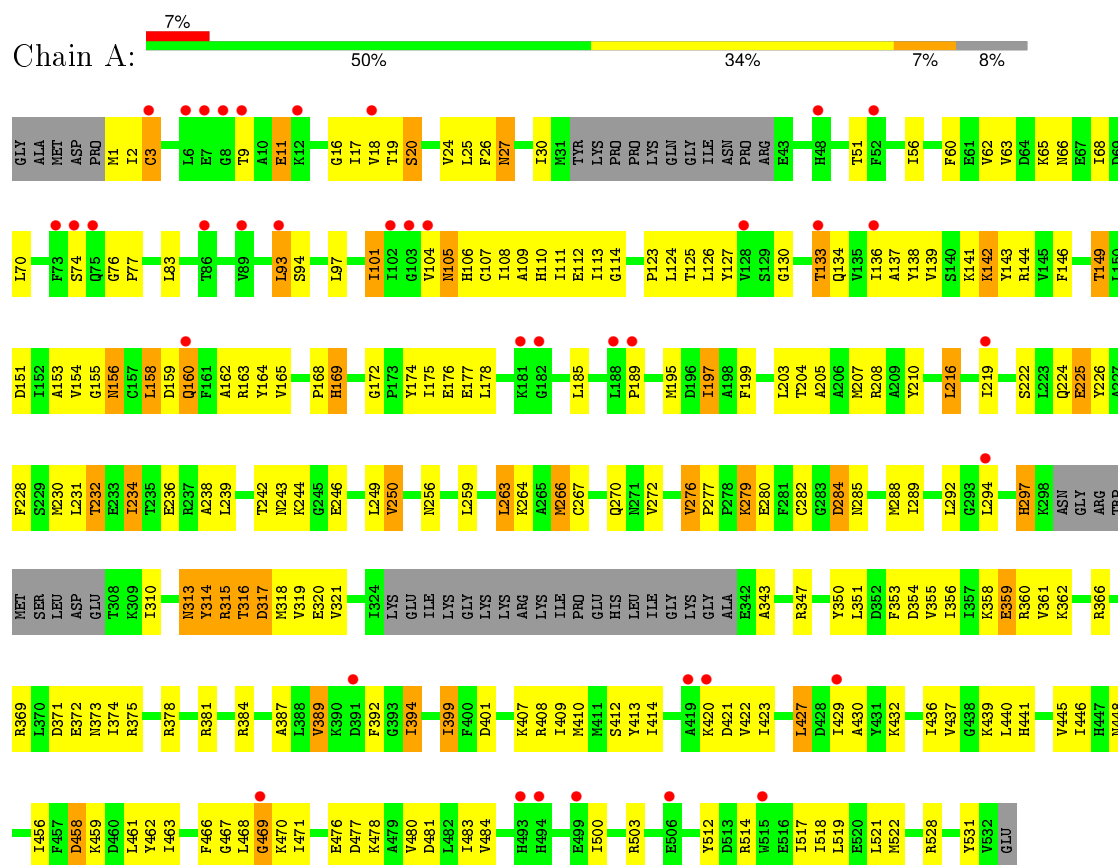
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Br	Ta		
3	B	1	18	12	6	0	0

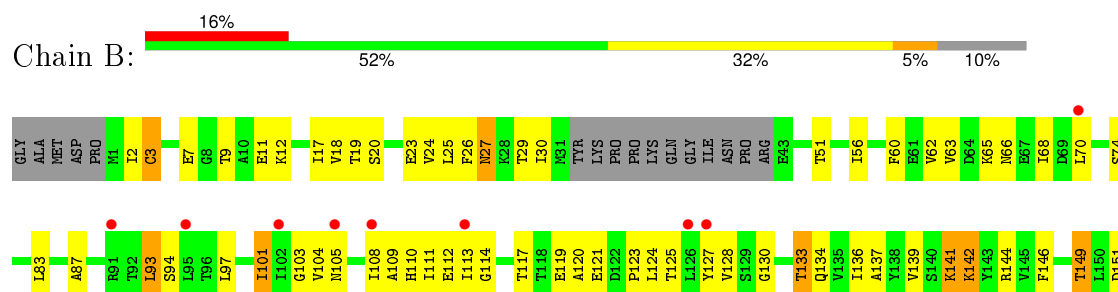
### 3 Residue-property plots

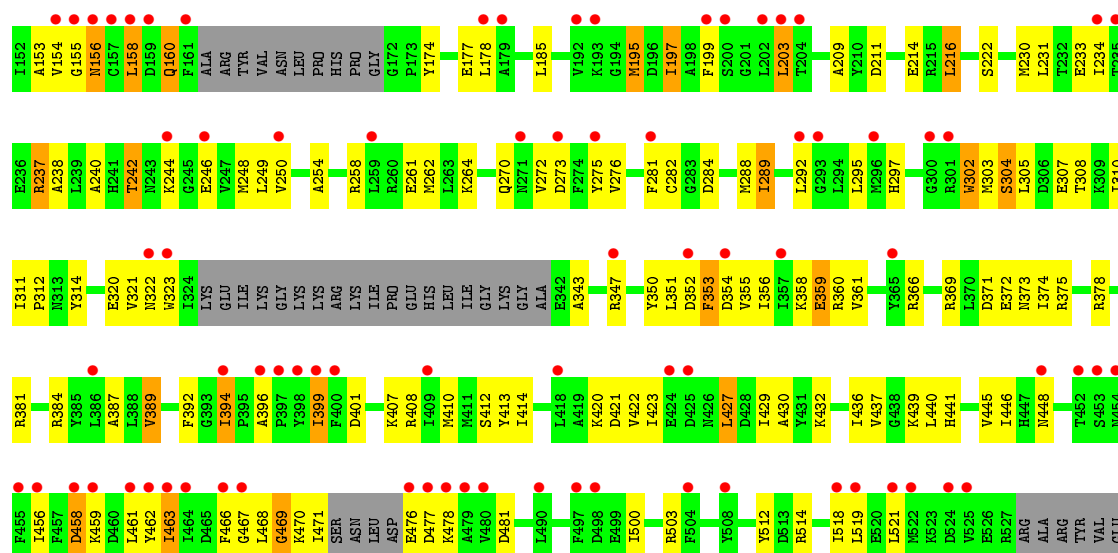
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Putative O-sialoglycoprotein endopeptidase

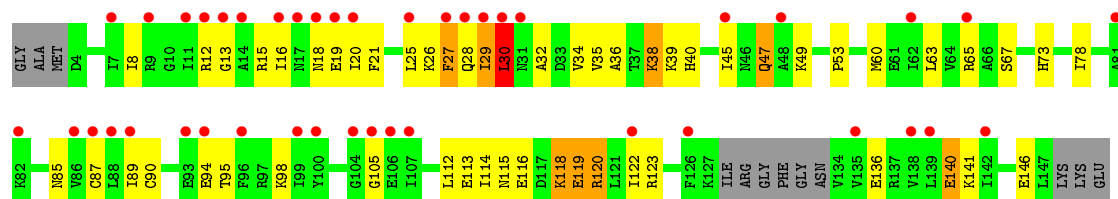


#### • Molecule 1: Putative O-sialoglycoprotein endopeptidase

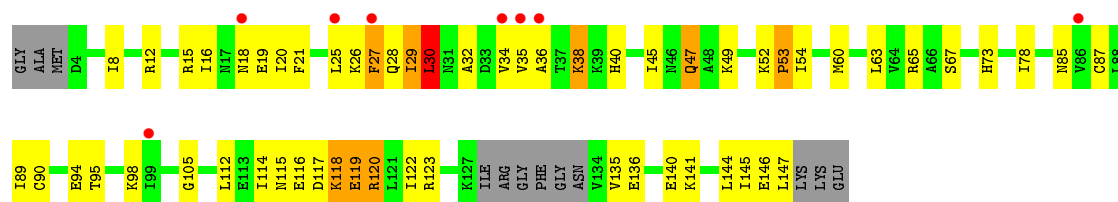




• Molecule 2: Uncharacterized protein MJ0187



• Molecule 2: Uncharacterized protein MJ0187





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.99Å 106.91Å 209.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.92 – 3.60 72.26 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (94.92-3.60) 100.0 (72.26-3.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, $R_{free}$	0.271 , 0.324 0.287 , 0.343	Depositor DCC
$R_{free}$ test set	1052 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	146.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 144.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 20739 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: TBR

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	0.35	0/3994	0.56	0/5387
1	B	0.35	0/3921	0.54	0/5284
2	C	0.36	0/1119	0.59	1/1499 (0.1%)
2	D	0.37	0/1119	0.59	1/1499 (0.1%)
All	All	0.35	0/10153	0.56	2/13669 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	30	LEU	CA-CB-CG	5.80	128.65	115.30
2	C	30	LEU	CA-CB-CG	5.72	128.47	115.30

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	3926	0	3959	168	0
1	B	3856	0	3887	140	0
2	C	1108	0	1168	31	0
2	D	1108	0	1168	34	0
3	A	72	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	72	0	0	5	0
All	All	10142	0	10182	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 18.

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:A:11:GLU:OE2	3:A:5769:TBR:BR5	2.09	1.25
2:C:114:ILE:HD11	2:C:119:GLU:HB3	1.33	1.09
2:D:114:ILE:HD11	2:D:119:GLU:HB3	1.35	1.08
1:A:394:ILE:HD12	1:A:436:ILE:HB	1.47	0.96
1:B:394:ILE:HD12	1:B:436:ILE:HB	1.47	0.95
1:B:133:THR:HG22	1:B:153:ALA:HA	1.57	0.87
1:B:258:ARG:HH12	1:B:262:MET:HB3	1.40	0.86
1:A:133:THR:HG22	1:A:153:ALA:HA	1.57	0.85
1:A:159:ASP:HB3	3:A:5769:TBR:BRB	2.32	0.84
1:A:104:VAL:HG21	1:A:289:ILE:HB	1.57	0.84
2:D:27:PHE:CE1	2:D:95:THR:HB	2.13	0.84
1:B:56:ILE:HD11	1:B:93:LEU:HD21	1.61	0.83
1:A:384:ARG:HG3	2:D:147:LEU:HD22	1.61	0.83
1:A:56:ILE:HD11	1:A:93:LEU:HD21	1.64	0.80
2:C:27:PHE:CE1	2:C:95:THR:HB	2.16	0.80
1:B:113:ILE:HG12	1:B:288:MET:HB2	1.63	0.80
1:A:154:VAL:HG21	1:A:231:LEU:HD11	1.65	0.78
1:B:351:LEU:HG	2:C:39:LYS:HG3	1.67	0.77
1:A:159:ASP:OD2	3:A:5769:TBR:BR3	2.58	0.77
1:B:113:ILE:HG12	1:B:288:MET:CB	2.16	0.76
1:A:160:GLN:HE21	1:A:203:LEU:HD21	1.49	0.76
2:D:12:ARG:O	2:D:105:GLY:HA3	1.87	0.74
2:C:12:ARG:O	2:C:105:GLY:HA3	1.89	0.73
1:A:387:ALA:HB2	1:A:399:ILE:HD11	1.69	0.73
1:A:11:GLU:CD	3:A:5769:TBR:BR1	2.83	0.73
1:A:3:CYS:HB2	1:A:70:LEU:HB3	1.71	0.72
1:B:3:CYS:HB2	1:B:70:LEU:HB3	1.71	0.72
1:A:355:VAL:HG12	1:A:412:SER:HA	1.72	0.72
1:A:384:ARG:HG3	2:D:147:LEU:CD2	2.20	0.71
1:B:195:MET:HG2	1:B:237:ARG:HE	1.54	0.71
1:B:352:ASP:HB2	2:C:39:LYS:HE2	1.73	0.70
1:B:154:VAL:HG21	1:B:231:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:HD3	1:A:169:HIS:HE1	1.55	0.70
1:B:355:VAL:HG12	1:B:412:SER:HA	1.74	0.69
1:B:456:ILE:HD11	1:B:462:TYR:HB2	1.73	0.69
1:A:456:ILE:HD11	1:A:462:TYR:HB2	1.74	0.69
1:B:270:GLN:HG2	1:B:272:VAL:HG22	1.75	0.68
1:B:387:ALA:HB2	1:B:399:ILE:HD11	1.74	0.68
1:A:1:MET:HB2	3:A:6769:TBR:BR6	2.48	0.68
1:A:315:ARG:NH1	1:A:317:ASP:HB2	2.07	0.68
1:A:124:LEU:HD11	1:A:238:ALA:HB1	1.75	0.68
1:A:77:PRO:HD3	1:A:314:TYR:HB3	1.75	0.68
1:A:427:LEU:HD22	1:A:503:ARG:HD3	1.74	0.68
1:A:297:HIS:CE1	3:A:6769:TBR:BR7	3.02	0.67
1:B:427:LEU:HD22	1:B:503:ARG:HD3	1.77	0.67
1:B:104:VAL:HB	1:B:292:LEU:HD12	1.75	0.67
1:B:7:GLU:HB2	1:B:289:ILE:CD1	2.23	0.67
1:A:106:HIS:HE1	1:A:284:ASP:HB3	1.60	0.66
1:B:238:ALA:O	1:B:242:THR:OG1	2.12	0.66
1:B:113:ILE:HD13	1:B:281:PHE:HB3	1.78	0.66
1:B:133:THR:CG2	1:B:153:ALA:HA	2.26	0.66
1:A:133:THR:CG2	1:A:153:ALA:HA	2.24	0.66
1:B:19:THR:HG23	1:B:25:LEU:HD21	1.78	0.65
1:B:130:GLY:HA2	1:B:155:GLY:HA3	1.78	0.65
1:A:3:CYS:HB3	1:A:294:LEU:HD23	1.78	0.64
1:A:355:VAL:HA	1:A:413:TYR:H	1.63	0.64
2:D:36:ALA:HB3	2:D:40:HIS:HB2	1.79	0.64
1:B:297:HIS:HE1	3:B:3769:TBR:BRB	2.35	0.64
1:A:134:GLN:HG3	1:A:136:ILE:HD11	1.80	0.63
2:C:36:ALA:HB3	2:C:40:HIS:HB2	1.79	0.63
1:B:134:GLN:HG3	1:B:136:ILE:HD11	1.79	0.63
1:A:130:GLY:HA2	1:A:155:GLY:HA3	1.81	0.63
1:A:19:THR:HG23	1:A:25:LEU:HD21	1.80	0.63
1:B:355:VAL:HA	1:B:413:TYR:H	1.63	0.62
1:A:231:LEU:O	1:A:234:ILE:HD13	1.99	0.62
2:C:28:GLN:NE2	2:C:63:LEU:HB2	2.15	0.61
1:A:159:ASP:OD2	3:A:5769:TBR:BR6	2.73	0.61
2:D:120:ARG:HD3	2:D:120:ARG:N	2.15	0.61
1:A:249:LEU:HB3	1:A:276:VAL:HG12	1.82	0.61
1:A:2:ILE:HG22	1:A:19:THR:HA	1.83	0.60
1:A:259:LEU:O	1:A:263:LEU:HB2	2.01	0.60
1:B:139:VAL:HG21	1:B:146:PHE:HZ	1.65	0.59
2:C:120:ARG:HD3	2:C:120:ARG:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ILE:HG22	1:B:19:THR:HA	1.84	0.59
1:B:7:GLU:HB2	1:B:289:ILE:HD11	1.83	0.59
1:A:168:PRO:HB2	1:A:174:TYR:HE2	1.67	0.59
1:A:159:ASP:CB	3:A:5769:TBR:BRB	3.03	0.59
1:A:138:TYR:CE1	1:A:321:VAL:HG21	2.38	0.58
2:D:32:ALA:HB3	2:D:85:ASN:HD22	1.69	0.58
1:B:74:SER:HB3	1:B:289:ILE:HG21	1.85	0.58
1:A:164:TYR:CD2	1:A:207:MET:HE2	2.38	0.58
1:A:162:ALA:HB2	1:A:175:ILE:HD11	1.85	0.58
2:D:32:ALA:HA	2:D:35:VAL:HG12	1.85	0.58
1:A:476:GLU:HG2	1:A:521:LEU:HD11	1.86	0.58
2:D:28:GLN:NE2	2:D:63:LEU:HB2	2.18	0.58
1:A:222:SER:HA	1:A:225:GLU:HB2	1.86	0.57
2:C:47:GLN:HG3	2:C:65:ARG:HH21	1.69	0.57
1:B:121:GLU:OE1	3:B:7769:TBR:BR8	2.77	0.57
1:A:242:THR:HB	1:A:244:LYS:HD3	1.86	0.57
2:D:38:LYS:HG3	2:D:112:LEU:HD13	1.86	0.57
1:A:441:HIS:HD2	1:A:478:LYS:HB3	1.68	0.57
1:B:141:LYS:O	1:B:321:VAL:HG22	2.04	0.56
2:C:115:ASN:H	2:C:118:LYS:HD3	1.69	0.56
2:C:32:ALA:HB3	2:C:85:ASN:HD22	1.70	0.56
1:B:360:ARG:HH12	1:B:378:ARG:CB	2.18	0.56
1:A:112:GLU:HG3	1:A:292:LEU:HD13	1.88	0.56
2:D:115:ASN:H	2:D:118:LYS:HD3	1.69	0.56
1:A:18:VAL:HG12	1:A:24:VAL:HA	1.88	0.56
1:B:112:GLU:HG3	1:B:292:LEU:HD23	1.86	0.56
1:B:476:GLU:HG2	1:B:521:LEU:HD11	1.87	0.56
1:A:105:ASN:ND2	1:A:108:ILE:H	2.03	0.56
1:B:105:ASN:HD22	1:B:108:ILE:H	1.52	0.56
1:A:11:GLU:OE2	3:A:5769:TBR:BR1	2.79	0.56
1:A:139:VAL:HG21	1:A:146:PHE:HZ	1.70	0.56
2:C:45:ILE:O	2:C:49:LYS:HB2	2.06	0.56
1:A:437:VAL:HA	1:A:440:LEU:HD12	1.87	0.56
1:A:387:ALA:CB	2:D:144:LEU:HD11	2.36	0.56
1:B:311:ILE:HB	1:B:314:TYR:HB2	1.87	0.56
1:A:369:ARG:O	1:A:373:ASN:HB2	2.06	0.56
1:B:369:ARG:O	1:B:373:ASN:HB2	2.06	0.56
2:D:27:PHE:HB3	2:D:90:CYS:HA	1.88	0.56
1:B:289:ILE:H	1:B:289:ILE:HD13	1.69	0.55
1:A:197:ILE:HD11	1:A:234:ILE:HD12	1.88	0.55
1:B:436:ILE:HA	1:B:439:LYS:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLU:HB2	1:B:289:ILE:HD12	1.89	0.55
1:B:87:ALA:HB2	1:B:310:ILE:HG23	1.89	0.55
1:B:441:HIS:HD2	1:B:478:LYS:HB3	1.72	0.55
1:B:105:ASN:ND2	1:B:108:ILE:H	2.05	0.55
2:D:45:ILE:O	2:D:49:LYS:HB2	2.06	0.54
1:B:94:SER:HB3	1:B:101:ILE:HG23	1.90	0.54
1:A:315:ARG:O	1:A:318:MET:HG2	2.06	0.54
1:A:105:ASN:HD22	1:A:108:ILE:H	1.53	0.54
1:B:429:ILE:HG23	1:B:461:LEU:HD11	1.90	0.54
1:B:185:LEU:HB2	1:B:369:ARG:NH1	2.23	0.54
2:D:47:GLN:HE21	2:D:47:GLN:HA	1.73	0.54
1:A:185:LEU:HB2	1:A:369:ARG:NH1	2.23	0.53
1:B:111:ILE:HG23	1:B:125:THR:HG21	1.90	0.53
2:C:38:LYS:HG3	2:C:112:LEU:HD13	1.88	0.53
1:A:111:ILE:HG23	1:A:125:THR:HG21	1.90	0.53
2:C:27:PHE:HB3	2:C:90:CYS:HA	1.91	0.53
1:A:168:PRO:HB2	1:A:174:TYR:CE2	2.44	0.53
1:A:360:ARG:HH12	1:A:378:ARG:CB	2.21	0.53
1:A:74:SER:HB3	1:A:289:ILE:HG21	1.90	0.53
1:B:30:ILE:HD12	1:B:51:THR:HG23	1.91	0.53
1:A:313:ASN:ND2	1:A:313:ASN:H	2.06	0.53
2:C:32:ALA:HA	2:C:35:VAL:HG12	1.92	0.52
1:A:185:LEU:HD22	1:A:222:SER:HB3	1.91	0.52
1:A:94:SER:HB3	1:A:101:ILE:HG23	1.92	0.52
1:B:83:LEU:HD23	1:B:310:ILE:HB	1.92	0.52
1:B:117:THR:HG21	1:B:281:PHE:CD1	2.44	0.52
1:A:236:GLU:HA	1:A:266:MET:HE3	1.90	0.52
1:B:437:VAL:HA	1:B:440:LEU:HD12	1.91	0.51
1:A:163:ARG:CZ	3:A:5769:TBR:BR8	3.14	0.51
1:A:228:PHE:CD1	1:A:259:LEU:HD12	2.45	0.51
1:B:310:ILE:HD12	1:B:312:PRO:HD3	1.93	0.51
1:B:119:GLU:HG3	1:B:275:TYR:HE1	1.75	0.51
2:C:87:CYS:HB3	2:C:112:LEU:CD2	2.41	0.51
1:B:389:VAL:O	1:B:394:ILE:HG23	2.11	0.51
2:C:47:GLN:HE21	2:C:47:GLN:HA	1.76	0.51
2:D:47:GLN:HG3	2:D:65:ARG:HH21	1.76	0.51
1:A:204:THR:O	1:A:208:ARG:HG3	2.10	0.51
1:B:249:LEU:HG	1:B:254:ALA:HB1	1.92	0.51
1:B:18:VAL:HG12	1:B:24:VAL:HA	1.93	0.50
1:B:30:ILE:HB	1:B:51:THR:HG21	1.93	0.50
1:A:113:ILE:HG12	1:A:288:MET:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ARG:HG3	1:B:371:ASP:HB2	1.94	0.50
1:A:436:ILE:HA	1:A:439:LYS:HG3	1.91	0.50
1:B:246:GLU:HA	1:B:273:ASP:HB3	1.93	0.50
1:A:429:ILE:HG23	1:A:461:LEU:HD11	1.94	0.50
1:B:347:ARG:HG2	1:B:356:ILE:HG22	1.94	0.50
1:B:360:ARG:HH12	1:B:378:ARG:HB2	1.76	0.50
1:A:11:GLU:HG2	3:A:5769:TBR:BR1	2.67	0.50
2:D:120:ARG:HD3	2:D:120:ARG:H	1.77	0.50
1:B:297:HIS:CE1	3:B:3769:TBR:BRB	3.20	0.49
1:A:226:TYR:O	1:A:230:MET:HG2	2.11	0.49
1:A:422:VAL:HG23	1:A:429:ILE:HD13	1.94	0.49
1:B:459:LYS:HA	1:B:459:LYS:HE2	1.93	0.49
1:B:272:VAL:HG23	1:B:273:ASP:N	2.27	0.49
1:B:399:ILE:O	2:C:140:GLU:HB2	2.11	0.49
2:C:16:ILE:HD11	2:C:29:ILE:HD11	1.94	0.49
2:D:16:ILE:HD11	2:D:29:ILE:HD11	1.93	0.49
1:A:267:CYS:HB2	1:A:272:VAL:HG23	1.94	0.49
1:A:18:VAL:HG23	1:A:294:LEU:HD21	1.95	0.49
1:B:414:ILE:HD11	1:B:458:ASP:HB2	1.94	0.49
1:B:149:THR:HG23	1:B:151:ASP:H	1.77	0.49
1:A:104:VAL:CG2	1:A:289:ILE:HB	2.36	0.49
1:A:459:LYS:HA	1:A:459:LYS:HE2	1.94	0.49
1:A:347:ARG:HG2	1:A:356:ILE:HG22	1.95	0.48
1:B:470:LYS:HG3	1:B:471:ILE:H	1.77	0.48
1:A:66:ASN:ND2	1:A:66:ASN:H	2.11	0.48
1:A:142:LYS:HB2	1:A:144:ARG:NH2	2.28	0.48
1:A:149:THR:HG23	1:A:151:ASP:H	1.78	0.48
2:D:87:CYS:HB3	2:D:112:LEU:CD2	2.43	0.48
1:B:343:ALA:HA	1:B:361:VAL:HG12	1.95	0.48
1:B:185:LEU:HB2	1:B:369:ARG:HH11	1.79	0.48
1:B:422:VAL:HG23	1:B:429:ILE:HD13	1.95	0.48
1:A:343:ALA:HB1	1:A:360:ARG:HA	1.94	0.48
1:B:24:VAL:HG21	1:B:27:ASN:HB2	1.95	0.48
1:B:295:LEU:HD22	1:B:323:TRP:HB2	1.95	0.48
1:B:142:LYS:HB2	1:B:144:ARG:NH2	2.28	0.48
1:B:512:TYR:CZ	1:B:514:ARG:HB2	2.49	0.48
1:A:30:ILE:HD12	1:A:51:THR:HG23	1.95	0.48
1:A:483:ILE:HG23	1:A:522:MET:SD	2.54	0.48
2:C:34:VAL:HG13	2:C:122:ILE:HG13	1.96	0.48
1:A:470:LYS:HG3	1:A:471:ILE:H	1.78	0.48
1:A:165:VAL:HG11	1:A:216:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ARG:HH12	1:A:470:LYS:NZ	2.11	0.47
1:B:66:ASN:H	1:B:66:ASN:ND2	2.12	0.47
1:B:401:ASP:HB3	1:B:410:MET:HB3	1.96	0.47
1:B:423:ILE:HD11	1:B:430:ALA:HB2	1.96	0.47
1:B:195:MET:HG3	1:B:237:ARG:HH21	1.77	0.47
1:A:313:ASN:H	1:A:313:ASN:HD22	1.61	0.47
1:A:358:LYS:O	1:A:408:ARG:HA	2.14	0.47
1:A:106:HIS:CE1	1:A:284:ASP:HB3	2.47	0.47
2:C:120:ARG:HD3	2:C:120:ARG:H	1.79	0.47
2:D:47:GLN:NE2	2:D:47:GLN:HA	2.28	0.47
1:A:432:LYS:HB3	1:A:461:LEU:HD12	1.97	0.47
1:A:30:ILE:HB	1:A:51:THR:HG21	1.97	0.47
2:D:34:VAL:HG13	2:D:122:ILE:HG13	1.96	0.47
1:A:154:VAL:HG22	1:A:199:PHE:CZ	2.50	0.47
1:A:297:HIS:HE1	3:A:6769:TBR:BR8	2.53	0.47
1:A:423:ILE:HD11	1:A:430:ALA:HB2	1.97	0.47
1:A:381:ARG:HD3	1:A:470:LYS:HD2	1.96	0.47
1:B:231:LEU:O	1:B:234:ILE:HG13	2.14	0.47
1:A:185:LEU:HB2	1:A:369:ARG:HH11	1.80	0.47
1:B:137:ALA:HB1	1:B:244:LYS:HE3	1.97	0.47
1:A:355:VAL:HA	1:A:413:TYR:N	2.29	0.46
1:B:321:VAL:HA	1:B:323:TRP:CZ3	2.49	0.46
1:B:174:TYR:HA	1:B:177:GLU:HB2	1.96	0.46
1:A:343:ALA:HA	1:A:361:VAL:HG12	1.97	0.46
1:A:358:LYS:HB2	1:A:409:ILE:HG22	1.97	0.46
1:B:110:HIS:HB3	1:B:250:VAL:HG21	1.96	0.46
1:A:11:GLU:HB2	3:A:5769:TBR:BR5	2.70	0.46
1:B:103:GLY:H	1:B:303:MET:HG3	1.80	0.46
1:B:127:TYR:O	1:B:133:THR:HA	2.16	0.46
2:C:8:ILE:HG22	2:C:89:ILE:HG12	1.98	0.46
1:A:285:ASN:ND2	1:A:288:MET:HB2	2.30	0.46
1:A:315:ARG:O	1:A:317:ASP:N	2.49	0.46
2:D:67:SER:HB2	2:D:78:ILE:HD11	1.98	0.46
1:B:19:THR:OG1	1:B:23:GLU:HG2	2.16	0.45
1:B:343:ALA:HB1	1:B:360:ARG:HA	1.98	0.45
1:A:108:ILE:HA	1:A:111:ILE:HD12	1.97	0.45
2:D:27:PHE:HB2	2:D:89:ILE:O	2.16	0.45
1:A:232:THR:HG23	1:A:263:LEU:HD22	1.99	0.45
1:A:414:ILE:HD11	1:A:458:ASP:HB2	1.98	0.45
1:B:359:GLU:OE1	1:B:408:ARG:HB3	2.16	0.45
2:D:8:ILE:HG22	2:D:89:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:ARG:HD2	2:D:85:ASN:HB3	1.98	0.45
1:A:110:HIS:O	1:A:250:VAL:HG11	2.17	0.45
1:A:24:VAL:HG21	1:A:27:ASN:HB2	1.98	0.45
1:A:456:ILE:CD1	1:A:462:TYR:HB2	2.44	0.45
1:A:20:SER:HA	1:A:294:LEU:HD13	1.99	0.45
1:A:366:ARG:HG3	1:A:371:ASP:HB2	1.98	0.45
1:A:389:VAL:O	1:A:394:ILE:HG23	2.17	0.45
1:B:109:ALA:O	1:B:113:ILE:HG13	2.16	0.45
1:A:228:PHE:O	1:A:232:THR:OG1	2.34	0.45
2:C:47:GLN:NE2	2:C:47:GLN:HA	2.32	0.45
1:A:360:ARG:HH12	1:A:378:ARG:HB2	1.82	0.45
1:A:114:GLY:HA2	1:A:277:PRO:HG3	1.99	0.45
1:A:512:TYR:CZ	1:A:514:ARG:HB2	2.51	0.45
1:A:110:HIS:HE1	1:A:282:CYS:O	2.00	0.45
1:B:209:ALA:O	1:B:214:GLU:HB2	2.17	0.45
1:A:123:PRO:HA	1:A:246:GLU:HG3	1.98	0.45
1:A:17:ILE:HD13	1:A:63:VAL:HG11	1.99	0.45
1:A:11:GLU:CB	3:A:5769:TBR:BR5	3.20	0.45
1:A:387:ALA:HB1	2:D:144:LEU:HD11	1.99	0.44
1:A:109:ALA:O	1:A:113:ILE:HG13	2.17	0.44
1:A:189:PRO:HD3	1:A:205:ALA:CB	2.46	0.44
1:A:401:ASP:HB3	1:A:410:MET:HB3	1.97	0.44
1:B:156:ASN:HD22	1:B:156:ASN:C	2.19	0.44
1:A:384:ARG:HH12	1:A:470:LYS:HZ3	1.64	0.44
2:C:27:PHE:HB2	2:C:89:ILE:O	2.17	0.44
1:B:355:VAL:HA	1:B:413:TYR:N	2.29	0.44
1:B:381:ARG:HD3	1:B:470:LYS:HD2	1.99	0.44
2:C:12:ARG:HD2	2:C:85:ASN:HB3	2.00	0.44
1:B:60:PHE:CD1	1:B:65:LYS:HG2	2.52	0.44
1:B:9:THR:HA	1:B:83:LEU:HD12	1.98	0.44
1:B:197:ILE:CG2	1:B:230:MET:HB3	2.48	0.44
1:A:60:PHE:CD1	1:A:65:LYS:HG2	2.52	0.44
1:B:154:VAL:HG22	1:B:199:PHE:CZ	2.53	0.44
1:B:125:THR:HG22	1:B:248:MET:HB3	2.00	0.44
1:B:139:VAL:HG21	1:B:146:PHE:CZ	2.50	0.44
1:B:353:PHE:CE2	2:C:136:GLU:HG2	2.53	0.44
1:A:76:GLY:HA2	1:A:314:TYR:HD1	1.83	0.44
2:C:67:SER:HB2	2:C:78:ILE:HD11	1.99	0.44
1:A:514:ARG:HA	1:A:517:ILE:HD13	2.00	0.43
1:A:448:ASN:ND2	1:A:469:GLY:HA2	2.33	0.43
1:B:456:ILE:CD1	1:B:462:TYR:HB2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ILE:HA	1:B:439:LYS:CG	2.48	0.43
1:B:83:LEU:HD22	1:B:312:PRO:HA	1.99	0.43
1:A:16:GLY:HA2	1:A:26:PHE:O	2.18	0.43
1:B:358:LYS:O	1:B:408:ARG:HA	2.18	0.43
1:A:362:LYS:HB2	1:A:371:ASP:OD2	2.17	0.43
1:A:9:THR:HA	1:A:83:LEU:HD12	2.01	0.43
1:A:126:LEU:HD11	1:A:231:LEU:HD22	2.01	0.43
1:A:127:TYR:O	1:A:133:THR:HA	2.19	0.43
1:A:210:TYR:HA	1:A:219:ILE:HD13	2.01	0.43
1:A:17:ILE:HG22	1:A:26:PHE:HB3	2.00	0.43
1:B:178:LEU:HD13	1:B:216:LEU:HD13	2.00	0.43
1:A:359:GLU:OE1	1:A:408:ARG:HB3	2.19	0.43
1:A:480:VAL:O	1:A:484:VAL:HG23	2.19	0.43
2:C:113:GLU:HG2	2:C:113:GLU:H	1.70	0.43
1:A:436:ILE:HA	1:A:439:LYS:CG	2.49	0.43
1:B:394:ILE:CD1	1:B:436:ILE:HB	2.35	0.43
1:B:356:ILE:HG23	1:B:413:TYR:HB2	2.01	0.42
1:A:174:TYR:HA	1:A:177:GLU:HB2	2.00	0.42
1:B:448:ASN:HB2	1:B:468:LEU:HD12	2.01	0.42
1:A:11:GLU:CG	3:A:5769:TBR:BR1	3.22	0.42
1:A:315:ARG:HH11	1:A:315:ARG:HB3	1.84	0.42
1:B:17:ILE:HG22	1:B:26:PHE:HB3	2.01	0.42
1:A:448:ASN:HD22	1:A:469:GLY:HA2	1.84	0.42
1:B:17:ILE:HD13	1:B:63:VAL:HG11	2.02	0.42
1:B:17:ILE:HG21	1:B:63:VAL:HG11	2.02	0.42
1:B:108:ILE:HA	1:B:111:ILE:HD12	2.01	0.42
1:A:143:TYR:O	1:A:317:ASP:HA	2.20	0.42
1:B:123:PRO:HB2	1:B:248:MET:HB2	2.01	0.42
1:B:160:GLN:HB3	1:B:203:LEU:HD11	2.01	0.42
1:B:432:LYS:HB3	1:B:461:LEU:HD12	2.00	0.42
1:A:351:LEU:HA	1:A:351:LEU:HD12	1.97	0.42
1:A:446:ILE:HD11	1:A:481:ASP:HB2	2.02	0.42
1:B:476:GLU:OE1	3:B:2769:TBR:BR9	2.93	0.42
1:A:66:ASN:H	1:A:66:ASN:HD22	1.67	0.42
1:A:142:LYS:HG3	1:A:319:VAL:O	2.20	0.42
1:A:156:ASN:HD22	1:A:156:ASN:C	2.23	0.42
1:A:133:THR:HG23	1:A:149:THR:HB	2.02	0.42
1:B:446:ILE:HD11	1:B:481:ASP:HB2	2.02	0.42
1:B:288:MET:HG3	1:B:289:ILE:N	2.35	0.41
1:A:138:TYR:HB2	1:A:143:TYR:CE1	2.54	0.41
1:A:124:LEU:HD12	1:A:137:ALA:HB2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:VAL:HG13	1:A:210:TYR:CZ	2.56	0.41
1:B:124:LEU:HD12	1:B:137:ALA:HB2	2.02	0.41
1:A:17:ILE:HG21	1:A:63:VAL:HG11	2.02	0.41
2:D:52:LYS:HA	2:D:53:PRO:HD3	1.96	0.41
1:A:93:LEU:O	1:A:97:LEU:HB2	2.19	0.41
2:C:28:GLN:HE22	2:C:63:LEU:HB2	1.85	0.41
1:B:121:GLU:HB2	3:B:7769:TBR:BR4	2.75	0.41
2:D:34:VAL:HG12	2:D:34:VAL:O	2.20	0.41
1:A:124:LEU:HD11	1:A:238:ALA:CB	2.48	0.41
1:A:105:ASN:HD21	1:A:107:CYS:HB2	1.85	0.41
1:B:114:GLY:HA3	1:B:248:MET:HE3	2.01	0.41
1:B:396:ALA:HB2	1:B:463:ILE:HD12	2.02	0.41
1:B:93:LEU:O	1:B:97:LEU:HB2	2.21	0.41
1:B:154:VAL:O	1:B:158:LEU:HB2	2.20	0.41
1:B:384:ARG:HH12	1:B:470:LYS:NZ	2.19	0.41
1:A:381:ARG:HD3	1:A:470:LYS:CD	2.51	0.41
1:A:445:VAL:HA	1:A:471:ILE:HG22	2.01	0.41
1:A:154:VAL:O	1:A:158:LEU:HB2	2.21	0.41
2:D:117:ASP:HA	2:D:120:ARG:NE	2.36	0.41
1:A:448:ASN:HB2	1:A:468:LEU:HD12	2.02	0.41
2:D:135:VAL:HG23	2:D:136:GLU:HG3	2.03	0.41
1:B:133:THR:HG23	1:B:149:THR:HB	2.02	0.41
1:A:356:ILE:HG23	1:A:413:TYR:HB2	2.03	0.41
1:B:185:LEU:HA	1:B:222:SER:OG	2.21	0.41
2:C:34:VAL:HG12	2:C:34:VAL:O	2.21	0.41
2:D:30:LEU:HD12	2:D:63:LEU:HD22	2.03	0.41
1:A:178:LEU:HD13	1:A:216:LEU:HD13	2.03	0.41
1:B:350:TYR:HB2	1:B:410:MET:SD	2.61	0.41
1:B:156:ASN:O	1:B:160:GLN:HB2	2.20	0.41
1:B:448:ASN:ND2	1:B:469:GLY:HA2	2.36	0.41
1:A:163:ARG:HD3	1:A:169:HIS:CE1	2.45	0.41
1:B:120:ALA:HB1	1:B:123:PRO:HG3	2.03	0.41
1:B:445:VAL:HA	1:B:471:ILE:HG22	2.03	0.41
1:B:142:LYS:HE2	1:B:320:GLU:HA	2.03	0.40
2:D:78:ILE:H	2:D:78:ILE:HG13	1.82	0.40
1:B:128:VAL:HG23	1:B:254:ALA:HB2	2.03	0.40
1:B:12:LYS:HB3	1:B:29:THR:CG2	2.51	0.40
1:B:113:ILE:HG21	1:B:288:MET:HA	2.03	0.40
1:A:76:GLY:HA2	1:A:314:TYR:HB2	2.03	0.40
1:B:87:ALA:HB2	1:B:310:ILE:CG2	2.51	0.40
1:A:176:GLU:HA	1:A:224:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:ILE:HG22	2:D:65:ARG:HH11	1.86	0.40
1:A:350:TYR:CG	1:A:351:LEU:N	2.87	0.40
1:A:394:ILE:CD1	1:A:436:ILE:HB	2.34	0.40
2:C:30:LEU:HB2	2:C:87:CYS:SG	2.62	0.40
1:B:302:TRP:HZ3	1:B:304:SER:HA	1.85	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	487/540 (90%)	423 (87%)	57 (12%)	7 (1%)	14	59
1	B	475/540 (88%)	421 (89%)	50 (10%)	4 (1%)	24	69
2	C	134/150 (89%)	115 (86%)	11 (8%)	8 (6%)	2	24
2	D	134/150 (89%)	115 (86%)	11 (8%)	8 (6%)	2	24
All	All	1230/1380 (89%)	1074 (87%)	129 (10%)	27 (2%)	8	51

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	THR
1	B	240	ALA
2	D	21	PHE
1	A	467	GLY
2	C	21	PHE
2	C	25	LEU
2	D	25	LEU
1	A	256	ASN
1	B	467	GLY
2	C	19	GLU

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Mol	Chain	Res	Type
2	D	18	ASN
2	D	19	GLU
2	D	119	GLU
1	A	172	GLY
2	C	18	ASN
2	C	119	GLU
1	A	279	LYS
1	B	469	GLY
1	A	141	LYS
1	A	469	GLY
1	B	141	LYS
2	C	20	ILE
2	D	20	ILE
2	C	53	PRO
2	D	145	ILE
2	D	53	PRO
2	C	13	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	421/460 (92%)	357 (85%)	64 (15%)	3	24
1	B	415/460 (90%)	360 (87%)	55 (13%)	5	30
2	C	120/128 (94%)	102 (85%)	18 (15%)	3	25
2	D	120/128 (94%)	102 (85%)	18 (15%)	3	25
All	All	1076/1176 (92%)	921 (86%)	155 (14%)	4	26

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	CYS
1	A	11	GLU
1	A	20	SER
1	A	27	ASN

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Mol	Chain	Res	Type
1	A	62	VAL
1	A	68	ILE
1	A	93	LEU
1	A	101	ILE
1	A	105	ASN
1	A	133	THR
1	A	142	LYS
1	A	149	THR
1	A	156	ASN
1	A	158	LEU
1	A	160	GLN
1	A	169	HIS
1	A	195	MET
1	A	197	ILE
1	A	216	LEU
1	A	225	GLU
1	A	232	THR
1	A	234	ILE
1	A	239	LEU
1	A	243	ASN
1	A	250	VAL
1	A	263	LEU
1	A	264	LYS
1	A	266	MET
1	A	270	GLN
1	A	276	VAL
1	A	279	LYS
1	A	280	GLU
1	A	284	ASP
1	A	297	HIS
1	A	310	ILE
1	A	313	ASN
1	A	314	TYR
1	A	315	ARG
1	A	316	THR
1	A	317	ASP
1	A	320	GLU
1	A	353	PHE
1	A	354	ASP
1	A	359	GLU
1	A	372	GLU
1	A	374	ILE

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Mol	Chain	Res	Type
1	A	375	ARG
1	A	389	VAL
1	A	392	PHE
1	A	394	ILE
1	A	399	ILE
1	A	407	LYS
1	A	420	LYS
1	A	421	ASP
1	A	427	LEU
1	A	458	ASP
1	A	463	ILE
1	A	466	PHE
1	A	477	ASP
1	A	500	ILE
1	A	518	ILE
1	A	519	LEU
1	A	528	ARG
1	A	531	TYR
1	B	3	CYS
1	B	11	GLU
1	B	20	SER
1	B	27	ASN
1	B	62	VAL
1	B	68	ILE
1	B	93	LEU
1	B	101	ILE
1	B	133	THR
1	B	142	LYS
1	B	149	THR
1	B	156	ASN
1	B	158	LEU
1	B	160	GLN
1	B	195	MET
1	B	197	ILE
1	B	203	LEU
1	B	211	ASP
1	B	216	LEU
1	B	233	GLU
1	B	237	ARG
1	B	242	THR
1	B	261	GLU
1	B	264	LYS

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Mol	Chain	Res	Type
1	B	276	VAL
1	B	282	CYS
1	B	284	ASP
1	B	289	ILE
1	B	302	TRP
1	B	304	SER
1	B	305	LEU
1	B	307	GLU
1	B	308	THR
1	B	322	ASN
1	B	353	PHE
1	B	354	ASP
1	B	359	GLU
1	B	372	GLU
1	B	374	ILE
1	B	375	ARG
1	B	389	VAL
1	B	392	PHE
1	B	394	ILE
1	B	399	ILE
1	B	407	LYS
1	B	420	LYS
1	B	421	ASP
1	B	427	LEU
1	B	458	ASP
1	B	463	ILE
1	B	466	PHE
1	B	477	ASP
1	B	500	ILE
1	B	518	ILE
1	B	519	LEU
2	C	15	ARG
2	C	26	LYS
2	C	27	PHE
2	C	29	ILE
2	C	30	LEU
2	C	38	LYS
2	C	47	GLN
2	C	60	MET
2	C	73	HIS
2	C	94	GLU
2	C	98	LYS

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Mol	Chain	Res	Type
2	C	116	GLU
2	C	118	LYS
2	C	120	ARG
2	C	123	ARG
2	C	140	GLU
2	C	141	LYS
2	C	146	GLU
2	D	15	ARG
2	D	26	LYS
2	D	27	PHE
2	D	29	ILE
2	D	30	LEU
2	D	38	LYS
2	D	47	GLN
2	D	60	MET
2	D	73	HIS
2	D	94	GLU
2	D	98	LYS
2	D	116	GLU
2	D	118	LYS
2	D	120	ARG
2	D	123	ARG
2	D	140	GLU
2	D	141	LYS
2	D	146	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	66	ASN
1	A	105	ASN
1	A	156	ASN
1	A	160	GLN
1	A	166	ASN
1	A	169	HIS
1	A	224	GLN
1	A	257	ASN
1	A	270	GLN
1	A	297	HIS
1	A	313	ASN
1	A	441	HIS

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Mol	Chain	Res	Type
1	B	27	ASN
1	B	66	ASN
1	B	105	ASN
1	B	156	ASN
1	B	297	HIS
1	B	322	ASN
1	B	441	HIS
2	C	46	ASN
2	C	47	GLN
2	D	46	ASN
2	D	47	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](#)

8 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	TBR	A	1769	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	A	4769	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	A	5769	-	0,36,36	0.00	-	0,180,180	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TBR	A	6769	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	B	2769	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	B	3769	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	B	7769	-	0,36,36	0.00	-	0,180,180	0.00	-
3	TBR	B	8769	-	0,36,36	0.00	-	0,180,180	0.00	-

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	TBR	A	1769	-	-	0/0/696/696	0/0/19/19
3	TBR	A	4769	-	-	0/0/696/696	0/0/19/19
3	TBR	A	5769	-	-	0/0/696/696	0/0/19/19
3	TBR	A	6769	-	-	0/0/696/696	0/0/19/19
3	TBR	B	2769	-	-	0/0/696/696	0/0/19/19
3	TBR	B	3769	-	-	0/0/696/696	0/0/19/19
3	TBR	B	7769	-	-	0/0/696/696	0/0/19/19
3	TBR	B	8769	-	-	0/0/696/696	0/0/19/19

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5769	TBR	12	0
3	A	6769	TBR	3	0
3	B	2769	TBR	1	0
3	B	3769	TBR	2	0
3	B	7769	TBR	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	495/540 (91%)	0.56	38 (7%) 16 11	70, 102, 104, 115	2 (0%)
1	B	485/540 (89%)	0.94	88 (18%) 2 2	99, 103, 120, 126	6 (1%)
2	C	138/150 (92%)	1.22	42 (30%) 1 1	101, 106, 114, 116	1 (0%)
2	D	138/150 (92%)	0.48	8 (5%) 26 18	101, 106, 114, 116	2 (1%)
All	All	1256/1380 (91%)	0.77	176 (14%) 4 3	70, 103, 114, 126	11 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	GLY	9.6
1	B	461	LEU	6.4
1	B	455	PHE	6.1
1	B	463	ILE	5.9
1	A	9	THR	5.5
1	B	400	PHE	5.4
2	C	107	ILE	5.4
1	A	7	GLU	5.3
2	C	19	GLU	5.2
1	B	161	PHE	4.9
2	C	11	ILE	4.8
1	B	158	LEU	4.8
1	B	504	PHE	4.8
2	C	106	GLU	4.8
1	B	454	ASN	4.7
1	B	244	LYS	4.5
2	C	104	GLY	4.5
1	B	464	ILE	4.5
1	B	273	ASP	4.5
1	A	493	HIS	4.4
1	B	199	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
2	C	30	LEU	4.1
1	A	73	PHE	4.1
1	B	293	GLY	4.1
1	B	203	LEU	4.0
1	B	301	ARG	4.0
1	A	75	GLN	4.0
2	C	88	LEU	4.0
1	B	323	TRP	4.0
2	C	31	ASN	4.0
1	B	250	VAL	4.0
2	C	82	LYS	3.9
2	C	16	ILE	3.9
2	C	20	ILE	3.9
1	B	159	ASP	3.8
1	B	386	LEU	3.8
2	C	105	GLY	3.8
1	B	397	PRO	3.7
1	A	419	ALA	3.7
1	A	499	GLU	3.7
1	B	300	GLY	3.7
2	D	25	LEU	3.6
1	B	399	ILE	3.4
1	A	74	SER	3.4
1	B	518	ILE	3.3
1	B	453	SER	3.3
1	B	497	PHE	3.3
1	B	462	TYR	3.3
2	C	89	ILE	3.3
1	A	104	VAL	3.2
1	B	193	LYS	3.2
2	D	35	VAL	3.2
1	A	86	THR	3.2
1	B	322	ASN	3.2
2	C	18	ASN	3.1
1	B	202	LEU	3.1
1	B	479	ALA	3.1
1	B	157	CYS	3.0
1	A	182	GLY	3.0
1	B	178	LEU	3.0
2	D	36	ALA	3.0
2	C	48	ALA	3.0
2	C	29	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	160	GLN	3.0
1	A	506	GLU	2.9
2	C	27	PHE	2.9
1	B	480	VAL	2.9
2	C	13	GLY	2.9
1	B	95	LEU	2.9
1	B	398	TYR	2.9
1	B	490	LEU	2.9
1	B	126	LEU	2.9
2	C	62	ILE	2.9
1	A	103	GLY	2.8
1	B	508	TYR	2.8
1	B	154	VAL	2.8
2	C	28	GLN	2.8
1	B	396	ALA	2.8
1	B	156	ASN	2.8
2	C	45	ILE	2.7
2	C	86	VAL	2.7
1	B	467	GLY	2.7
1	B	235	THR	2.6
1	B	192	VAL	2.6
1	B	448	ASN	2.6
1	B	519	LEU	2.6
1	B	521	LEU	2.6
2	C	138	VAL	2.6
2	C	139	LEU	2.6
1	A	48	HIS	2.6
1	B	476	GLU	2.5
1	A	429	ILE	2.5
1	B	354	ASP	2.5
1	B	456	ILE	2.5
2	C	126	PHE	2.5
1	B	459	LYS	2.5
1	B	522	MET	2.5
1	A	3	CYS	2.5
1	B	424	GLU	2.5
2	C	9	ARG	2.5
2	D	34	VAL	2.5
2	C	100	TYR	2.5
1	B	91	ARG	2.5
2	C	12	ARG	2.5
1	B	70	LEU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	122	ILE	2.5
1	B	102	ILE	2.5
1	B	113	ILE	2.4
1	A	52	PHE	2.4
1	B	409	ILE	2.4
1	B	155	GLY	2.4
1	B	127	TYR	2.4
1	A	102	ILE	2.4
1	A	6	LEU	2.3
1	B	352	ASP	2.3
1	A	12	LYS	2.3
1	B	477	ASP	2.3
1	B	271	ASN	2.3
1	A	133	THR	2.3
2	C	99	ILE	2.3
1	A	420	LYS	2.3
1	B	200	SER	2.3
1	B	466	PHE	2.3
1	B	105	ASN	2.3
1	B	296	MET	2.3
2	C	81	ALA	2.3
2	C	96	PHE	2.3
1	A	219	ILE	2.3
1	B	275	TYR	2.3
1	A	181	LYS	2.3
2	C	94	GLU	2.3
1	A	469	GLY	2.3
1	A	189	PRO	2.3
2	C	142	ILE	2.3
1	B	108	ILE	2.3
1	A	515	TRP	2.2
2	C	17	ASN	2.2
1	B	365	TYR	2.2
2	C	14	ALA	2.2
2	C	135	VAL	2.2
1	A	128	VAL	2.2
1	B	394	ILE	2.2
2	D	99	ILE	2.2
1	B	425	ASP	2.2
1	B	347	ARG	2.1
1	B	418	LEU	2.1
1	B	478	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	452	THR	2.1
1	B	525	VAL	2.1
2	C	25	LEU	2.1
1	B	281	PHE	2.1
1	B	292	LEU	2.1
1	A	18	VAL	2.1
1	B	179	ALA	2.1
1	B	357	ILE	2.1
2	C	87	CYS	2.1
1	B	259	LEU	2.1
1	B	246	GLU	2.1
1	B	498	ASP	2.1
2	C	93	GLU	2.1
1	A	391	ASP	2.1
2	C	65	ARG	2.1
2	D	27	PHE	2.1
1	B	204	THR	2.1
1	B	234	ILE	2.0
2	D	86	VAL	2.0
1	B	458	ASP	2.0
1	A	136	ILE	2.0
2	C	7	ILE	2.0
1	A	93	LEU	2.0
1	B	524	ASP	2.0
1	A	294	LEU	2.0
1	A	494	HIS	2.0
1	A	89	VAL	2.0
1	A	188	LEU	2.0
2	D	18	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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( $\text{\AA}^2$ )	Q<0.9
3	TBR	A	4769	18/18	0.96	0.43	1.84	151,222,500,500	18
3	TBR	A	6769	18/18	0.97	0.39	0.96	83,119,191,196	18
3	TBR	B	7769	18/18	0.84	0.45	0.90	79,159,374,500	18
3	TBR	B	2769	18/18	0.98	0.43	0.08	25,81,98,244	18
3	TBR	B	3769	18/18	0.98	0.39	-0.50	122,181,265,500	18
3	TBR	A	5769	18/18	0.90	0.28	-0.98	72,127,269,500	18
3	TBR	A	1769	18/18	0.99	0.33	-1.08	67,105,143,170	18
3	TBR	B	8769	18/18	0.87	0.63	-	51,146,180,230	18

## 6.5 Other polymers

There are no such residues in this entry.