



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:27 AM GMT

PDB ID : 4ENE  
Title : Structure of the N- and C-terminal trimmed ClC-ec1 Cl<sup>-</sup>/H<sup>+</sup> antiporter and Fab Complex  
Authors : Hyun-Ho Lim; Shane, T.; Miller, C.  
Deposited on : 2012-04-13  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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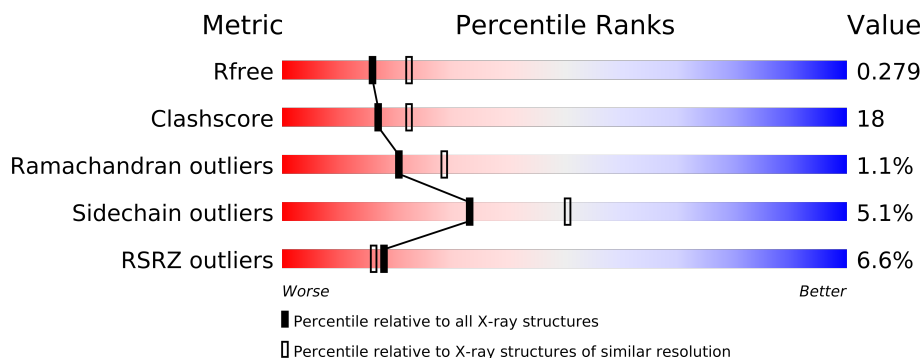
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	446	
1	B	446	
2	C	222	
2	E	222	
3	D	211	
3	F	211	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	DMU	A	504	-	X
6	MAL	B	507	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13691 atoms, of which 0 are hydrogen and 0 are deuterium.

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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	560	563	20			
1	B	442	Total	C	N	O	S	0	0	0
			3315	2180	557	558	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	EXPRESSION TAG	UNP P37019
A	461	LYS	-	EXPRESSION TAG	UNP P37019
B	16	MET	-	EXPRESSION TAG	UNP P37019
B	461	LYS	-	EXPRESSION TAG	UNP P37019

- Molecule 2 is a protein called heavy chain of Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1681	1082	275	318	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

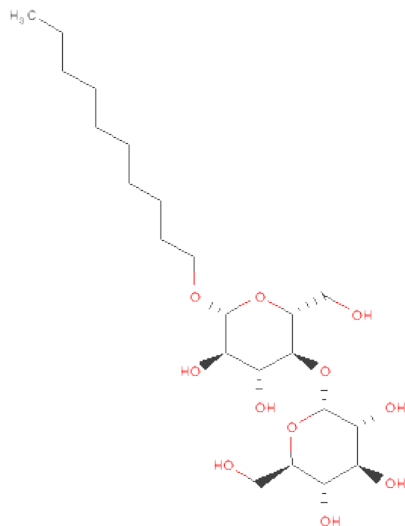
- Molecule 3 is a protein called light chain of Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

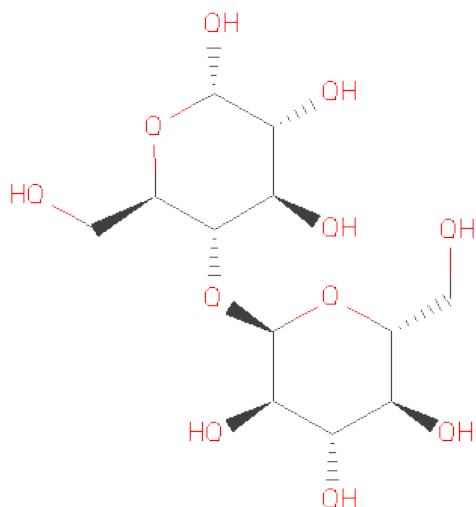
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Cl	0	0
			3	3		
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			33	22	11		
5	A	1	Total	C	O	0	0
			33	22	11		
5	A	1	Total	C	O	0	0
			33	22	11		
5	A	1	Total	C	O	0	0
			33	22	11		
5	B	1	Total	C	O	0	0
			33	22	11		
5	B	1	Total	C	O	0	0
			33	22	11		

- Molecule 6 is SUGAR (MALTOSE) (three-letter code: MAL) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			23	12	11		
6	B	1	Total	C	O	0	0
			23	12	11		
6	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 7 is water.

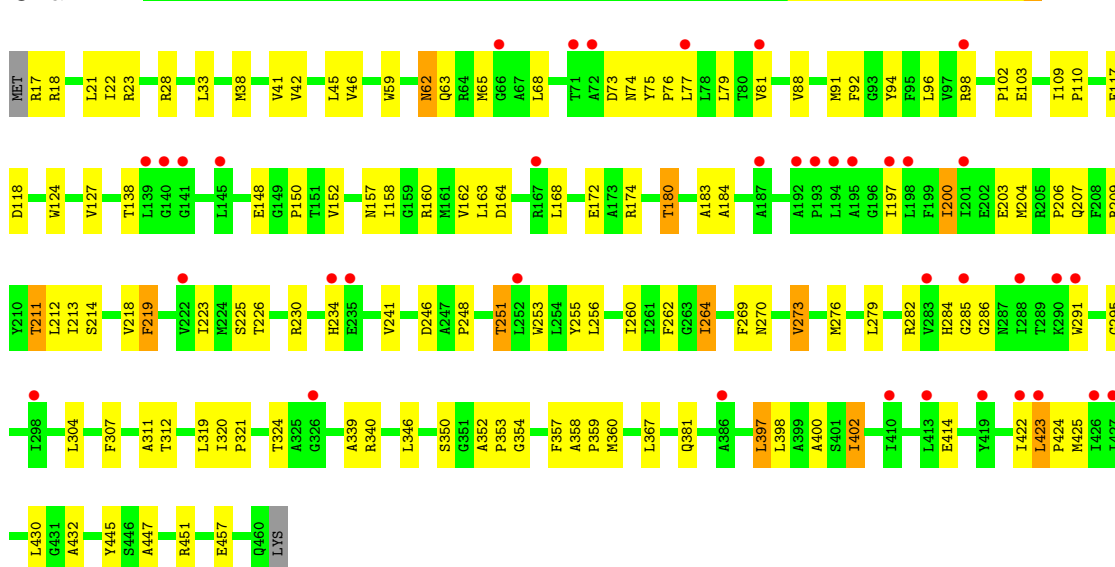
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total	O	0	0
			17	17		
7	B	34	Total	O	0	0
			34	34		
7	C	45	Total	O	0	0
			45	45		
7	D	24	Total	O	0	0
			24	24		
7	E	22	Total	O	0	0
			22	22		
7	F	34	Total	O	0	0
			34	34		

### 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.

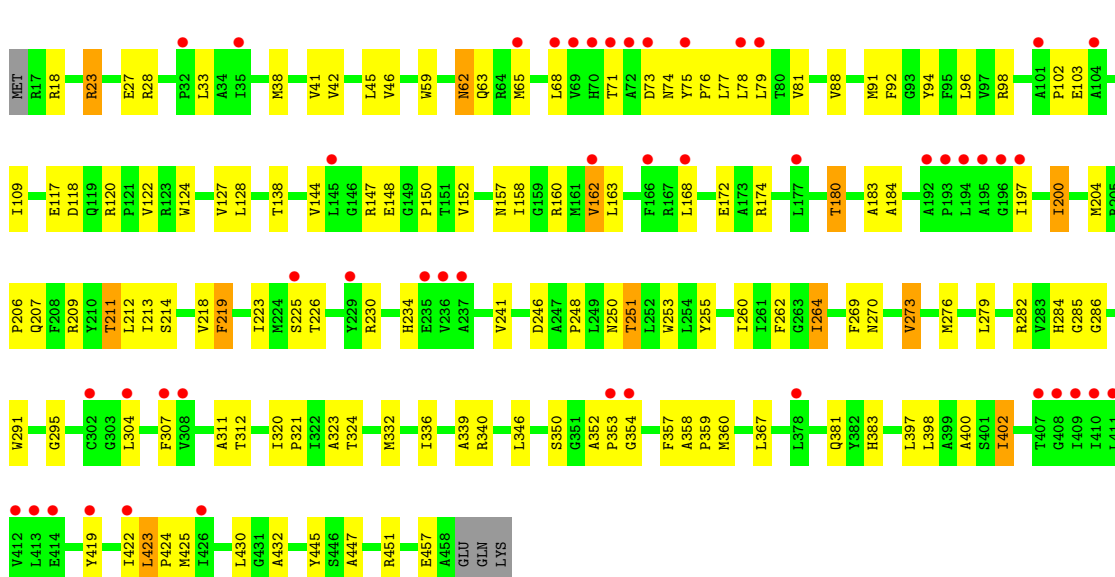
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain A:



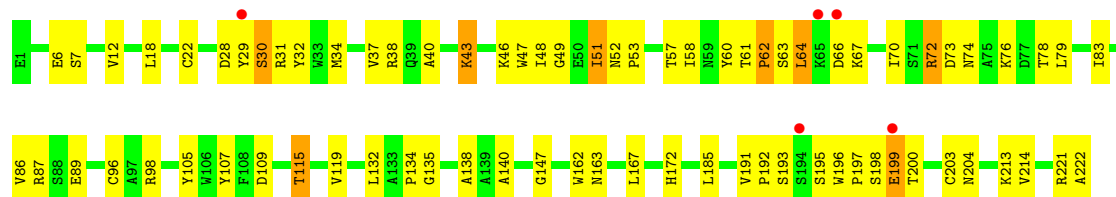
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain B:



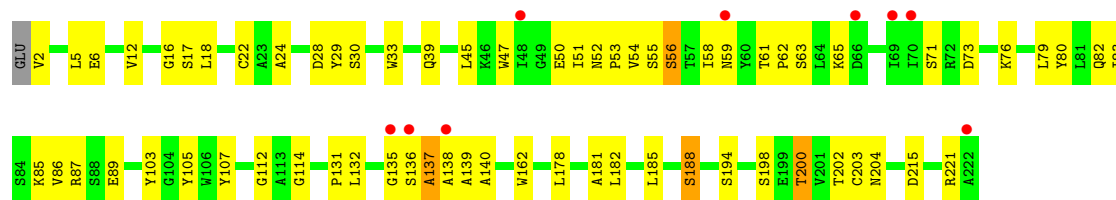
- Molecule 2: heavy chain of Fab fragment

Chain C: 



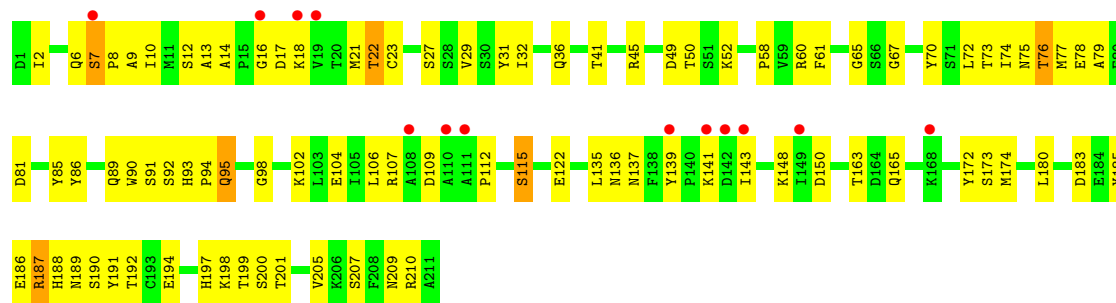
- Molecule 2: heavy chain of Fab fragment

Chain E: 



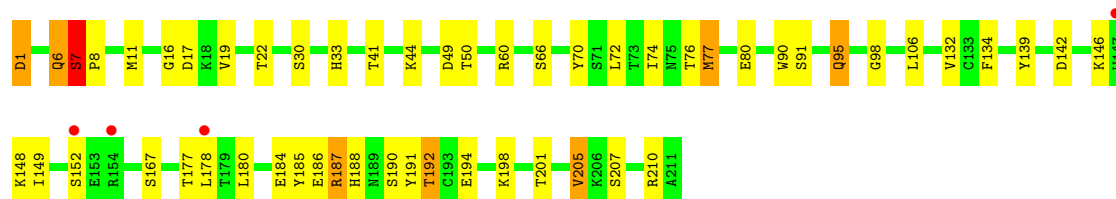
- Molecule 3: light chain of Fab fragment

Chain D: 



- Molecule 3: light chain of Fab fragment

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.26Å 97.52Å 173.96Å 90.00° 132.87° 90.00°	Depositor
Resolution (Å)	24.87 – 2.40 58.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (24.87-2.40) 97.5 (58.80-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.239 , 0.278 0.240 , 0.279	Depositor DCC
$R_{free}$ test set	6187 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.6	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.8	EDS
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 123348 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13691	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, DMU, MAL

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	0/3405	0.50	0/4621
1	B	0.39	0/3387	0.51	0/4597
2	C	0.51	0/1730	0.63	0/2367
2	E	0.43	0/1721	0.61	0/2355
3	D	0.44	0/1660	0.61	0/2257
3	F	0.49	0/1660	0.68	1/2257 (0.0%)
All	All	0.43	0/13563	0.57	1/18454 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	SER	C-N-CD	7.37	143.88	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3333	0	3484	114	0
1	B	3315	0	3470	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1681	0	1663	56	0
2	E	1672	0	1654	44	0
3	D	1621	0	1546	83	1
3	F	1621	0	1546	55	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
5	A	132	0	168	30	1
5	B	66	0	84	16	0
6	B	69	0	66	9	0
7	A	17	0	0	2	0
7	B	34	0	0	4	0
7	C	45	0	0	2	1
7	D	24	0	0	3	0
7	E	22	0	0	1	0
7	F	34	0	0	3	1
All	All	13691	0	13681	481	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (481) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:95:GLN:N	3:D:95:GLN:OE1	1.69	1.24
1:A:207:GLN:HG2	1:B:28:ARG:HD2	1.17	1.13
1:A:28:ARG:HD2	1:B:207:GLN:HG2	1.23	1.11
3:F:95:GLN:N	3:F:95:GLN:OE1	1.90	1.04
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.44	0.99
3:F:7:SER:HB3	3:F:22:THR:HB	1.45	0.99
3:F:95:GLN:H	3:F:95:GLN:CD	1.59	0.97
1:B:422:ILE:HA	1:B:425:MET:HE3	1.47	0.96
3:D:187:ARG:CG	3:D:187:ARG:HH11	1.79	0.95
3:D:192:THR:HG22	3:D:207:SER:CB	1.98	0.94
1:A:422:ILE:HA	1:A:425:MET:HE3	1.52	0.92
5:B:505:DMU:H29	5:B:506:DMU:H11	1.51	0.92
1:B:250:ASN:OD1	7:B:625:HOH:O	1.87	0.90
2:C:51:ILE:HD12	2:C:58:ILE:HG12	1.53	0.89
3:D:187:ARG:HH11	3:D:187:ARG:HG3	1.37	0.88
3:F:95:GLN:N	3:F:95:GLN:CD	2.22	0.87
2:C:163:ASN:HD22	2:C:167:LEU:HD13	1.41	0.85
3:D:192:THR:HG22	3:D:207:SER:HB2	1.57	0.84
3:F:194:GLU:HG2	3:F:205:VAL:HB	1.62	0.82
3:F:192:THR:HB	3:F:207:SER:HB3	1.61	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:PRO:HG2	1:A:211:THR:HG21	1.62	0.81
3:D:17:ASP:OD1	3:D:18:LYS:N	2.13	0.81
1:B:147:ARG:NH2	7:B:606:HOH:O	1.92	0.80
3:D:95:GLN:H	3:D:95:GLN:CD	1.85	0.79
1:A:207:GLN:HG2	1:B:28:ARG:CD	2.09	0.79
3:D:6:GLN:NE2	3:D:85:TYR:O	2.15	0.79
3:D:197:HIS:CG	3:D:198:LYS:H	2.01	0.78
1:A:241:VAL:HG21	1:A:324:THR:HG21	1.66	0.77
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.66	0.77
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.18	0.76
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.15	0.76
1:A:430:LEU:HD22	1:B:223:ILE:HD11	1.68	0.76
1:B:241:VAL:HG21	1:B:324:THR:HG21	1.69	0.75
2:E:135:GLY:O	2:E:137:ALA:N	2.20	0.75
3:D:185:TYR:CZ	3:D:210:ARG:HD3	2.22	0.74
1:A:164:ASP:HB3	5:A:503:DMU:H9	1.70	0.73
5:A:505:DMU:H10	5:A:505:DMU:H5	1.70	0.73
3:F:90:TRP:CD2	3:F:95:GLN:HG3	2.25	0.72
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.71	0.72
3:D:187:ARG:NH1	3:D:187:ARG:HG3	2.03	0.72
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.90	0.71
3:F:7:SER:OG	3:F:8:PRO:CD	2.38	0.71
6:B:507:MAL:H1	6:B:507:MAL:H6'1	1.71	0.71
2:E:85:LYS:HE2	2:E:85:LYS:H	1.56	0.70
5:A:505:DMU:O6	7:A:617:HOH:O	2.09	0.70
3:F:90:TRP:CE2	3:F:95:GLN:HG3	2.27	0.70
5:B:505:DMU:O5	5:B:505:DMU:H8	1.91	0.69
1:A:28:ARG:CD	1:B:207:GLN:HG2	2.12	0.69
1:B:253:TRP:HB3	5:B:505:DMU:H7	1.74	0.69
1:A:160:ARG:HD3	7:A:608:HOH:O	1.91	0.69
1:A:447:ALA:O	1:A:451:ARG:HG3	1.92	0.68
2:C:37:VAL:HG13	2:C:46:LYS:O	1.92	0.68
2:E:135:GLY:HA2	2:E:221:ARG:HD2	1.76	0.67
1:A:346:LEU:O	1:A:350:SER:HB3	1.94	0.67
3:F:7:SER:O	3:F:8:PRO:C	2.30	0.67
1:B:346:LEU:O	1:B:350:SER:HB3	1.95	0.67
2:C:7:SER:HA	2:C:115:THR:HG21	1.77	0.67
1:A:253:TRP:HB3	5:A:506:DMU:H7	1.77	0.67
1:A:33:LEU:HD23	1:A:33:LEU:O	1.94	0.66
1:B:447:ALA:O	1:B:451:ARG:HG3	1.95	0.66
5:A:504:DMU:O49	5:A:504:DMU:H8	1.96	0.66
3:D:31:TYR:HA	3:D:50:THR:OG1	1.95	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.61	0.66
1:B:214:SER:HA	6:B:502:MAL:O3'	1.95	0.66
1:A:241:VAL:CG2	1:A:324:THR:HG21	2.25	0.66
1:B:241:VAL:CG2	1:B:324:THR:HG21	2.26	0.66
2:C:163:ASN:HD22	2:C:167:LEU:CD1	2.09	0.66
2:E:188:SER:HB2	3:F:134:PHE:CE2	2.31	0.66
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.62	0.65
3:F:7:SER:HB2	3:F:8:PRO:HD3	1.79	0.65
3:D:14:ALA:O	3:D:17:ASP:HB3	1.97	0.64
5:A:503:DMU:H4	5:A:503:DMU:C5	2.18	0.64
1:B:23:ARG:CG	1:B:23:ARG:HH11	2.10	0.64
3:F:41:THR:HB	7:F:311:HOH:O	1.97	0.64
1:B:269:PHE:O	1:B:273:VAL:HG12	1.98	0.64
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.33	0.64
2:E:194:SER:O	2:E:198:SER:HB3	1.97	0.64
2:C:86:VAL:CG1	2:C:119:VAL:HG21	2.28	0.63
1:B:422:ILE:HA	1:B:425:MET:CE	2.26	0.63
1:A:270:ASN:O	1:A:273:VAL:HG13	1.99	0.63
5:B:505:DMU:C57	5:B:506:DMU:H11	2.28	0.63
2:E:59:ASN:HB3	7:F:326:HOH:O	1.99	0.63
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.64	0.63
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.81	0.63
1:B:33:LEU:HD23	1:B:33:LEU:O	1.99	0.62
1:A:223:ILE:HD11	1:B:430:LEU:HD22	1.81	0.62
5:B:505:DMU:H29	5:B:506:DMU:O16	1.99	0.62
1:A:223:ILE:CD1	1:B:430:LEU:HD22	2.30	0.62
2:C:30:SER:O	2:C:31:ARG:HB2	1.99	0.62
1:A:269:PHE:O	1:A:273:VAL:HG12	2.00	0.62
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.68	0.62
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.82	0.62
1:B:148:GLU:O	1:B:152:VAL:HG23	2.00	0.61
3:F:7:SER:CB	3:F:8:PRO:CD	2.78	0.61
5:A:505:DMU:C6	5:A:505:DMU:H10	2.30	0.61
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.83	0.61
2:C:172:HIS:HE1	3:D:136:ASN:ND2	1.98	0.60
3:D:187:ARG:HH11	3:D:187:ARG:HG2	1.63	0.60
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.66	0.60
2:C:40:ALA:O	2:C:43:LYS:HB2	2.01	0.60
1:A:226:THR:O	1:A:230:ARG:HG2	2.01	0.60
3:F:148:LYS:HA	3:F:152:SER:O	2.01	0.60
1:B:457:GLU:O	1:B:457:GLU:HG3	2.02	0.60
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.16	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.84	0.59
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.84	0.59
3:F:185:TYR:O	3:F:191:TYR:OH	2.20	0.59
1:B:270:ASN:O	1:B:273:VAL:HG13	2.03	0.59
5:A:503:DMU:O55	5:A:503:DMU:O16	2.16	0.59
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.84	0.59
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.83	0.59
1:B:42:VAL:O	1:B:46:VAL:HG23	2.03	0.59
3:D:189:ASN:O	3:D:209:ASN:HA	2.03	0.59
5:A:503:DMU:H4	5:A:503:DMU:H32	1.85	0.59
5:A:503:DMU:C57	5:A:503:DMU:H6	2.34	0.58
5:A:503:DMU:O2	5:A:503:DMU:O3	2.21	0.58
3:D:150:ASP:HA	3:D:190:SER:OG	2.04	0.58
1:A:17:ARG:HH22	1:A:21:LEU:HD13	1.68	0.58
3:D:197:HIS:CG	3:D:198:LYS:N	2.71	0.58
1:A:206:PRO:HG2	1:A:211:THR:CG2	2.31	0.58
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.19	0.58
1:A:17:ARG:NH2	1:A:21:LEU:HD13	2.19	0.57
3:F:6:GLN:HB3	7:F:331:HOH:O	2.02	0.57
1:A:423:LEU:HD13	1:B:230:ARG:CZ	2.34	0.57
5:B:505:DMU:O49	5:B:505:DMU:H4	2.05	0.57
3:F:187:ARG:O	3:F:188:HIS:CG	2.58	0.57
1:A:207:GLN:HG3	6:B:502:MAL:H6'1	1.86	0.57
3:D:192:THR:HG22	3:D:207:SER:HB3	1.81	0.57
6:B:507:MAL:O3'	6:B:508:MAL:H6'2	2.05	0.57
2:E:85:LYS:HE2	2:E:85:LYS:N	2.18	0.57
1:B:248:PRO:O	1:B:251:THR:HB	2.05	0.57
3:D:75:ASN:O	3:D:76:THR:HG22	2.05	0.57
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.39	0.56
3:D:29:VAL:HG11	3:D:89:GLN:HB2	1.88	0.56
3:F:186:GLU:O	3:F:210:ARG:NH2	2.38	0.56
3:D:12:SER:HA	3:D:104:GLU:O	2.05	0.56
3:F:7:SER:CB	3:F:8:PRO:HD3	2.35	0.56
3:D:36:GLN:HG3	3:D:85:TYR:CE2	2.41	0.56
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.19	0.56
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.88	0.56
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.40	0.56
3:F:192:THR:HB	3:F:207:SER:CB	2.34	0.56
3:F:66:SER:HA	3:F:70:TYR:CZ	2.41	0.56
1:A:68:LEU:HD23	1:A:81:VAL:HG23	1.88	0.56
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.20	0.56
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:29:VAL:O	3:D:70:TYR:OH	2.17	0.55
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.41	0.55
2:E:24:ALA:HB3	2:E:29:TYR:CD1	2.42	0.55
2:C:12:VAL:HG21	2:C:18:LEU:HD23	1.89	0.55
1:B:68:LEU:HD23	1:B:81:VAL:HG23	1.89	0.55
2:E:50:GLU:HG2	2:E:59:ASN:HB2	1.88	0.55
3:D:141:LYS:HB3	3:D:172:TYR:CD1	2.41	0.55
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.89	0.55
1:A:248:PRO:O	1:A:251:THR:HB	2.07	0.55
5:B:506:DMU:C2	5:B:506:DMU:O1	2.54	0.55
1:A:256:LEU:HD23	5:A:505:DMU:H17	1.87	0.55
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.89	0.55
1:B:284:HIS:C	1:B:286:GLY:H	2.10	0.54
3:D:6:GLN:OE1	3:D:98:GLY:HA3	2.07	0.54
2:C:73:ASP:HB3	2:C:76:LYS:HB2	1.89	0.54
3:F:191:TYR:O	3:F:207:SER:HB2	2.07	0.54
3:F:180:LEU:HD22	3:F:184:GLU:HG2	1.89	0.54
3:D:106:LEU:HD23	3:D:107:ARG:H	1.73	0.54
3:D:115:SER:HB2	7:D:304:HOH:O	2.07	0.54
3:D:186:GLU:O	3:D:210:ARG:NH2	2.41	0.54
1:A:62:ASN:O	1:A:65:MET:N	2.40	0.54
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.90	0.53
5:A:505:DMU:H32	5:A:505:DMU:H4	1.90	0.53
2:C:72:ARG:HD3	2:C:74:ASN:OD1	2.07	0.53
5:A:506:DMU:O55	5:A:506:DMU:H32	2.08	0.53
1:A:284:HIS:C	1:A:286:GLY:H	2.12	0.53
2:C:52:ASN:CG	2:C:57:THR:HG22	2.28	0.53
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.24	0.53
1:B:23:ARG:HG3	1:B:23:ARG:HH11	1.74	0.53
1:B:226:THR:O	1:B:230:ARG:HG2	2.09	0.53
1:A:262:PHE:CZ	1:A:367:LEU:HD23	2.44	0.53
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.90	0.53
3:D:197:HIS:CD2	3:D:198:LYS:H	2.26	0.53
1:B:276:MET:HA	1:B:276:MET:HE2	1.91	0.53
2:C:195:SER:O	2:C:199:GLU:HG3	2.08	0.53
2:C:86:VAL:CG1	2:C:119:VAL:CG2	2.87	0.53
1:A:230:ARG:CZ	1:B:423:LEU:HD13	2.39	0.53
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.43	0.53
1:A:276:MET:HE2	1:A:276:MET:HA	1.89	0.53
1:A:381:GLN:N	1:A:381:GLN:OE1	2.32	0.53
2:C:60:TYR:CE2	2:C:70:ILE:HD12	2.44	0.53
3:D:7:SER:CB	3:D:8:PRO:HD3	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:204:ASN:HD22	2:E:215:ASP:HB3	1.73	0.52
1:B:402:ILE:HG13	1:B:402:ILE:O	2.09	0.52
2:E:80:TYR:OH	7:E:307:HOH:O	2.15	0.52
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.90	0.52
5:B:505:DMU:H29	5:B:506:DMU:C22	2.33	0.52
3:D:58:PRO:HG2	3:D:61:PHE:CE1	2.45	0.52
1:B:23:ARG:CG	1:B:23:ARG:NH1	2.72	0.52
2:C:51:ILE:HG12	2:C:72:ARG:HG2	1.92	0.52
5:A:505:DMU:O61	5:A:506:DMU:H4	2.09	0.52
2:C:86:VAL:HG11	2:C:119:VAL:HG22	1.91	0.52
3:D:106:LEU:HD23	3:D:107:ARG:N	2.24	0.52
2:E:131:PRO:O	2:E:132:LEU:HD23	2.10	0.52
3:F:7:SER:OG	3:F:8:PRO:HD2	2.10	0.52
2:C:87:ARG:HH21	2:C:89:GLU:CD	2.12	0.52
3:D:76:THR:HG23	3:D:76:THR:O	2.10	0.52
1:A:422:ILE:HA	1:A:425:MET:CE	2.33	0.52
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.92	0.52
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.44	0.51
1:B:206:PRO:HG2	1:B:211:THR:CG2	2.36	0.51
3:D:60:ARG:HD2	3:D:76:THR:O	2.10	0.51
1:B:197:ILE:HD11	1:B:219:PHE:CD2	2.45	0.51
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.92	0.51
3:D:141:LYS:HB3	3:D:172:TYR:CE1	2.44	0.51
1:A:92:PHE:O	1:A:96:LEU:HD23	2.10	0.51
1:B:27:GLU:O	6:B:502:MAL:H62	2.11	0.51
1:B:360:MET:HE3	1:B:398:LEU:HD23	1.92	0.51
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.46	0.51
5:A:505:DMU:H9	5:A:506:DMU:O49	2.10	0.51
5:A:504:DMU:H6	5:A:504:DMU:H15	1.93	0.51
1:B:214:SER:HA	6:B:502:MAL:HO3'	1.76	0.51
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.92	0.51
1:B:62:ASN:O	1:B:65:MET:N	2.43	0.51
3:F:132:VAL:HG22	3:F:177:THR:HG23	1.93	0.51
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.46	0.50
3:F:1:ASP:OD1	3:F:1:ASP:N	2.27	0.50
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.92	0.50
3:D:76:THR:CG2	3:D:76:THR:O	2.59	0.50
2:E:6:GLU:OE1	2:E:112:GLY:HA3	2.10	0.50
1:A:148:GLU:O	1:A:152:VAL:HG23	2.12	0.50
1:A:226:THR:CG2	1:B:423:LEU:HD11	2.41	0.50
1:A:423:LEU:HD11	1:B:226:THR:CG2	2.41	0.50
2:C:213:LYS:N	7:C:342:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:86:VAL:HG11	2:C:119:VAL:CG2	2.41	0.50
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.47	0.50
5:A:503:DMU:H6	5:A:503:DMU:O61	2.11	0.50
3:D:136:ASN:HB3	3:D:137:ASN:HD22	1.75	0.50
1:A:311:ALA:O	1:A:340:ARG:HD2	2.12	0.50
3:F:95:GLN:O	3:F:95:GLN:NE2	2.45	0.49
5:A:505:DMU:H7	5:A:506:DMU:C2	2.43	0.49
1:B:74:ASN:O	1:B:77:LEU:N	2.45	0.49
2:C:163:ASN:ND2	2:C:167:LEU:HD22	2.27	0.49
3:D:7:SER:O	3:D:9:ALA:N	2.45	0.49
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.92	0.49
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.95	0.49
3:D:150:ASP:OD1	3:D:188:HIS:HB3	2.12	0.49
1:A:42:VAL:O	1:A:46:VAL:HG23	2.12	0.49
1:A:109:ILE:HG23	1:A:204:MET:SD	2.52	0.49
2:C:32:TYR:CE2	2:C:98:ARG:HD3	2.47	0.49
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.31	0.49
5:A:505:DMU:C18	5:A:506:DMU:H2	2.43	0.49
2:C:105:TYR:CD2	3:D:91:SER:HA	2.47	0.49
2:E:178:LEU:HD11	2:E:181:ALA:HA	1.94	0.49
3:F:6:GLN:HA	3:F:22:THR:O	2.13	0.49
2:E:178:LEU:HD12	2:E:182:LEU:O	2.13	0.49
2:C:185:LEU:C	2:C:185:LEU:HD12	2.34	0.48
2:C:51:ILE:HD12	2:C:58:ILE:CG1	2.33	0.48
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.28	0.48
1:B:402:ILE:HD12	1:B:445:TYR:CE1	2.48	0.48
1:B:92:PHE:O	1:B:96:LEU:HD23	2.12	0.48
5:A:505:DMU:H7	5:A:506:DMU:H2	1.94	0.48
2:C:7:SER:HA	2:C:115:THR:CG2	2.43	0.48
2:C:172:HIS:HE1	3:D:136:ASN:CG	2.16	0.48
2:E:73:ASP:OD1	2:E:76:LYS:HB2	2.13	0.48
2:E:17:SER:HB2	2:E:83:ILE:O	2.14	0.48
3:F:186:GLU:C	3:F:188:HIS:H	2.16	0.48
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.96	0.48
1:B:158:ILE:O	1:B:162:VAL:HG13	2.13	0.48
3:D:74:ILE:HD13	3:D:81:ASP:OD2	2.13	0.48
1:A:402:ILE:O	1:A:402:ILE:HG13	2.12	0.48
2:E:162:TRP:CH2	2:E:203:CYS:HB3	2.48	0.48
5:B:505:DMU:H3	5:B:506:DMU:O49	2.14	0.48
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.95	0.48
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.95	0.48
1:A:180:THR:HB	1:A:218:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:10:ILE:HG23	3:D:102:LYS:HB3	1.95	0.48
2:C:29:TYR:HE2	2:C:74:ASN:OD1	1.97	0.47
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.81	0.47
2:C:87:ARG:NH2	2:C:89:GLU:OE1	2.41	0.47
2:E:54:VAL:HG23	2:E:56:SER:H	1.79	0.47
2:C:18:LEU:HD11	2:C:83:ILE:HD12	1.96	0.47
1:A:262:PHE:CE2	1:A:367:LEU:HD23	2.49	0.47
1:A:197:ILE:HD11	1:A:219:PHE:CD2	2.48	0.47
6:B:507:MAL:C3'	6:B:508:MAL:H6'2	2.44	0.47
1:B:311:ALA:O	1:B:340:ARG:HD2	2.15	0.47
1:B:109:ILE:HG23	1:B:204:MET:SD	2.54	0.47
1:A:158:ILE:O	1:A:162:VAL:HG13	2.13	0.47
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.96	0.47
1:B:381:GLN:OE1	1:B:381:GLN:N	2.33	0.47
1:A:414:GLU:HG2	1:B:419:TYR:CZ	2.50	0.47
1:B:172:GLU:HG3	1:B:212:LEU:HB3	1.96	0.47
2:E:47:TRP:CG	3:F:95:GLN:NE2	2.82	0.47
3:F:6:GLN:O	3:F:7:SER:O	2.33	0.47
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.96	0.47
1:A:94:TYR:CE1	1:A:295:GLY:HA3	2.50	0.47
1:B:98:ARG:HH21	1:B:102:PRO:HB3	1.78	0.47
1:B:41:VAL:O	1:B:45:LEU:HG	2.14	0.47
2:E:87:ARG:HE	2:E:89:GLU:CD	2.17	0.47
1:B:118:ASP:CG	1:B:174:ARG:HH21	2.18	0.47
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.95	0.47
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.93	0.47
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.44	0.47
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.95	0.47
1:B:75:TYR:O	1:B:79:LEU:HG	2.14	0.47
1:A:75:TYR:O	1:A:79:LEU:HG	2.14	0.47
2:C:135:GLY:O	2:C:138:ALA:HB2	2.15	0.47
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.18	0.47
3:D:89:GLN:O	3:D:95:GLN:HB2	2.14	0.47
3:F:184:GLU:HA	3:F:187:ARG:HH11	1.79	0.47
3:F:6:GLN:OE1	3:F:98:GLY:HA3	2.15	0.47
1:B:197:ILE:CD1	1:B:219:PHE:CD2	2.98	0.47
1:B:59:TRP:O	1:B:63:GLN:HG2	2.15	0.47
1:B:117:GLU:O	1:B:118:ASP:HB2	2.14	0.46
1:B:260:ILE:O	1:B:264:ILE:HG23	2.15	0.46
2:C:61:THR:O	2:C:63:SER:N	2.48	0.46
1:A:255:TYR:CD1	1:A:424:PRO:HB3	2.50	0.46
1:A:98:ARG:NH1	1:A:291:TRP:CZ3	2.84	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:117:GLU:HA	1:B:117:GLU:OE1	2.15	0.46
3:D:191:TYR:O	3:D:207:SER:HB2	2.15	0.46
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.97	0.46
3:F:60:ARG:HG3	3:F:74:ILE:CG2	2.46	0.46
3:F:77:MET:HE2	3:F:77:MET:HB3	1.81	0.46
2:E:18:LEU:O	2:E:82:GLN:HA	2.15	0.46
3:D:109:ASP:HA	3:D:139:TYR:O	2.15	0.46
1:A:74:ASN:O	1:A:77:LEU:N	2.48	0.46
1:A:260:ILE:O	1:A:264:ILE:HG23	2.15	0.46
3:F:72:LEU:C	3:F:72:LEU:HD23	2.35	0.46
2:E:188:SER:HB2	3:F:134:PHE:CD2	2.51	0.46
1:B:255:TYR:CD1	1:B:424:PRO:HB3	2.51	0.46
1:B:262:PHE:CE2	1:B:367:LEU:HD23	2.51	0.46
3:F:16:GLY:HA2	3:F:76:THR:HB	1.97	0.46
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.97	0.46
1:B:211:THR:HB	1:B:213:ILE:HG13	1.97	0.46
2:C:28:ASP:O	2:C:30:SER:O	2.34	0.46
7:C:322:HOH:O	3:D:122:GLU:HG2	2.16	0.46
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.98	0.46
5:A:503:DMU:H6	5:A:503:DMU:H29	1.97	0.46
2:E:24:ALA:HB3	2:E:29:TYR:HD1	1.81	0.46
1:A:59:TRP:O	1:A:63:GLN:HG2	2.15	0.46
1:A:109:ILE:N	1:A:110:PRO:CD	2.79	0.45
3:D:22:THR:CG2	3:D:23:CYS:N	2.79	0.45
3:D:199:THR:O	3:D:200:SER:HB2	2.16	0.45
5:B:506:DMU:H17	5:B:506:DMU:H10	1.68	0.45
3:D:143:ILE:HG13	3:D:197:HIS:HA	1.97	0.45
3:F:49:ASP:O	3:F:50:THR:HB	2.16	0.45
1:B:120:ARG:HE	1:B:120:ARG:HB3	1.53	0.45
3:F:80:GLU:HA	3:F:167:SER:O	2.16	0.45
1:A:360:MET:HE2	1:A:360:MET:HB2	1.81	0.45
2:E:138:ALA:O	2:E:140:ALA:N	2.48	0.45
3:D:89:GLN:NE2	3:D:95:GLN:HA	2.31	0.45
2:E:2:VAL:HG22	2:E:2:VAL:O	2.16	0.45
1:A:160:ARG:HD2	1:A:160:ARG:HA	1.76	0.45
3:D:74:ILE:HG21	3:D:81:ASP:OD2	2.15	0.45
1:B:103:GLU:OE1	1:B:103:GLU:N	2.38	0.45
1:B:183:ALA:HB2	1:B:200:ILE:HG12	1.98	0.45
2:E:185:LEU:HD12	2:E:185:LEU:C	2.37	0.45
5:A:506:DMU:H13	5:A:506:DMU:H6	1.65	0.45
1:B:38:MET:O	1:B:42:VAL:HG23	2.17	0.45
5:A:505:DMU:H7	5:A:506:DMU:O55	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:505:DMU:O16	5:A:506:DMU:H2	2.16	0.45
1:B:445:TYR:HB2	7:B:604:HOH:O	2.17	0.45
6:B:507:MAL:C6'	6:B:507:MAL:H1	2.41	0.45
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.98	0.45
3:D:79:ALA:C	3:D:81:ASP:H	2.20	0.45
1:B:94:TYR:CE1	1:B:295:GLY:HA3	2.51	0.45
1:B:38:MET:HA	1:B:41:VAL:HG13	1.99	0.45
1:A:211:THR:HB	1:A:213:ILE:HG13	1.98	0.44
1:A:319:LEU:C	1:A:319:LEU:HD12	2.38	0.44
5:B:505:DMU:O49	5:B:505:DMU:H36	2.17	0.44
1:A:117:GLU:HA	1:A:117:GLU:OE1	2.17	0.44
5:A:505:DMU:C5	5:A:505:DMU:H4	2.40	0.44
1:B:180:THR:HB	1:B:218:VAL:HA	2.00	0.44
2:E:28:ASP:O	2:E:30:SER:O	2.35	0.44
3:D:194:GLU:HG2	3:D:205:VAL:CG1	2.29	0.44
1:B:148:GLU:HG3	1:B:357:PHE:HB3	2.00	0.44
2:C:162:TRP:CH2	2:C:203:CYS:HB3	2.52	0.44
3:D:29:VAL:CG1	3:D:89:GLN:HB2	2.46	0.44
1:A:117:GLU:O	1:A:118:ASP:HB2	2.18	0.44
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.66	0.44
1:A:18:ARG:O	1:A:22:ILE:HG13	2.18	0.44
1:B:332:MET:O	1:B:336:ILE:HG13	2.17	0.44
3:D:29:VAL:CG1	3:D:32:ILE:HD11	2.48	0.44
3:F:30:SER:HA	3:F:70:TYR:OH	2.18	0.44
2:E:52:ASN:HB2	2:E:53:PRO:CD	2.48	0.44
3:D:135:LEU:HD23	3:D:135:LEU:N	2.32	0.44
5:B:506:DMU:H2	5:B:506:DMU:O1	2.18	0.43
5:B:506:DMU:H35	5:B:506:DMU:O55	2.18	0.43
1:A:183:ALA:HB2	1:A:200:ILE:HG12	2.00	0.43
3:D:72:LEU:HD23	3:D:73:THR:N	2.33	0.43
3:D:93:HIS:CG	3:D:94:PRO:HA	2.53	0.43
5:B:506:DMU:H14	5:B:506:DMU:H21	1.74	0.43
3:F:149:ILE:HG12	3:F:191:TYR:CD2	2.53	0.43
1:A:197:ILE:CD1	1:A:219:PHE:CD2	3.01	0.43
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.51	0.43
1:A:279:LEU:HA	1:A:282:ARG:HH11	1.82	0.43
2:E:6:GLU:CD	2:E:114:GLY:H	2.21	0.43
1:A:172:GLU:HG3	1:A:212:LEU:HB3	1.99	0.43
1:A:163:LEU:HD12	1:A:168:LEU:HB2	2.00	0.43
2:C:132:LEU:HD12	2:C:147:GLY:HA3	2.00	0.43
1:B:284:HIS:O	1:B:286:GLY:N	2.51	0.43
2:C:52:ASN:ND2	2:C:57:THR:HG22	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:41:VAL:O	1:A:45:LEU:HG	2.19	0.43
1:B:312:THR:HG22	1:B:339:ALA:CB	2.49	0.43
2:C:22:CYS:O	2:C:78:THR:HG23	2.19	0.43
2:E:47:TRP:CB	3:F:95:GLN:NE2	2.81	0.43
3:D:112:PRO:HG3	3:D:143:ILE:HD11	2.00	0.43
3:D:104:GLU:HB3	3:D:165:GLN:OE1	2.19	0.43
1:A:226:THR:HG21	1:B:423:LEU:HD11	2.00	0.43
1:B:38:MET:HG3	1:B:168:LEU:HD11	2.00	0.43
2:E:105:TYR:HD2	3:F:91:SER:HA	1.82	0.43
3:D:13:ALA:HA	7:D:309:HOH:O	2.17	0.43
1:A:103:GLU:N	1:A:103:GLU:OE1	2.44	0.43
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.49	0.43
3:F:187:ARG:HG3	3:F:188:HIS:CD2	2.53	0.43
2:E:16:GLY:O	2:E:86:VAL:HB	2.19	0.43
1:A:88:VAL:HA	1:A:91:MET:HE2	2.01	0.43
1:B:88:VAL:HA	1:B:91:MET:HE2	2.00	0.42
1:A:312:THR:HG22	1:A:339:ALA:CB	2.49	0.42
2:E:39:GLN:HB2	2:E:45:LEU:HD23	2.01	0.42
3:F:149:ILE:HD11	3:F:178:LEU:HD21	2.01	0.42
1:A:148:GLU:HG3	1:A:357:PHE:HB3	2.00	0.42
2:C:38:ARG:HD3	2:C:48:ILE:HD11	2.01	0.42
3:F:11:MET:CE	3:F:19:VAL:HG13	2.47	0.42
1:A:430:LEU:CD2	1:B:223:ILE:HD12	2.49	0.42
3:F:106:LEU:HA	3:F:139:TYR:OH	2.19	0.42
2:C:61:THR:OG1	2:C:62:PRO:HD2	2.19	0.42
2:C:6:GLU:OE2	2:C:96:CYS:N	2.42	0.42
1:A:98:ARG:HA	1:A:98:ARG:NE	2.35	0.42
3:D:186:GLU:HA	3:D:210:ARG:NH2	2.35	0.42
3:F:187:ARG:O	3:F:188:HIS:CD2	2.73	0.42
1:A:423:LEU:HD11	1:B:226:THR:HG21	2.01	0.42
1:A:423:LEU:HD11	1:B:226:THR:HG22	2.02	0.42
1:A:62:ASN:O	1:A:63:GLN:C	2.57	0.42
3:D:49:ASP:HB2	3:D:52:LYS:HD3	2.01	0.41
3:D:78:GLU:HA	3:D:78:GLU:OE2	2.20	0.41
2:C:196:TRP:HA	2:C:197:PRO:HA	1.83	0.41
1:A:164:ASP:HB3	5:A:503:DMU:C19	2.47	0.41
3:F:184:GLU:HA	3:F:187:ARG:NH1	2.35	0.41
1:B:279:LEU:HA	1:B:282:ARG:HH11	1.84	0.41
2:C:47:TRP:CD2	3:D:95:GLN:NE2	2.87	0.41
1:A:214:SER:O	1:A:218:VAL:HG23	2.20	0.41
2:E:200:THR:HG23	2:E:202:THR:HG23	2.02	0.41
1:B:98:ARG:NE	1:B:98:ARG:HA	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:172:GLU:OE1	6:B:502:MAL:O3	2.35	0.41
2:C:29:TYR:CE2	2:C:74:ASN:OD1	2.72	0.41
1:B:160:ARG:HD2	1:B:160:ARG:HA	1.80	0.41
1:B:122:VAL:HB	1:B:160:ARG:HG2	2.02	0.41
2:C:221:ARG:O	2:C:222:ALA:HB3	2.21	0.41
2:E:61:THR:O	2:E:63:SER:N	2.54	0.41
5:A:504:DMU:H15	5:A:504:DMU:H21	1.89	0.41
1:A:38:MET:HA	1:A:41:VAL:HG13	2.03	0.41
1:A:402:ILE:HD12	1:A:445:TYR:CE1	2.56	0.41
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.50	0.41
3:D:7:SER:CB	3:D:8:PRO:CD	2.99	0.41
1:A:98:ARG:HH21	1:A:102:PRO:HB3	1.82	0.41
1:B:68:LEU:HD22	1:B:78:LEU:HD22	2.02	0.41
2:E:204:ASN:ND2	2:E:215:ASP:HB3	2.35	0.41
1:A:38:MET:O	1:A:42:VAL:HG23	2.20	0.41
1:A:172:GLU:HG3	1:A:212:LEU:O	2.21	0.41
1:B:323:ALA:HA	7:B:621:HOH:O	2.21	0.41
5:B:505:DMU:H30	5:B:505:DMU:O3	2.21	0.41
2:C:53:PRO:O	2:C:74:ASN:ND2	2.53	0.41
1:A:226:THR:HG22	1:B:423:LEU:HD11	2.03	0.41
1:B:71:THR:O	1:B:78:LEU:HD23	2.21	0.41
3:D:163:THR:OG1	3:D:173:SER:HB2	2.21	0.41
5:A:503:DMU:H4	5:A:503:DMU:H36	1.29	0.40
2:C:86:VAL:HG12	2:C:119:VAL:HG11	2.03	0.40
1:A:68:LEU:HD13	1:A:307:PHE:CD1	2.55	0.40
3:F:17:ASP:O	3:F:76:THR:HA	2.20	0.40
1:A:203:GLU:HA	1:A:203:GLU:OE1	2.21	0.40
5:B:506:DMU:C9	5:B:506:DMU:O55	2.68	0.40
3:D:60:ARG:NE	3:D:78:GLU:HG2	2.37	0.40
1:B:276:MET:HB2	1:B:276:MET:HE3	1.93	0.40
2:E:52:ASN:HD21	2:E:56:SER:HB3	1.86	0.40
3:D:16:GLY:N	3:D:77:MET:O	2.54	0.40
3:D:58:PRO:HG2	3:D:61:PHE:HE1	1.85	0.40
2:C:134:PRO:HA	7:D:318:HOH:O	2.20	0.40
2:C:107:TYR:CD1	3:D:45:ARG:HD3	2.57	0.40
1:B:172:GLU:HG3	1:B:212:LEU:O	2.22	0.40
1:B:68:LEU:HD13	1:B:307:PHE:CD1	2.57	0.40
1:B:128:LEU:HA	1:B:128:LEU:HD23	1.87	0.40
2:C:191:VAL:HB	2:C:192:PRO:CD	2.51	0.40
1:A:253:TRP:HB3	5:A:506:DMU:C18	2.50	0.40
1:B:94:TYR:OH	1:B:352:ALA:HB2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:183:ASP:OD2	5:A:503:DMU:O2[3_545]	1.78	0.42
7:C:342:HOH:O	7:F:321:HOH:O[2_555]	1.82	0.38

## 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	442/446 (99%)	410 (93%)	29 (7%)	3 (1%)	30	43
1	B	440/446 (99%)	413 (94%)	23 (5%)	4 (1%)	25	35
2	C	220/222 (99%)	209 (95%)	8 (4%)	3 (1%)	16	22
2	E	219/222 (99%)	200 (91%)	14 (6%)	5 (2%)	10	10
3	D	209/211 (99%)	182 (87%)	25 (12%)	2 (1%)	22	32
3	F	209/211 (99%)	196 (94%)	11 (5%)	2 (1%)	22	32
All	All	1739/1758 (99%)	1610 (93%)	110 (6%)	19 (1%)	21	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	64	LEU
2	E	65	LYS
2	E	136	SER
3	F	7	SER
2	C	140	ALA
3	D	67	GLY
2	E	139	ALA
1	A	457	GLU
1	B	234	HIS
3	D	7	SER
3	F	187	ARG
1	A	234	HIS
2	E	137	ALA
1	B	18	ARG

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Mol	Chain	Res	Type
1	B	285	GLY
1	B	144	VAL
2	E	62	PRO
1	A	285	GLY
2	C	62	PRO

### 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	335/337 (99%)	320 (96%)	15 (4%)	38	57
1	B	333/337 (99%)	317 (95%)	16 (5%)	35	53
2	C	182/182 (100%)	170 (93%)	12 (7%)	24	35
2	E	181/182 (100%)	174 (96%)	7 (4%)	43	64
3	D	185/185 (100%)	174 (94%)	11 (6%)	28	42
3	F	185/185 (100%)	174 (94%)	11 (6%)	28	42
All	All	1401/1408 (100%)	1329 (95%)	72 (5%)	33	50

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	62	ASN
1	A	73	ASP
1	A	180	THR
1	A	200	ILE
1	A	211	THR
1	A	219	PHE
1	A	246	ASP
1	A	251	THR
1	A	264	ILE
1	A	273	VAL
1	A	304	LEU
1	A	397	LEU
1	A	402	ILE

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Mol	Chain	Res	Type
1	A	423	LEU
1	B	23	ARG
1	B	62	ASN
1	B	73	ASP
1	B	162	VAL
1	B	180	THR
1	B	200	ILE
1	B	211	THR
1	B	219	PHE
1	B	246	ASP
1	B	251	THR
1	B	264	ILE
1	B	273	VAL
1	B	304	LEU
1	B	397	LEU
1	B	402	ILE
1	B	423	LEU
2	C	30	SER
2	C	43	LYS
2	C	51	ILE
2	C	66	ASP
2	C	72	ARG
2	C	115	THR
2	C	193	SER
2	C	198	SER
2	C	199	GLU
2	C	200	THR
2	C	204	ASN
2	C	214	VAL
3	D	21	MET
3	D	22	THR
3	D	41	THR
3	D	76	THR
3	D	92	SER
3	D	95	GLN
3	D	115	SER
3	D	174	MET
3	D	180	LEU
3	D	187	ARG
3	D	201	THR
2	E	5	LEU
2	E	55	SER

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Mol	Chain	Res	Type
2	E	56	SER
2	E	71	SER
2	E	103	TYR
2	E	188	SER
2	E	200	THR
3	F	1	ASP
3	F	6	GLN
3	F	44	LYS
3	F	77	MET
3	F	95	GLN
3	F	142	ASP
3	F	190	SER
3	F	192	THR
3	F	198	LYS
3	F	201	THR
3	F	205	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	157	ASN
1	A	207	GLN
1	A	270	ASN
1	B	157	ASN
1	B	250	ASN
1	B	270	ASN
2	C	163	ASN
2	C	172	HIS
3	D	136	ASN
3	D	137	ASN
3	D	144	ASN
3	D	188	HIS
2	E	172	HIS
2	E	179	GLN
3	F	136	ASN
3	F	137	ASN
3	F	188	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	DMU	A	503	-	34,34,34	0.48	0	45,45,45	1.33	6 (13%)
5	DMU	A	504	-	34,34,34	0.54	0	45,45,45	1.20	3 (6%)
5	DMU	A	505	-	34,34,34	0.47	0	45,45,45	1.13	4 (8%)
5	DMU	A	506	-	34,34,34	0.41	0	45,45,45	1.21	4 (8%)
6	MAL	B	502	-	24,24,24	0.57	0	35,35,35	1.26	3 (8%)
5	DMU	B	505	-	34,34,34	0.45	0	45,45,45	1.09	3 (6%)
5	DMU	B	506	-	34,34,34	0.47	0	45,45,45	1.08	3 (6%)
6	MAL	B	507	-	24,24,24	0.47	0	35,35,35	0.92	0
6	MAL	B	508	-	24,24,24	0.61	0	35,35,35	1.38	4 (11%)

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
5	DMU	A	503	-	-	0/19/59/59	0/2/2/2
5	DMU	A	504	-	-	0/19/59/59	0/2/2/2
5	DMU	A	505	-	-	0/19/59/59	0/2/2/2
5	DMU	A	506	-	-	0/19/59/59	0/2/2/2
6	MAL	B	502	-	-	0/8/48/48	0/2/2/2
5	DMU	B	505	-	-	0/19/59/59	0/2/2/2
5	DMU	B	506	-	-	0/19/59/59	0/2/2/2
6	MAL	B	507	-	-	0/8/48/48	0/2/2/2
6	MAL	B	508	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	508	MAL	C1-C2-C3	4.14	118.05	110.00
5	A	503	DMU	C8-C7-C5	-3.71	103.97	110.82
5	A	504	DMU	C6-O5-C4	3.38	120.30	113.73
6	B	502	MAL	C1-O5-C5	3.34	120.22	113.73
5	A	506	DMU	C2-C3-C4	-3.32	103.39	110.85
6	B	502	MAL	C2'-C3'-C4'	3.30	116.78	109.61
6	B	508	MAL	C1-O5-C5	3.27	120.09	113.73
6	B	508	MAL	O5-C1-C2	3.06	116.59	110.31
5	A	505	DMU	C7-C8-C9	3.06	115.67	110.20
5	A	503	DMU	O5-C4-C3	3.00	115.97	109.70
5	A	503	DMU	O2-C8-C7	-2.79	104.09	110.35
5	B	505	DMU	C10-O1-C9	-2.74	108.39	113.73
5	A	504	DMU	O16-C6-C1	2.64	111.54	108.18
5	B	505	DMU	C7-C8-C9	2.62	114.89	110.20
5	B	506	DMU	C6-O5-C4	-2.61	108.64	113.73
5	A	503	DMU	C10-O7-C3	-2.60	111.35	117.99
5	B	506	DMU	C1-C2-C3	2.57	115.20	109.61
5	A	505	DMU	O1-C9-C8	2.55	114.48	109.76
5	A	504	DMU	C10-O7-C3	-2.42	111.83	117.99
5	A	506	DMU	C6-C1-C2	2.37	114.61	110.00
6	B	508	MAL	C3'-C4'-C5'	-2.36	105.55	110.85
5	A	503	DMU	C6-C1-C2	-2.35	105.42	110.00
5	B	505	DMU	C18-O16-C6	-2.34	109.74	113.96
5	A	506	DMU	C18-O16-C6	-2.28	109.85	113.96
5	A	506	DMU	C6-O5-C4	-2.13	109.58	113.73
5	A	505	DMU	O7-C3-C4	2.11	114.83	109.33
6	B	502	MAL	O5'-C5'-C4'	2.08	114.05	109.70
5	B	506	DMU	O55-C2-C1	-2.08	105.69	110.35
5	A	503	DMU	C2-C3-C4	2.01	115.36	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	505	DMU	O2-C8-C7	-2.00	105.86	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	444/446 (99%)	0.65	38 (8%) 11 9	27, 47, 78, 118	0
1	B	442/446 (99%)	0.72	48 (10%) 6 6	27, 46, 79, 106	0
2	C	222/222 (100%)	-0.01	5 (2%) 57 55	15, 40, 76, 102	0
2	E	221/222 (99%)	0.17	9 (4%) 35 33	19, 43, 75, 124	0
3	D	211/211 (100%)	0.31	13 (6%) 20 18	26, 48, 70, 86	0
3	F	211/211 (100%)	0.15	4 (1%) 64 61	16, 37, 76, 99	0
All	All	1751/1758 (99%)	0.42	117 (6%) 18 16	15, 45, 78, 124	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	PHE	10.2
1	A	72	ALA	5.9
2	E	136	SER	5.6
1	A	71	THR	5.2
1	B	72	ALA	4.9
1	B	68	LEU	4.7
2	E	69	ILE	4.5
2	C	194	SER	4.2
2	E	222	ALA	4.2
1	B	75	TYR	4.1
1	B	304	LEU	4.1
1	B	410	ILE	4.0
2	E	135	GLY	4.0
1	B	195	ALA	4.0
1	A	291	TRP	3.9
1	B	145	LEU	3.8
1	B	78	LEU	3.7
1	B	354	GLY	3.7
3	F	147	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	29	TYR	3.7
2	C	65	LYS	3.7
1	B	422	ILE	3.6
1	B	65	MET	3.5
1	A	283	VAL	3.5
1	B	79	LEU	3.4
1	B	168	LEU	3.4
1	B	104	ALA	3.4
1	B	412	VAL	3.3
1	B	166	PHE	3.3
1	A	326	GLY	3.2
1	B	229	TYR	3.2
1	A	194	LEU	3.2
1	B	194	LEU	3.1
1	A	140	GLY	3.1
3	D	110	ALA	3.1
1	B	235	GLU	3.1
1	A	193	PRO	3.1
1	A	234	HIS	3.1
2	E	70	ILE	3.0
1	B	73	ASP	2.9
1	B	413	LEU	2.9
1	B	71	THR	2.9
1	A	198	LEU	2.9
3	D	141	LYS	2.8
1	A	77	LEU	2.8
1	B	69	VAL	2.8
1	B	411	LEU	2.8
3	F	152	SER	2.8
1	B	236	VAL	2.8
3	F	154	ARG	2.8
1	A	197	ILE	2.8
1	B	409	ILE	2.7
1	A	413	LEU	2.7
3	D	111	ALA	2.7
1	A	410	ILE	2.7
1	B	419	TYR	2.7
1	B	193	PRO	2.7
1	A	426	ILE	2.6
1	B	197	ILE	2.6
1	B	408	GLY	2.6
1	B	162	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	139	TYR	2.6
1	B	35	ILE	2.6
2	E	59	ASN	2.6
1	A	386	ALA	2.6
1	B	196	GLY	2.6
1	B	32	PRO	2.6
1	A	167	ARG	2.5
1	A	290	LYS	2.5
1	B	192	ALA	2.5
3	D	7	SER	2.5
1	A	422	ILE	2.5
1	B	353	PRO	2.5
3	D	18	LYS	2.5
1	B	407	THR	2.4
1	B	426	ILE	2.4
2	E	48	ILE	2.4
1	A	285	GLY	2.4
1	B	414	GLU	2.4
1	A	141	GLY	2.4
3	D	142	ASP	2.3
1	A	187	ALA	2.3
1	A	66	GLY	2.3
3	D	149	ILE	2.3
1	A	139	LEU	2.3
1	B	378	LEU	2.3
3	D	143	ILE	2.3
1	A	81	VAL	2.3
1	A	222	VAL	2.3
1	B	177	LEU	2.3
1	B	101	ALA	2.3
1	A	288	ILE	2.3
1	A	298	ILE	2.3
1	B	308	VAL	2.2
1	A	195	ALA	2.2
1	B	237	ALA	2.2
1	A	201	ILE	2.2
1	A	252	LEU	2.2
1	A	145	LEU	2.1
1	A	423	LEU	2.1
2	E	66	ASP	2.1
1	A	235	GLU	2.1
1	A	427	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	70	HIS	2.1
1	A	98	ARG	2.1
3	F	178	LEU	2.1
1	B	302	CYS	2.1
2	C	199	GLU	2.1
3	D	16	GLY	2.0
3	D	19	VAL	2.0
1	A	419	TYR	2.0
2	E	138	ALA	2.0
3	D	108	ALA	2.0
1	B	225	SER	2.0
1	A	192	ALA	2.0
2	C	66	ASP	2.0
3	D	168	LYS	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	MAL	B	507	23/23	0.23	56.33	80,91,102,105	0
5	DMU	A	504	33/33	0.21	6.47	69,81,91,92	0
6	MAL	B	508	23/23	0.27	1.43	72,85,97,100	0
5	DMU	B	506	33/33	0.18	1.30	54,65,84,87	0
5	DMU	A	503	33/33	0.22	0.59	43,72,80,83	0
5	DMU	B	505	33/33	0.17	-0.33	38,68,90,95	0
5	DMU	A	505	33/33	0.15	-0.49	61,72,80,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MAL	B	502	23/23	0.16	-0.64	59,77,84,85	0
4	CL	A	502	1/1	0.11	-1.03	60,60,60,60	0
4	CL	B	501	1/1	0.16	-1.30	65,65,65,65	0
5	DMU	A	506	33/33	0.16	-1.51	48,72,96,98	0
4	CL	B	504	1/1	0.12	-2.14	49,49,49,49	0
4	CL	B	503	1/1	0.09	-2.93	43,43,43,43	0
4	CL	A	501	1/1	0.07	-3.40	42,42,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.