



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:29 PM 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 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

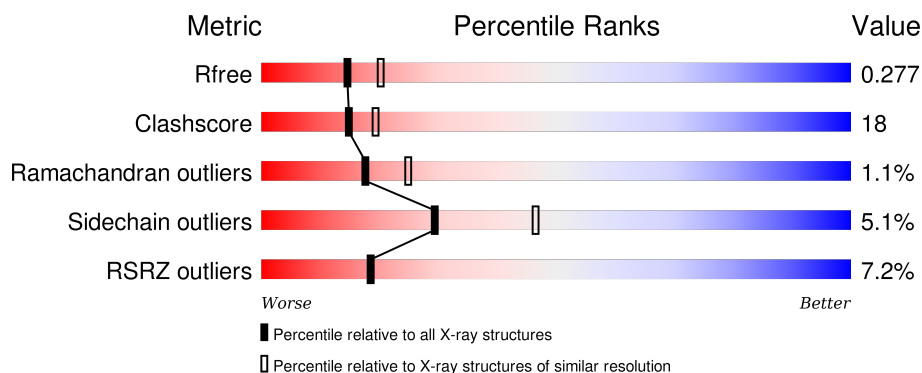
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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. 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	446	<div> <div>10%</div> <div>71%</div> <div>26%</div> <div>.</div> </div>
1	B	446	<div> <div>12%</div> <div>69%</div> <div>27%</div> <div>..</div> </div>
2	C	222	<div> <div>4%</div> <div>66%</div> <div>30%</div> <div>.</div> </div>
2	E	222	<div> <div>3%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>
3	D	211	<div> <div>5%</div> <div>57%</div> <div>40%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	211	

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
6	MAL	B	508	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13691 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 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			

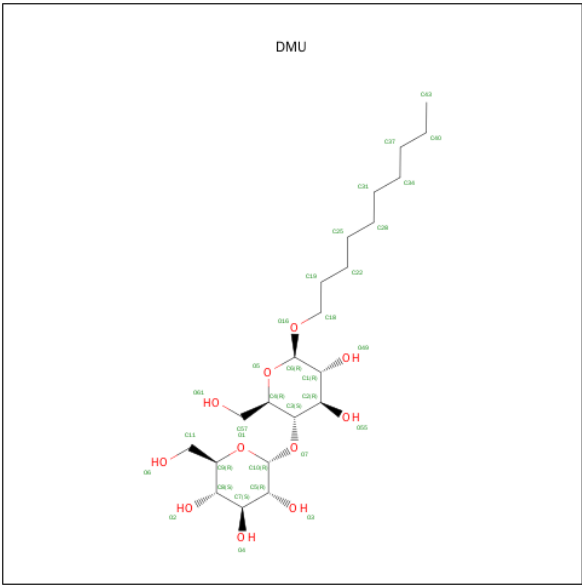
- Molecule 3 is a protein called light chain of Fab fragment.

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).

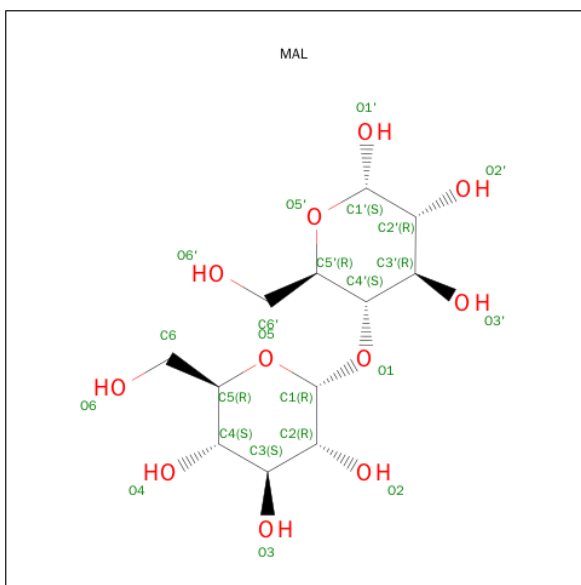
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Cl	0	0
			3	3		
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



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		

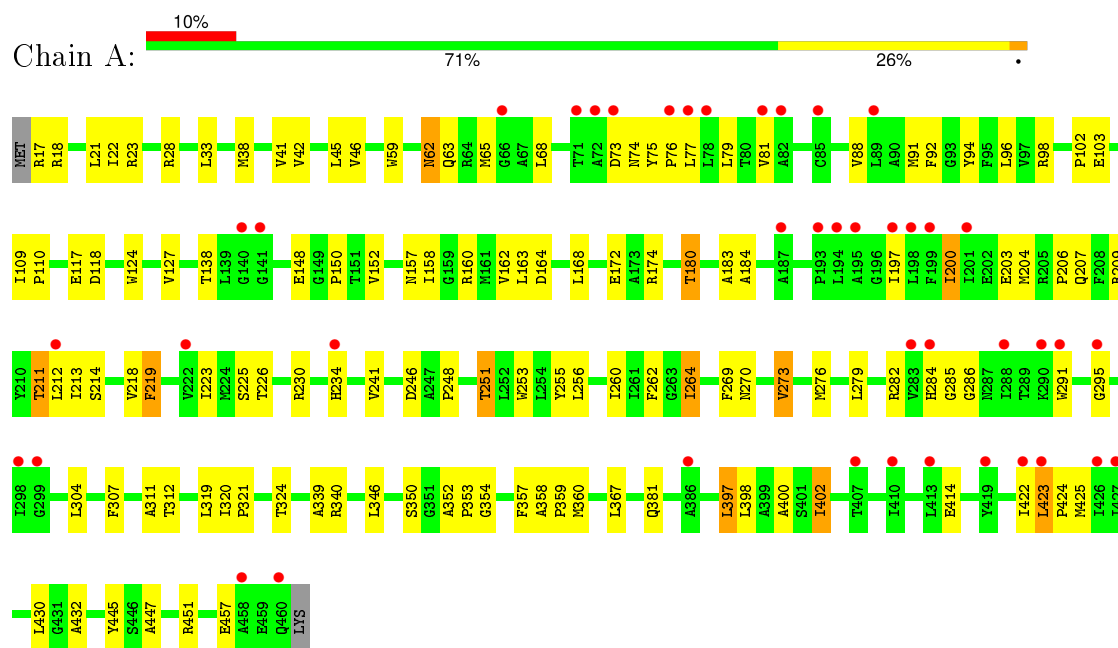
- Molecule 7 is water.

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		

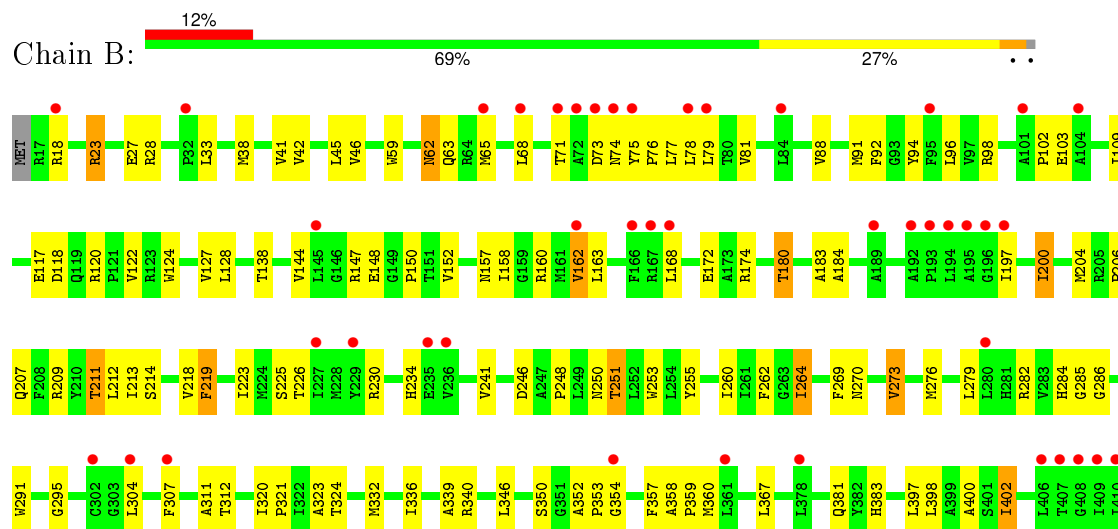
### 3 Residue-property plots [i](#)

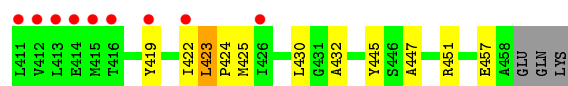
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

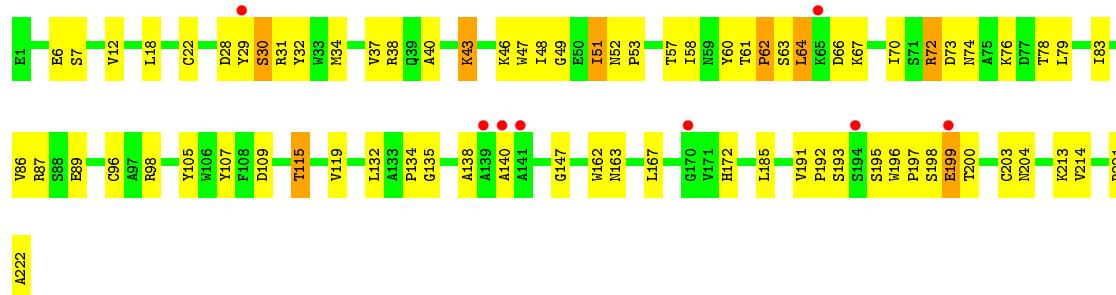


- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

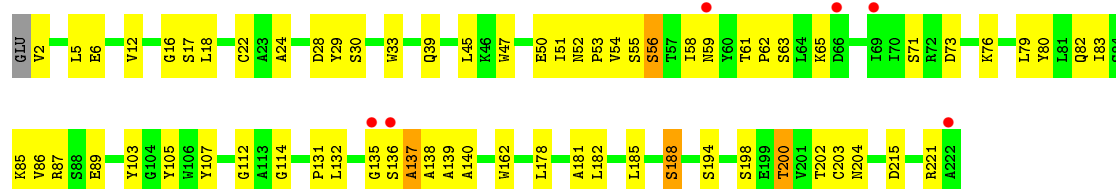




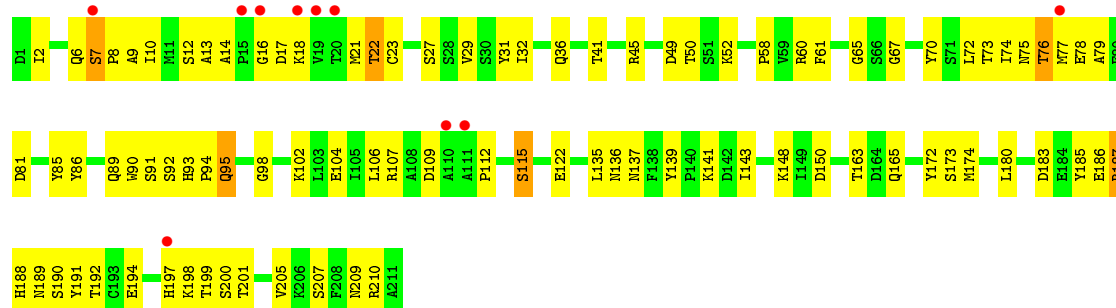
- Molecule 2: heavy chain of Fab fragment



- Molecule 2: heavy chain of Fab fragment



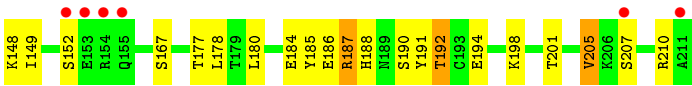
- Molecule 3: light chain of Fab fragment



- Molecule 3: light chain of Fab fragment







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.26 Å 97.52 Å 173.96 Å 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 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.239 , 0.278 0.238 , 0.277	Depositor DCC
$R_{free}$ test set	5504 reflections (5.33%)	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> )	0.34 , 54.4	EDS
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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.

<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

### 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 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	3333	0	3484	114	0
1	B	3315	0	3470	120	0
2	C	1681	0	1663	56	0
2	E	1672	0	1654	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 (481) 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)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:31:TYR:HA	3:D:50:THR:OG1	1.95	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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%)	26	38
1	B	440/446 (99%)	413 (94%)	23 (5%)	4 (1%)	21	30
2	C	220/222 (99%)	209 (95%)	8 (4%)	3 (1%)	14	19
2	E	219/222 (99%)	200 (91%)	14 (6%)	5 (2%)	8	8
3	D	209/211 (99%)	182 (87%)	25 (12%)	2 (1%)	19	28
3	F	209/211 (99%)	196 (94%)	11 (5%)	2 (1%)	19	28
All	All	1739/1758 (99%)	1610 (93%)	110 (6%)	19 (1%)	17	25



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
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%)	34	52
1	B	333/337 (99%)	317 (95%)	16 (5%)	31	49
2	C	182/182 (100%)	170 (93%)	12 (7%)	21	32
2	E	181/182 (100%)	174 (96%)	7 (4%)	39	59
3	D	185/185 (100%)	174 (94%)	11 (6%)	24	38
3	F	185/185 (100%)	174 (94%)	11 (6%)	24	38
All	All	1401/1408 (100%)	1329 (95%)	72 (5%)	29	46

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [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](#)

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	1.32	7 (15%)
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	1.14	3 (6%)
5	DMU	A	506	-	34,34,34	0.41	0	45,45,45	1.21	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAL	B	502	-	24,24,24	0.58	0	35,35,35	1.25	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	0.48	0	35,35,35	0.91	0
6	MAL	B	508	-	24,24,24	0.62	0	35,35,35	1.37	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(°)
5	A	503	DMU	C8-C7-C5	-3.66	103.97	110.79
5	A	506	DMU	C2-C3-C4	-3.30	103.39	110.84
5	A	503	DMU	O2-C8-C7	-2.77	104.09	110.34
5	B	505	DMU	C10-O1-C9	-2.76	108.39	113.75
5	B	506	DMU	C6-O5-C4	-2.63	108.64	113.75
5	A	503	DMU	C10-O7-C3	-2.55	111.35	118.01
5	B	505	DMU	C18-O16-C6	-2.40	109.74	113.94
5	A	504	DMU	C10-O7-C3	-2.37	111.83	118.01
5	A	506	DMU	C18-O16-C6	-2.34	109.85	113.94
6	B	508	MAL	C3'-C4'-C5'	-2.34	105.55	110.84
5	A	503	DMU	C6-C1-C2	-2.31	105.42	109.97
5	A	506	DMU	C6-O5-C4	-2.14	109.58	113.75
5	B	506	DMU	O55-C2-C1	-2.06	105.69	110.34
5	A	503	DMU	C18-O16-C6	-2.05	110.36	113.94
5	A	503	DMU	C2-C3-C4	2.00	115.36	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	502	MAL	O5'-C5'-C4'	2.04	114.05	109.75
5	A	505	DMU	O7-C3-C4	2.10	114.83	109.32
5	A	506	DMU	C6-C1-C2	2.35	114.61	109.97
5	B	506	DMU	C1-C2-C3	2.55	115.20	109.60
5	A	505	DMU	O1-C9-C8	2.56	114.48	109.68
5	B	505	DMU	C7-C8-C9	2.69	114.89	110.20
5	A	504	DMU	O16-C6-C1	2.77	111.54	108.04
5	A	503	DMU	O5-C4-C3	2.95	115.97	109.75
6	B	508	MAL	O5-C1-C2	3.08	116.59	110.28
5	A	505	DMU	C7-C8-C9	3.14	115.67	110.20
6	B	502	MAL	C2'-C3'-C4'	3.27	116.78	109.60
6	B	508	MAL	C1-O5-C5	3.27	120.09	113.75
6	B	502	MAL	C1-O5-C5	3.34	120.22	113.75
5	A	504	DMU	C6-O5-C4	3.38	120.30	113.75
6	B	508	MAL	C1-C2-C3	4.10	118.05	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	DMU	10	1
5	A	504	DMU	3	0
5	A	505	DMU	13	0
5	A	506	DMU	11	0
6	B	502	MAL	5	0
5	B	505	DMU	10	0
5	B	506	DMU	11	0
6	B	507	MAL	4	0
6	B	508	MAL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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%)	0.66	43 (9%)	10 9	27, 47, 78, 118	0
1	B	442/446 (99%)	0.71	52 (11%)	6 6	27, 46, 79, 106	0
2	C	222/222 (100%)	-0.00	8 (3%)	46 47	15, 40, 76, 102	0
2	E	221/222 (99%)	0.12	6 (2%)	58 57	19, 43, 75, 124	0
3	D	211/211 (100%)	0.33	10 (4%)	35 36	26, 48, 70, 86	0
3	F	211/211 (100%)	0.17	7 (3%)	50 50	16, 37, 76, 99	0
All	All	1751/1758 (99%)	0.42	126 (7%)	18 18	15, 45, 78, 124	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	PHE	7.0
1	A	72	ALA	6.4
1	B	72	ALA	6.3
1	A	71	THR	5.0
2	C	194	SER	4.9
2	E	136	SER	4.9
2	E	222	ALA	4.7
1	B	410	ILE	4.6
1	A	291	TRP	4.4
1	B	104	ALA	4.3
1	B	195	ALA	4.2
2	C	65	LYS	4.1
1	B	78	LEU	3.8
1	B	422	ILE	3.7
1	A	197	ILE	3.7
3	F	152	SER	3.6
1	A	460	GLN	3.5
1	B	194	LEU	3.5
1	B	75	TYR	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	194	LEU	3.4
1	B	71	THR	3.4
1	B	412	VAL	3.4
1	B	73	ASP	3.4
1	B	197	ILE	3.4
1	B	235	GLU	3.4
2	E	66	ASP	3.4
1	B	145	LEU	3.3
1	A	140	GLY	3.3
3	D	16	GLY	3.3
1	A	77	LEU	3.3
1	A	198	LEU	3.3
1	A	81	VAL	3.2
3	D	110	ALA	3.2
1	B	304	LEU	3.2
1	B	409	ILE	3.1
1	A	426	ILE	3.1
1	B	354	GLY	3.1
3	F	155	GLN	3.0
1	A	290	LYS	3.0
1	B	68	LEU	3.0
1	A	193	PRO	3.0
1	A	201	ILE	3.0
3	D	19	VAL	3.0
1	A	234	HIS	3.0
1	B	236	VAL	3.0
1	B	84	LEU	3.0
1	B	408	GLY	3.0
1	B	229	TYR	3.0
2	E	69	ILE	3.0
3	D	7	SER	2.9
1	A	78	LEU	2.9
1	A	413	LEU	2.9
3	F	154	ARG	2.9
1	B	413	LEU	2.9
3	F	153	GLU	2.8
1	B	168	LEU	2.8
3	D	18	LYS	2.8
2	E	135	GLY	2.8
1	B	426	ILE	2.8
2	C	139	ALA	2.8
1	A	141	GLY	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	29	TYR	2.8
1	A	82	ALA	2.8
1	B	411	LEU	2.7
1	B	166	PHE	2.7
1	B	193	PRO	2.7
1	A	66	GLY	2.7
1	A	283	VAL	2.7
3	F	207	SER	2.7
1	A	284	HIS	2.6
3	D	111	ALA	2.6
1	B	196	GLY	2.6
2	C	141	ALA	2.5
1	B	167	ARG	2.5
1	A	410	ILE	2.5
1	A	386	ALA	2.5
1	B	407	THR	2.5
1	A	298	ILE	2.5
1	B	79	LEU	2.4
2	C	140	ALA	2.4
1	B	280	LEU	2.4
1	A	458	ALA	2.4
3	F	211	ALA	2.4
1	B	378	LEU	2.4
1	B	192	ALA	2.4
3	D	77	MET	2.4
1	B	101	ALA	2.4
1	A	422	ILE	2.3
1	B	406	LEU	2.3
1	A	76	PRO	2.3
3	D	15	PRO	2.3
1	B	302	CYS	2.3
1	A	195	ALA	2.3
1	A	427	ILE	2.3
1	A	423	LEU	2.3
1	B	414	GLU	2.3
1	A	89	LEU	2.3
2	E	59	ASN	2.3
1	B	32	PRO	2.3
1	B	419	TYR	2.2
1	B	162	VAL	2.2
1	B	74	ASN	2.2
1	B	65	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	415	MET	2.2
1	B	361	LEU	2.2
1	A	187	ALA	2.2
1	B	189	ALA	2.2
1	A	85	CYS	2.2
1	B	18	ARG	2.2
2	C	199	GLU	2.1
1	A	73	ASP	2.1
1	B	95	PHE	2.1
1	A	295	GLY	2.1
1	A	419	TYR	2.1
1	B	227	ILE	2.1
3	D	20	THR	2.1
3	F	147	TRP	2.1
1	A	288	ILE	2.1
3	D	197	HIS	2.0
1	A	212	LEU	2.0
1	A	407	THR	2.0
1	B	416	THR	2.0
1	A	222	VAL	2.0
1	A	199	PHE	2.0
1	A	299	GLY	2.0
2	C	170	GLY	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( $\text{\AA}^2$ )	Q<0.9
6	MAL	B	508	23/23	0.69	0.38	2.35	72,85,97,100	0
5	DMU	A	503	33/33	0.85	0.21	1.09	43,72,80,83	0
5	DMU	B	505	33/33	0.86	0.18	-0.15	38,68,90,95	0
4	CL	B	501	1/1	0.94	0.19	-0.22	65,65,65,65	0
5	DMU	A	505	33/33	0.90	0.14	-0.62	61,72,80,83	0
6	MAL	B	502	23/23	0.83	0.16	-0.67	59,77,84,85	0
4	CL	A	502	1/1	0.83	0.12	-0.98	60,60,60,60	0
5	DMU	A	506	33/33	0.88	0.16	-1.19	48,72,96,98	0
4	CL	B	504	1/1	0.97	0.10	-2.93	49,49,49,49	0
4	CL	B	503	1/1	0.95	0.10	-3.11	43,43,43,43	0
4	CL	A	501	1/1	0.92	0.09	-3.55	42,42,42,42	0
6	MAL	B	507	23/23	0.78	0.31	-	80,91,102,105	0
5	DMU	A	504	33/33	0.84	0.23	-	69,81,91,92	0
5	DMU	B	506	33/33	0.91	0.16	-	54,65,84,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.