



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:43 PM GMT

PDB ID : 4PQK  
Title : C-Terminal domain of DNA binding protein  
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.K.  
Deposited on : 2014-03-03  
Resolution : 3.40 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

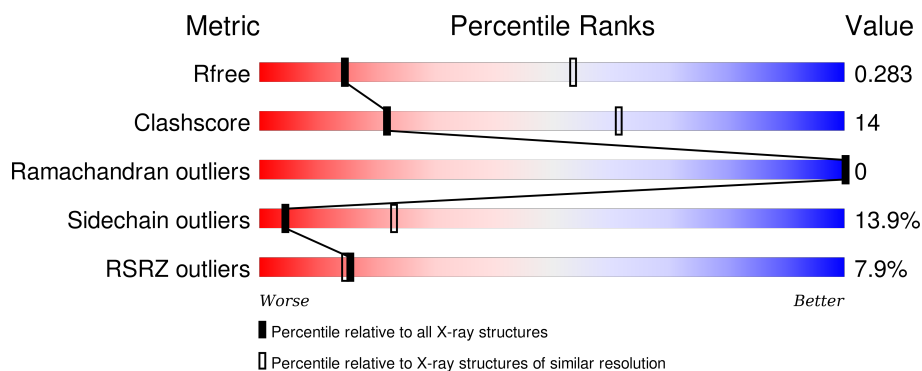
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	487	<div> <div>9%</div> <div>64% 30% . .</div> </div>
1	B	487	<div> <div>7%</div> <div>70% 26% . .</div> </div>
1	C	487	<div> <div>7%</div> <div>68% 25% 5% .</div> </div>
1	D	487	<div> <div>8%</div> <div>63% 28% 6% .</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14876 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.

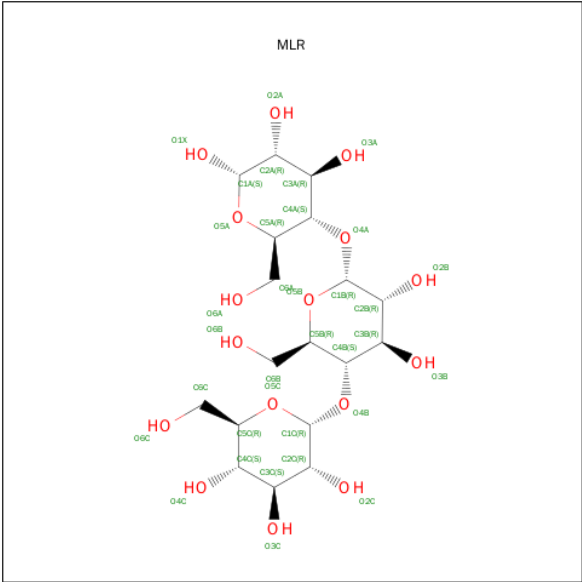
- Molecule 1 is a protein called Maltose ABC transporter periplasmic protein, Truncated replication protein RepA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3700	2371	603	713	13			
1	B	479	Total	C	N	O	S	0	0	0
			3722	2392	615	703	12			
1	C	476	Total	C	N	O	S	0	0	0
			3648	2346	601	690	11			
1	D	472	Total	C	N	O	S	0	0	0
			3670	2351	601	707	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP U6NJU2
B	1	MET	-	EXPRESSION TAG	UNP U6NJU2
C	1	MET	-	EXPRESSION TAG	UNP U6NJU2
D	1	MET	-	EXPRESSION TAG	UNP U6NJU2

- Molecule 2 is MALTOTRIOSE (three-letter code: MLR) (formula: C<sub>18</sub>H<sub>32</sub>O<sub>16</sub>).

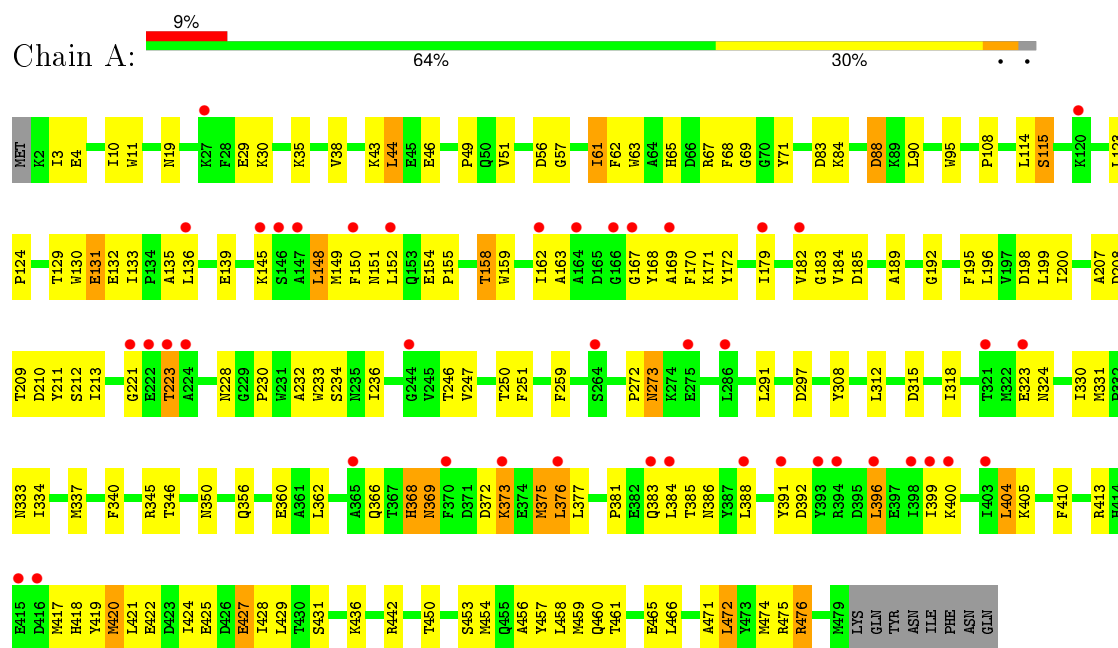


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			34	18	16		
2	B	1	Total	C	O	0	0
			34	18	16		
2	C	1	Total	C	O	0	0
			34	18	16		
2	D	1	Total	C	O	0	0
			34	18	16		

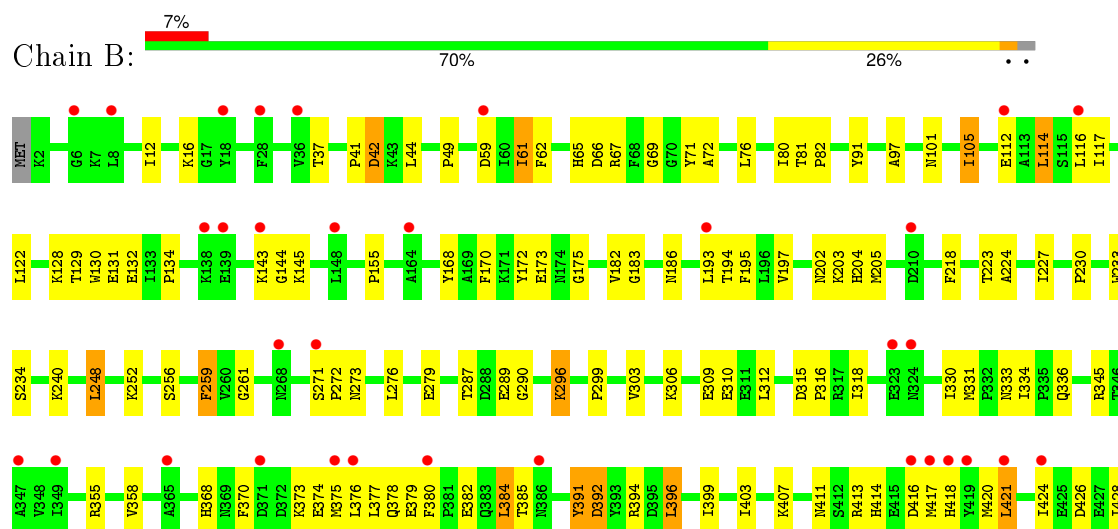
### 3 Residue-property plots

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: Maltose ABC transporter periplasmic protein, Truncated replication protein RepA

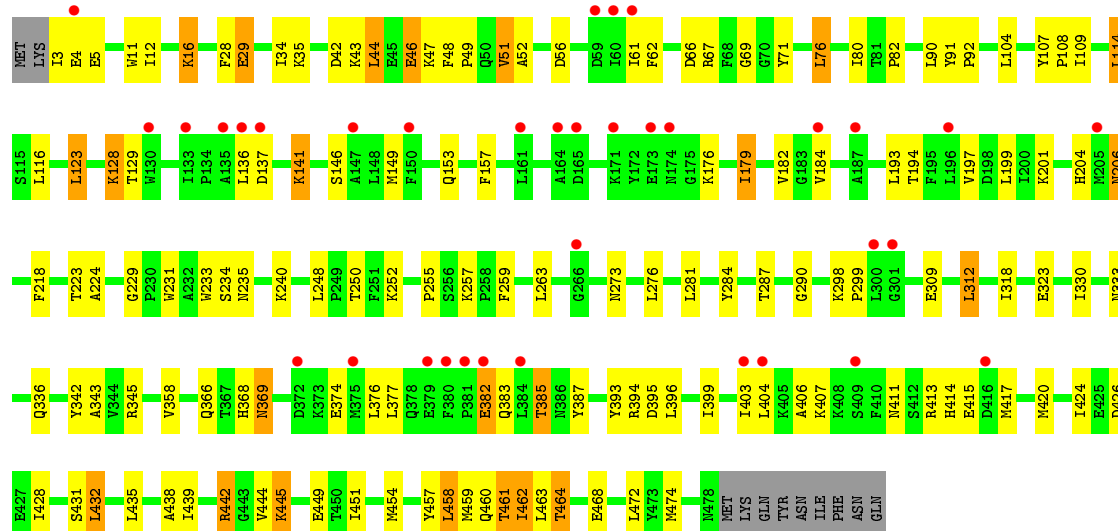


- Molecule 1: Maltose ABC transporter periplasmic protein, Truncated replication protein RepA

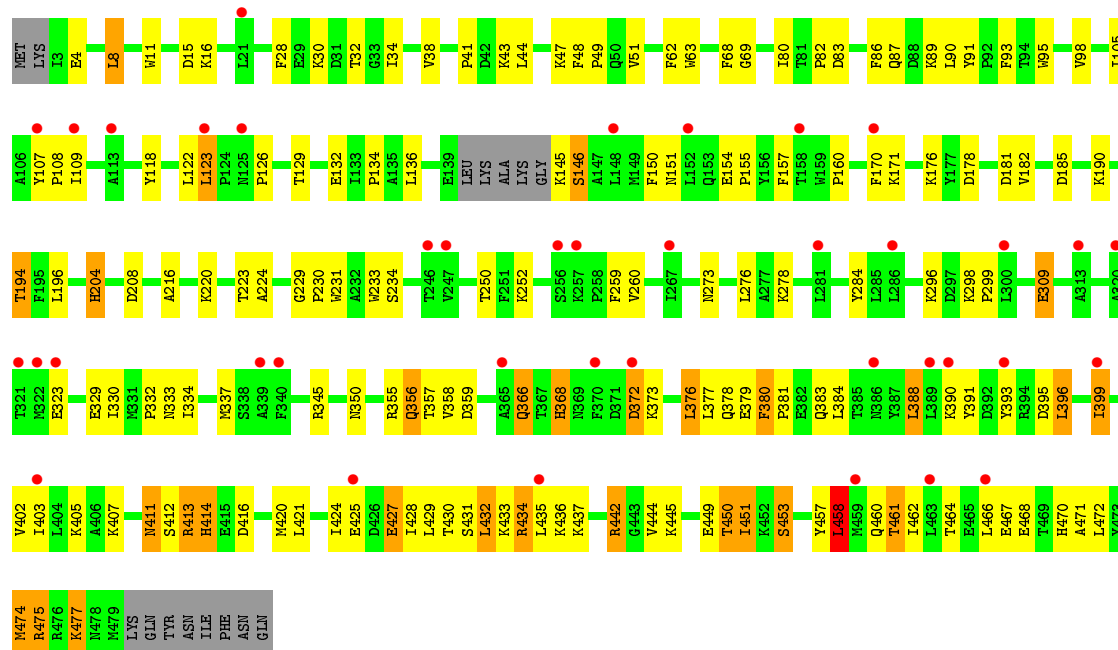




- Molecule 1: Maltose ABC transporter periplasmic protein, Truncated replication protein RepA



- Molecule 1: Maltose ABC transporter periplasmic protein, Truncated replication protein RepA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.22Å 93.67Å 100.81Å 107.67° 108.30° 84.93°	Depositor
Resolution (Å)	46.62 – 3.40 46.62 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.62-3.40) 63.2 (46.62-3.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.237 , 0.275 0.252 , 0.283	Depositor DCC
$R_{free}$ test set	1963 reflections (11.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.9	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 25.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 19628 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	14876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% 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: MLR

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	0.45	0/3784	0.57	0/5142
1	B	0.44	0/3805	0.54	0/5157
1	C	0.43	0/3730	0.63	1/5063 (0.0%)
1	D	0.45	0/3751	0.65	2/5090 (0.0%)
All	All	0.44	0/15070	0.60	3/20452 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8	LEU	CA-CB-CG	5.36	127.62	115.30
1	D	458	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	463	LEU	CA-CB-CG	5.02	126.84	115.30

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	3700	0	3562	116	0
1	B	3722	0	3663	87	0
1	C	3648	0	3540	85	0
1	D	3670	0	3560	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	34	0	31	7	0
2	B	34	0	32	7	0
2	C	34	0	31	5	0
2	D	34	0	32	6	0
All	All	14876	0	14451	411	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 14.

All (411) 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)
2:C:700:MLR:O5C	2:C:700:MLR:C5C	1.63	1.46
2:A:700:MLR:C5C	2:A:700:MLR:O5C	1.64	1.45
2:D:700:MLR:C5C	2:D:700:MLR:O5C	1.64	1.43
2:B:700:MLR:C5C	2:B:700:MLR:O5C	1.64	1.41
2:B:700:MLR:C1C	2:B:700:MLR:O5C	1.72	1.38
2:A:700:MLR:C1C	2:A:700:MLR:O5C	1.73	1.37
2:C:700:MLR:C1C	2:C:700:MLR:O5C	1.71	1.36
2:D:700:MLR:C1C	2:D:700:MLR:O5C	1.71	1.36
1:A:155:PRO:HD3	1:A:345:ARG:HG3	1.36	1.05
1:C:413:ARG:HG2	1:C:414:HIS:CE1	1.93	1.03
1:A:129:THR:HG22	1:A:250:THR:OG1	1.61	1.00
1:A:272:PRO:HG2	1:A:273:ASN:ND2	1.79	0.97
1:B:144:GLY:O	1:B:145:LYS:NZ	2.03	0.91
1:B:377:LEU:HD21	1:B:396:LEU:HD21	1.52	0.90
1:C:403:ILE:HD12	1:C:428:ILE:HD13	1.52	0.89
2:A:700:MLR:C1C	2:A:700:MLR:C5C	2.51	0.88
1:A:420:MET:CE	1:A:420:MET:HA	2.06	0.85
2:C:700:MLR:C1C	2:C:700:MLR:C5C	2.54	0.85
2:B:700:MLR:C5C	2:B:700:MLR:C1C	2.56	0.84
1:A:420:MET:HE2	1:A:420:MET:HA	1.59	0.84
1:A:155:PRO:CD	1:A:345:ARG:HG3	2.07	0.83
1:B:424:ILE:HG22	1:B:428:ILE:HG13	1.60	0.83
1:A:421:LEU:HD12	1:A:421:LEU:H	1.42	0.83
1:D:80:ILE:HG22	1:D:82:PRO:HD3	1.62	0.80
1:C:16:LYS:NZ	1:C:263:LEU:HD22	1.96	0.80
1:A:376:LEU:HD11	1:A:400:LYS:HD2	1.63	0.79
2:D:700:MLR:C1C	2:D:700:MLR:C5C	2.60	0.78
1:B:170:PHE:CD2	1:B:334:ILE:HD11	2.18	0.78
1:C:11:TRP:HB3	1:C:44:LEU:HD12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:HD3	1:A:345:ARG:CG	2.16	0.75
1:D:462:ILE:O	1:D:466:LEU:HD12	1.86	0.75
1:D:91:TYR:HE2	1:D:309:GLU:HG3	1.52	0.75
1:B:420:MET:HE3	1:B:421:LEU:H	1.52	0.75
1:B:407:LYS:O	1:B:411:ASN:ND2	2.20	0.74
1:C:5:GLU:O	1:C:273:ASN:ND2	2.20	0.73
1:B:296:LYS:HB3	1:B:296:LYS:HZ2	1.51	0.73
1:D:146:SER:HB2	1:D:223:THR:HG23	1.69	0.73
1:B:296:LYS:HB3	1:B:296:LYS:NZ	2.03	0.73
1:C:342:TYR:HD1	1:C:345:ARG:HH21	1.37	0.72
1:D:430:THR:O	1:D:434:ARG:HG2	1.88	0.72
1:C:16:LYS:HZ2	1:C:263:LEU:HD22	1.53	0.72
1:C:47:LYS:O	1:C:51:VAL:HG22	1.88	0.72
1:C:399:ILE:HD11	1:C:451:ILE:HG12	1.73	0.71
1:B:336:GLN:HE21	1:B:373:LYS:HG3	1.55	0.71
1:A:391:TYR:HB2	1:A:396:LEU:HD12	1.72	0.71
1:D:16:LYS:NZ	2:D:700:MLR:O2A	2.24	0.70
1:D:402:VAL:HG11	1:D:458:LEU:HG	1.72	0.70
1:D:368:HIS:O	1:D:368:HIS:ND1	2.23	0.70
1:C:179:ILE:H	1:C:179:ILE:HD12	1.57	0.70
1:D:34:ILE:HD13	1:D:276:LEU:HD21	1.71	0.69
1:B:382:GLU:O	1:B:385:THR:HG22	1.92	0.69
1:D:388:LEU:HB3	1:D:396:LEU:HD11	1.75	0.68
1:D:414:HIS:HD2	1:D:470:HIS:CD2	2.11	0.68
1:B:80:ILE:HG22	1:B:82:PRO:HD3	1.74	0.68
1:B:240:LYS:HA	1:C:240:LYS:HG3	1.74	0.68
1:A:155:PRO:HG3	1:A:345:ARG:HA	1.77	0.67
1:B:378:GLN:HG2	1:B:379:GLU:HG2	1.75	0.66
1:C:431:SER:OG	1:C:462:ILE:HG22	1.95	0.66
1:B:391:TYR:H	1:B:391:TYR:HD2	1.44	0.65
1:A:168:TYR:CE1	1:A:183:GLY:HA3	2.31	0.65
1:B:303:VAL:HG22	1:B:312:LEU:HD12	1.79	0.65
1:A:67:ARG:NH2	2:A:700:MLR:O3C	2.30	0.65
1:B:72:ALA:HB2	1:B:105:ILE:HG21	1.79	0.65
1:D:444:VAL:O	1:D:445:LYS:HB2	1.98	0.64
1:B:377:LEU:HD21	1:B:396:LEU:CD2	2.26	0.63
1:D:475:ARG:HH11	1:D:475:ARG:HG2	1.63	0.63
1:A:51:VAL:HB	1:A:56:ASP:OD2	1.98	0.63
1:B:97:ALA:HB2	1:B:330:ILE:HD11	1.81	0.63
1:C:206:ASN:N	1:C:206:ASN:OD1	2.31	0.62
1:A:129:THR:HG22	1:A:250:THR:HG1	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:ASP:OD1	1:C:451:ILE:CG2	2.48	0.62
1:A:410:PHE:HE2	1:A:419:TYR:CD1	2.18	0.62
1:D:182:VAL:O	1:D:366:GLN:NE2	2.32	0.62
1:B:129:THR:HG22	1:B:132:GLU:HG3	1.80	0.62
1:B:355:ARG:HG3	1:B:355:ARG:HH11	1.64	0.61
1:D:403:ILE:HD12	1:D:428:ILE:HD13	1.81	0.61
1:D:332:PRO:O	1:D:337:MET:HG3	2.01	0.61
1:D:413:ARG:HB2	1:D:414:HIS:ND1	2.15	0.61
1:A:410:PHE:HE2	1:A:419:TYR:CE1	2.18	0.61
1:D:69:GLY:HA3	1:D:333:ASN:O	2.01	0.61
1:D:384:LEU:HD23	1:D:425:GLU:HB2	1.82	0.61
1:A:376:LEU:HD13	1:A:376:LEU:O	2.01	0.60
1:B:424:ILE:CG2	1:B:428:ILE:HG13	2.30	0.60
1:D:98:VAL:O	1:D:105:ILE:HG13	2.01	0.60
1:A:450:THR:HG23	1:A:453:SER:H	1.66	0.60
1:C:458:LEU:O	1:C:462:ILE:HG23	2.02	0.59
1:C:137:ASP:OD2	1:C:204:HIS:HA	2.02	0.59
2:C:700:MLR:O5C	2:C:700:MLR:C6C	2.47	0.59
1:C:69:GLY:HA3	1:C:333:ASN:O	2.01	0.59
1:A:49:PRO:HG3	1:A:71:TYR:CE1	2.38	0.59
1:A:334:ILE:HG12	1:A:337:MET:HG2	1.84	0.59
1:C:343:ALA:HB2	1:C:369:ASN:ND2	2.18	0.59
1:D:462:ILE:HG22	1:D:466:LEU:HD11	1.85	0.59
1:C:80:ILE:HG22	1:C:82:PRO:HD3	1.84	0.59
1:A:345:ARG:NH2	2:A:700:MLR:O6C	2.36	0.59
1:A:135:ALA:O	1:A:139:GLU:HG3	2.04	0.58
1:A:169:ALA:O	1:A:170:PHE:CD2	2.57	0.57
1:A:410:PHE:CE2	1:A:419:TYR:CD1	2.92	0.57
1:B:131:GLU:OE1	1:B:131:GLU:N	2.38	0.57
1:A:246:THR:OG1	1:A:247:VAL:N	2.36	0.57
1:B:380:PHE:HD1	1:B:384:LEU:HD12	1.70	0.57
1:A:391:TYR:HB2	1:A:396:LEU:CD1	2.34	0.57
1:D:414:HIS:CD2	1:D:470:HIS:CD2	2.91	0.57
1:D:4:GLU:O	1:D:273:ASN:ND2	2.30	0.57
1:D:414:HIS:NE2	1:D:467:GLU:OE2	2.35	0.56
1:C:182:VAL:HG12	1:C:184:VAL:HG23	1.87	0.56
1:C:34:ILE:HD13	1:C:276:LEU:HD21	1.88	0.56
1:A:350:ASN:HB3	1:A:356:GLN:HG2	1.88	0.56
1:A:410:PHE:CE2	1:A:419:TYR:CE1	2.94	0.56
1:D:442:ARG:HG2	1:D:449:GLU:HG2	1.87	0.56
1:D:381:PRO:HG2	1:D:384:LEU:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TRP:HA	1:A:133:ILE:HD13	1.88	0.56
1:A:192:GLY:HA2	1:A:251:PHE:CE2	2.41	0.56
1:D:407:LYS:HG3	1:D:424:ILE:HD12	1.88	0.55
1:B:336:GLN:NE2	1:B:373:LYS:HG3	2.21	0.55
1:C:444:VAL:O	1:C:445:LYS:HD3	2.06	0.55
1:C:48:PHE:HA	1:C:51:VAL:CG2	2.36	0.55
1:D:123:LEU:HD22	1:D:224:ALA:HB1	1.88	0.55
1:C:457:TYR:O	1:C:461:THR:OG1	2.23	0.55
1:A:272:PRO:HG2	1:A:273:ASN:HD21	1.70	0.55
1:B:170:PHE:CE2	1:B:334:ILE:HD11	2.42	0.55
1:D:428:ILE:HG22	1:D:432:LEU:HD12	1.89	0.55
1:B:130:TRP:HB3	1:B:195:PHE:HE2	1.71	0.55
1:C:90:LEU:HD23	1:C:108:PRO:HG2	1.87	0.55
1:D:134:PRO:HA	1:D:204:HIS:CD2	2.42	0.54
1:A:381:PRO:O	1:A:385:THR:HG23	2.07	0.54
1:A:209:THR:HA	1:A:213:ILE:HD12	1.89	0.54
1:B:391:TYR:N	1:B:391:TYR:CD2	2.73	0.54
1:C:435:LEU:HD21	1:C:451:ILE:HD13	1.88	0.54
1:D:372:ASP:OD1	1:D:372:ASP:N	2.40	0.54
1:D:155:PRO:HG3	1:D:345:ARG:HA	1.89	0.54
1:B:49:PRO:HG3	1:B:71:TYR:CE1	2.42	0.54
1:D:185:ASP:O	1:D:190:LYS:NZ	2.41	0.54
1:D:399:ILE:HD11	1:D:451:ILE:HD11	1.90	0.54
1:B:65:HIS:CE1	1:B:331:MET:HB2	2.43	0.54
1:B:172:TYR:HE1	1:B:175:GLY:HA2	1.73	0.54
1:A:46:GLU:O	1:A:49:PRO:HD2	2.08	0.54
1:D:395:ASP:OD1	1:D:451:ILE:CG2	2.56	0.54
1:B:443:GLY:HA2	1:B:447:GLN:O	2.07	0.53
1:A:373:LYS:O	1:A:377:LEU:HG	2.07	0.53
1:B:218:PHE:HA	1:B:223:THR:HG22	1.89	0.53
1:C:229:GLY:HA3	1:C:231:TRP:CH2	2.44	0.53
1:C:16:LYS:HZ1	1:C:263:LEU:HD22	1.72	0.53
1:B:65:HIS:CD2	1:B:97:ALA:HB1	2.43	0.53
1:D:457:TYR:O	1:D:461:THR:OG1	2.25	0.53
1:B:66:ASP:OD1	1:B:66:ASP:N	2.40	0.53
1:D:260:VAL:HB	1:D:330:ILE:HD13	1.91	0.53
1:C:439:ILE:HD11	1:C:454:MET:HG3	1.91	0.53
1:D:129:THR:OG1	1:D:132:GLU:HG3	2.08	0.52
1:D:178:ASP:OD2	1:D:181:ASP:HB2	2.09	0.52
1:D:230:PRO:HA	1:D:233:TRP:CE2	2.44	0.52
1:C:29:GLU:HG3	1:C:35:LYS:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PRO:HG3	1:B:71:TYR:HE1	1.74	0.52
1:D:378:GLN:O	1:D:379:GLU:HG2	2.09	0.52
1:D:118:TYR:CE1	1:D:126:PRO:HD3	2.45	0.52
1:D:384:LEU:O	1:D:388:LEU:HD12	2.10	0.52
1:B:378:GLN:NE2	1:B:379:GLU:H	2.07	0.52
1:B:414:HIS:NE2	1:B:467:GLU:OE2	2.39	0.52
1:C:128:LYS:HD2	1:C:128:LYS:N	2.24	0.52
1:B:287:THR:HG23	1:B:290:GLY:H	1.73	0.52
1:D:47:LYS:O	1:D:51:VAL:HG22	2.09	0.52
1:A:29:GLU:OE2	1:A:35:LYS:HD3	2.10	0.51
1:A:115:SER:OG	1:A:324:ASN:ND2	2.43	0.51
1:C:406:ALA:HB3	1:C:462:ILE:HD11	1.93	0.51
1:C:234:SER:HB3	1:C:299:PRO:HD3	1.93	0.51
1:C:116:LEU:HB2	1:C:248:LEU:HD23	1.92	0.51
1:B:129:THR:CG2	1:B:132:GLU:HG3	2.39	0.51
1:D:471:ALA:O	1:D:475:ARG:HB2	2.11	0.51
1:D:134:PRO:HA	1:D:204:HIS:HD2	1.75	0.51
2:A:700:MLR:O2C	2:A:700:MLR:O3B	2.28	0.51
2:D:700:MLR:C6C	2:D:700:MLR:O5C	2.51	0.51
1:C:312:LEU:HB3	1:C:318:ILE:HD13	1.93	0.51
1:D:407:LYS:O	1:D:411:ASN:HB2	2.11	0.51
1:D:424:ILE:O	1:D:427:GLU:HG2	2.11	0.51
1:A:155:PRO:CG	1:A:345:ARG:HG3	2.41	0.50
1:C:179:ILE:H	1:C:179:ILE:CD1	2.18	0.50
1:D:32:THR:HG22	1:D:34:ILE:HD12	1.93	0.50
1:A:399:ILE:HG23	1:A:458:LEU:HD21	1.93	0.50
1:A:424:ILE:HG23	1:A:466:LEU:HD21	1.93	0.50
1:A:155:PRO:HG3	1:A:345:ARG:CA	2.41	0.50
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.46	0.50
1:A:129:THR:HB	1:A:131:GLU:HG2	1.94	0.50
1:D:424:ILE:HD13	1:D:466:LEU:HD21	1.94	0.50
1:D:86:PHE:O	1:D:89:LYS:HB2	2.12	0.50
1:B:144:GLY:C	1:B:145:LYS:HZ3	2.11	0.50
1:A:368:HIS:ND1	1:A:369:ASN:N	2.60	0.50
1:A:192:GLY:HA2	1:A:251:PHE:HE2	1.76	0.50
1:B:69:GLY:HA3	1:B:333:ASN:O	2.11	0.50
1:B:399:ILE:O	1:B:403:ILE:HG12	2.12	0.50
1:C:413:ARG:HG2	1:C:414:HIS:ND1	2.25	0.49
1:C:407:LYS:O	1:C:411:ASN:HB2	2.12	0.49
1:A:182:VAL:HG12	1:A:184:VAL:HG23	1.94	0.49
1:A:63:TRP:HB3	1:A:68:PHE:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD22	1:A:150:PHE:HD2	1.78	0.49
1:D:391:TYR:HB2	1:D:396:LEU:HD12	1.94	0.49
1:A:195:PHE:O	1:A:198:ASP:HB2	2.12	0.49
1:A:471:ALA:O	1:A:475:ARG:HG3	2.12	0.49
1:C:218:PHE:HA	1:C:223:THR:HG22	1.95	0.49
1:D:118:TYR:CE2	1:D:126:PRO:HG3	2.48	0.49
1:B:439:ILE:HG23	1:B:449:GLU:HB3	1.94	0.49
1:C:123:LEU:HD11	1:C:224:ALA:HB1	1.95	0.49
1:A:420:MET:CE	1:A:420:MET:CA	2.85	0.49
1:C:48:PHE:HA	1:C:51:VAL:HG23	1.95	0.49
1:C:49:PRO:HG3	1:C:71:TYR:CE1	2.48	0.49
1:A:376:LEU:CD1	1:A:400:LYS:HD2	2.38	0.48
1:D:474:MET:O	1:D:477:LYS:HD3	2.13	0.48
1:D:462:ILE:HG22	1:D:466:LEU:CD1	2.43	0.48
1:A:155:PRO:HD2	2:A:700:MLR:O6B	2.13	0.48
1:D:350:ASN:HB3	1:D:356:GLN:HB2	1.95	0.48
1:C:460:GLN:O	1:C:464:THR:OG1	2.31	0.48
1:C:395:ASP:OD1	1:C:451:ILE:HG21	2.11	0.48
1:A:49:PRO:HG3	1:A:71:TYR:HE1	1.77	0.48
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.48	0.48
1:A:376:LEU:HD11	1:A:400:LYS:CD	2.40	0.48
1:B:355:ARG:NH1	1:B:355:ARG:HG3	2.28	0.48
1:A:149:MET:HB2	1:A:223:THR:HG21	1.96	0.48
1:A:152:LEU:HD12	1:A:207:ALA:HA	1.95	0.48
1:A:129:THR:OG1	1:A:132:GLU:HG2	2.13	0.48
1:C:395:ASP:OD1	1:C:451:ILE:HG22	2.14	0.48
1:A:168:TYR:CE1	1:A:183:GLY:N	2.82	0.48
1:C:233:TRP:HB2	1:C:299:PRO:HG2	1.95	0.48
1:C:255:PRO:HG2	1:C:257:LYS:NZ	2.28	0.48
1:D:384:LEU:HD11	1:D:428:ILE:HG21	1.95	0.48
1:B:382:GLU:HA	1:B:385:THR:HG22	1.96	0.48
2:B:700:MLR:C6C	2:B:700:MLR:O5C	2.50	0.48
1:C:428:ILE:O	1:C:432:LEU:HD12	2.14	0.48
1:A:168:TYR:CE1	1:A:183:GLY:CA	2.96	0.48
1:B:16:LYS:NZ	2:B:700:MLR:O2A	2.39	0.47
1:B:248:LEU:HB3	1:B:256:SER:HB2	1.96	0.47
1:D:190:LYS:HD2	1:D:359:ASP:OD2	2.13	0.47
1:C:439:ILE:CD1	1:C:454:MET:HG3	2.44	0.47
1:D:435:LEU:HD22	1:D:458:LEU:HD22	1.96	0.47
1:D:442:ARG:HG2	1:D:449:GLU:CG	2.44	0.47
1:A:421:LEU:N	1:A:421:LEU:HD12	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:PHE:CE2	1:A:419:TYR:HD1	2.32	0.47
1:D:190:LYS:O	1:D:194:THR:OG1	2.32	0.47
1:B:91:TYR:HE2	1:B:309:GLU:HG2	1.78	0.47
1:B:41:PRO:HG2	1:B:44:LEU:HB3	1.97	0.47
1:A:90:LEU:CD1	1:A:108:PRO:HG2	2.45	0.47
1:A:424:ILE:HG22	1:A:428:ILE:HG13	1.96	0.47
1:A:159:TRP:CH2	1:A:340:PHE:HZ	2.33	0.46
1:B:312:LEU:HB3	1:B:318:ILE:HD13	1.97	0.46
1:A:151:ASN:HB3	1:A:211:TYR:N	2.29	0.46
1:A:83:ASP:N	1:A:83:ASP:OD1	2.48	0.46
1:A:123:LEU:HA	1:A:123:LEU:HD13	1.68	0.46
1:A:19:ASN:HB2	1:A:297:ASP:OD2	2.15	0.46
1:B:391:TYR:HB2	1:B:396:LEU:HD12	1.98	0.46
1:D:475:ARG:NH1	1:D:475:ARG:HG2	2.29	0.46
1:D:414:HIS:ND1	1:D:414:HIS:N	2.63	0.46
1:C:114:LEU:HD21	1:C:157:PHE:CD2	2.51	0.46
1:B:42:ASP:N	1:B:42:ASP:OD2	2.48	0.46
1:A:168:TYR:CD1	1:A:168:TYR:C	2.89	0.46
1:D:170:PHE:CD2	1:D:334:ILE:HD11	2.51	0.46
1:D:91:TYR:CE2	1:D:309:GLU:HG3	2.42	0.46
1:A:456:ALA:O	1:A:460:GLN:HG3	2.15	0.46
1:A:3:ILE:HG13	1:A:57:GLY:O	2.16	0.46
1:C:28:PHE:HD1	1:C:284:TYR:CD2	2.34	0.46
1:C:287:THR:HG23	1:C:290:GLY:H	1.79	0.46
1:A:472:LEU:O	1:A:476:ARG:HB2	2.16	0.46
1:B:155:PRO:HD3	1:B:345:ARG:HG3	1.97	0.45
1:D:458:LEU:O	1:D:462:ILE:HG13	2.16	0.45
1:B:130:TRP:HB3	1:B:195:PHE:CE2	2.50	0.45
1:C:229:GLY:HA3	1:C:231:TRP:CZ3	2.51	0.45
1:C:396:LEU:HA	1:C:396:LEU:HD23	1.80	0.45
1:D:28:PHE:HA	1:D:284:TYR:CE1	2.51	0.45
1:B:315:ASP:HA	1:B:316:PRO:HD2	1.83	0.45
1:B:114:LEU:HA	1:B:114:LEU:HD12	1.76	0.45
1:B:67:ARG:NH2	2:B:700:MLR:O3C	2.36	0.45
1:B:296:LYS:NZ	1:B:296:LYS:CB	2.73	0.45
1:A:200:ILE:HD13	1:A:207:ALA:HB2	1.98	0.45
1:B:116:LEU:HB2	1:B:248:LEU:HD12	1.97	0.45
1:A:90:LEU:HB2	1:A:95:TRP:NE1	2.32	0.45
1:A:457:TYR:O	1:A:461:THR:OG1	2.32	0.45
1:C:107:TYR:CD1	1:C:281:LEU:HD13	2.51	0.45
1:D:154:GLU:OE1	2:D:700:MLR:O6B	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:CG	1:A:172:TYR:O	2.69	0.45
1:C:194:THR:HA	1:C:358:VAL:HG21	1.99	0.45
1:B:252:LYS:HB3	1:B:252:LYS:HE2	1.78	0.45
1:C:382:GLU:HA	1:C:385:THR:OG1	2.16	0.45
1:B:145:LYS:HZ2	1:B:145:LYS:HA	1.82	0.45
1:D:32:THR:CG2	1:D:34:ILE:HD12	2.46	0.45
1:D:194:THR:HA	1:D:358:VAL:HG21	1.98	0.45
1:C:382:GLU:O	1:C:385:THR:OG1	2.29	0.45
1:B:61:ILE:HG13	1:B:62:PHE:N	2.31	0.45
1:C:411:ASN:O	1:C:414:HIS:O	2.34	0.44
1:A:145:LYS:HD2	1:A:221:GLY:O	2.17	0.44
1:D:63:TRP:HB3	1:D:68:PHE:HE1	1.82	0.44
1:B:193:LEU:O	1:B:197:VAL:HG23	2.18	0.44
1:A:162:ILE:HG23	1:A:189:ALA:HB1	1.99	0.44
1:B:91:TYR:CE1	1:B:306:LYS:HG2	2.51	0.44
1:A:384:LEU:O	1:A:388:LEU:HD23	2.17	0.44
1:C:407:LYS:HE3	1:C:420:MET:SD	2.58	0.44
1:A:158:THR:HG21	1:A:196:LEU:HD22	1.99	0.44
1:B:424:ILE:O	1:B:424:ILE:HG22	2.16	0.44
1:C:67:ARG:NH2	2:C:700:MLR:O3C	2.34	0.44
1:C:43:LYS:HB3	1:C:46:GLU:HG3	1.99	0.44
1:B:273:ASN:HB3	1:B:276:LEU:HB2	2.00	0.44
1:A:69:GLY:HA3	1:A:333:ASN:O	2.17	0.44
1:A:131:GLU:H	1:A:131:GLU:HG2	1.42	0.44
1:A:168:TYR:CD1	1:A:168:TYR:O	2.70	0.44
1:D:395:ASP:OD1	1:D:451:ILE:HG22	2.17	0.44
1:D:429:LEU:O	1:D:433:LYS:HG3	2.18	0.44
1:A:84:LYS:NZ	1:A:88:ASP:OD2	2.51	0.44
1:A:169:ALA:O	1:A:170:PHE:CG	2.71	0.44
1:C:449:GLU:HA	1:C:449:GLU:OE2	2.18	0.44
1:D:384:LEU:HD12	1:D:388:LEU:HD11	1.99	0.43
1:D:384:LEU:HD11	1:D:428:ILE:CG2	2.48	0.43
1:B:172:TYR:CE1	1:B:175:GLY:HA2	2.53	0.43
1:D:129:THR:HG22	1:D:250:THR:OG1	2.18	0.43
1:D:450:THR:O	1:D:453:SER:N	2.50	0.43
1:D:150:PHE:HZ	1:D:196:LEU:HD11	1.83	0.43
1:B:12:ILE:HA	1:B:62:PHE:HB2	1.99	0.43
1:A:383:GLN:HB3	1:A:425:GLU:OE2	2.18	0.43
1:A:154:GLU:HA	1:A:155:PRO:HD3	1.85	0.43
1:D:383:GLN:NE2	1:D:425:GLU:OE1	2.51	0.43
1:B:312:LEU:HB3	1:B:318:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASP:H	1:A:213:ILE:HD12	1.82	0.43
1:B:414:HIS:HD2	1:B:470:HIS:CD2	2.35	0.43
1:D:151:ASN:HB3	1:D:157:PHE:CD1	2.53	0.43
1:D:427:GLU:N	1:D:427:GLU:OE2	2.52	0.43
1:A:169:ALA:C	1:A:170:PHE:CD2	2.92	0.43
1:D:41:PRO:HB2	1:D:47:LYS:NZ	2.34	0.43
1:B:122:LEU:HD23	1:B:224:ALA:HB2	1.99	0.43
1:C:29:GLU:CG	1:C:35:LYS:HA	2.48	0.43
1:D:41:PRO:HG2	1:D:44:LEU:HB3	2.00	0.43
1:B:114:LEU:HG	1:B:227:ILE:HG22	2.00	0.43
1:B:112:GLU:HG2	1:B:261:GLY:O	2.18	0.43
1:C:377:LEU:HD23	1:C:377:LEU:C	2.39	0.43
1:D:229:GLY:HA3	1:D:231:TRP:CH2	2.53	0.43
1:A:372:ASP:HB3	1:A:375:MET:HB3	2.01	0.43
1:A:10:ILE:HB	1:A:38:VAL:HG22	2.00	0.43
1:C:49:PRO:HG3	1:C:71:TYR:HE1	1.82	0.43
1:A:421:LEU:H	1:A:421:LEU:CD1	2.20	0.43
1:A:43:LYS:HD3	1:A:46:GLU:OE2	2.18	0.43
1:D:157:PHE:O	1:D:160:PRO:HD2	2.19	0.42
1:A:185:ASP:CB	1:A:366:GLN:OE1	2.67	0.42
1:A:84:LYS:HA	1:A:84:LYS:HD2	1.81	0.42
1:D:107:TYR:OH	1:D:278:LYS:HD3	2.19	0.42
1:B:202:ASN:O	1:B:203:LYS:HB2	2.19	0.42
1:C:255:PRO:HG2	1:C:257:LYS:HZ2	1.83	0.42
1:B:128:LYS:HE2	1:B:128:LYS:HB3	1.88	0.42
1:A:427:GLU:HG3	1:A:466:LEU:HD23	2.00	0.42
1:C:438:ALA:O	1:C:442:ARG:HB2	2.19	0.42
1:B:392:ASP:OD1	1:B:392:ASP:N	2.52	0.42
1:D:83:ASP:N	1:D:83:ASP:OD1	2.52	0.42
1:B:134:PRO:HB3	1:B:204:HIS:NE2	2.35	0.42
1:D:62:PHE:HE1	1:D:109:ILE:HG13	1.83	0.42
1:B:259:PHE:HA	1:B:259:PHE:HD1	1.71	0.42
1:A:315:ASP:HB3	1:A:318:ILE:HG12	2.01	0.42
1:D:155:PRO:HG3	1:D:345:ARG:CA	2.49	0.42
1:A:410:PHE:CE2	1:A:419:TYR:HE1	2.38	0.42
1:A:420:MET:HE3	1:A:420:MET:HA	1.98	0.42
1:C:141:LYS:HE2	1:C:141:LYS:HB2	1.79	0.42
1:B:155:PRO:HD2	2:B:700:MLR:O6B	2.20	0.42
1:D:424:ILE:HG21	1:D:424:ILE:HD13	1.79	0.42
1:D:395:ASP:OD1	1:D:451:ILE:HG21	2.19	0.42
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:HIS:CE1	1:A:331:MET:HB2	2.55	0.42
1:C:250:THR:HG22	1:C:255:PRO:HA	2.02	0.42
1:D:298:LYS:HA	1:D:299:PRO:HD3	1.89	0.42
1:D:431:SER:HA	1:D:434:ARG:HG3	2.01	0.42
1:D:43:LYS:HE3	1:D:43:LYS:HB2	1.89	0.41
1:C:12:ILE:HA	1:C:62:PHE:HB2	2.02	0.41
1:B:117:ILE:HG22	1:B:218:PHE:CZ	2.54	0.41
1:C:377:LEU:HD21	1:C:385:THR:CG2	2.50	0.41
1:A:159:TRP:NE1	1:A:163:ALA:HB2	2.35	0.41
1:A:196:LEU:O	1:A:196:LEU:HG	2.20	0.41
1:D:87:GLN:HG3	1:D:95:TRP:CE2	2.55	0.41
1:B:463:LEU:HD23	1:B:463:LEU:HA	1.90	0.41
1:D:154:GLU:HA	1:D:155:PRO:HD3	1.96	0.41
1:C:66:ASP:HA	1:C:333:ASN:HA	2.02	0.41
1:D:11:TRP:HB3	1:D:44:LEU:HD13	2.03	0.41
1:A:123:LEU:HD13	1:A:124:PRO:HD2	2.02	0.41
1:C:91:TYR:HA	1:C:92:PRO:HD3	1.89	0.41
1:C:407:LYS:HE3	1:C:420:MET:HA	2.02	0.41
1:B:380:PHE:HD1	1:B:384:LEU:CD1	2.34	0.41
1:C:424:ILE:O	1:C:428:ILE:HG13	2.21	0.41
1:C:76:LEU:HD13	1:C:76:LEU:N	2.36	0.41
1:A:308:TYR:CE2	1:A:312:LEU:HD11	2.56	0.41
1:C:393:TYR:CE2	1:C:394:ARG:NH1	2.89	0.41
1:D:373:LYS:HG3	1:D:393:TYR:HD1	1.85	0.41
1:D:170:PHE:HE1	1:D:182:VAL:HG22	1.85	0.41
1:D:107:TYR:HA	1:D:108:PRO:HD3	1.87	0.41
1:D:424:ILE:HG22	1:D:428:ILE:HG13	2.03	0.41
1:A:404:LEU:HA	1:A:404:LEU:HD12	1.88	0.41
1:D:216:ALA:HB1	1:D:220:LYS:NZ	2.36	0.41
1:A:168:TYR:CD1	1:A:183:GLY:HA3	2.55	0.41
1:B:194:THR:HA	1:B:358:VAL:HG21	2.02	0.41
1:A:405:LYS:HE3	1:A:459:MET:HE2	2.03	0.41
1:D:48:PHE:HB3	1:D:49:PRO:HD3	2.03	0.41
1:C:179:ILE:CG2	1:C:336:GLN:HG2	2.50	0.40
1:A:368:HIS:C	1:A:368:HIS:ND1	2.74	0.40
1:A:184:VAL:HG12	1:A:362:LEU:HD22	2.02	0.40
1:C:382:GLU:H	1:C:382:GLU:HG2	1.45	0.40
1:D:90:LEU:HB2	1:D:95:TRP:NE1	2.36	0.40
1:D:68:PHE:HB3	1:D:105:ILE:HD13	2.03	0.40
1:B:168:TYR:CE2	1:B:183:GLY:HA3	2.56	0.40
1:C:52:ALA:HA	1:C:56:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:TRP:HB3	1:A:44:LEU:HD13	2.03	0.40
1:B:271:SER:HA	1:B:272:PRO:HD3	1.83	0.40
1:A:61:ILE:HG13	1:A:62:PHE:N	2.35	0.40
1:D:377:LEU:O	1:D:380:PHE:HB2	2.22	0.40
1:C:47:LYS:HB2	1:C:47:LYS:HE3	1.82	0.40
1:D:170:PHE:CE1	1:D:182:VAL:HG22	2.57	0.40
1:B:233:TRP:HB2	1:B:299:PRO:HG2	2.04	0.40
1:A:167:GLY:HA3	1:A:189:ALA:HB2	2.04	0.40
1:C:193:LEU:O	1:C:197:VAL:HG23	2.21	0.40
1:C:109:ILE:HD13	1:C:109:ILE:HA	1.84	0.40
1:D:376:LEU:HD23	1:D:396:LEU:HD23	2.03	0.40
1:C:235:ASN:OD1	1:C:298:LYS:HE3	2.21	0.40
1:A:232:ALA:O	1:A:236:ILE:HG13	2.21	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	476/487 (98%)	463 (97%)	13 (3%)	0	100	100
1	B	477/487 (98%)	472 (99%)	5 (1%)	0	100	100
1	C	474/487 (97%)	469 (99%)	5 (1%)	0	100	100
1	D	468/487 (96%)	464 (99%)	4 (1%)	0	100	100
All	All	1895/1948 (97%)	1868 (99%)	27 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	375/407 (92%)	326 (87%)	49 (13%)	5	25
1	B	380/407 (93%)	337 (89%)	43 (11%)	7	32
1	C	363/407 (89%)	308 (85%)	55 (15%)	3	19
1	D	375/407 (92%)	315 (84%)	60 (16%)	3	16
All	All	1493/1628 (92%)	1286 (86%)	207 (14%)	4	23

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	30	LYS
1	A	44	LEU
1	A	61	ILE
1	A	88	ASP
1	A	114	LEU
1	A	115	SER
1	A	131	GLU
1	A	136	LEU
1	A	148	LEU
1	A	158	THR
1	A	171	LYS
1	A	179	ILE
1	A	199	LEU
1	A	208	ASP
1	A	212	SER
1	A	223	THR
1	A	228	ASN
1	A	234	SER
1	A	259	PHE
1	A	273	ASN
1	A	323	GLU
1	A	330	ILE
1	A	346	THR

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Mol	Chain	Res	Type
1	A	360	GLU
1	A	368	HIS
1	A	369	ASN
1	A	373	LYS
1	A	375	MET
1	A	376	LEU
1	A	386	ASN
1	A	392	ASP
1	A	396	LEU
1	A	404	LEU
1	A	413	ARG
1	A	417	MET
1	A	418	HIS
1	A	420	MET
1	A	422	GLU
1	A	427	GLU
1	A	429	LEU
1	A	431	SER
1	A	436	LYS
1	A	442	ARG
1	A	454	MET
1	A	465	GLU
1	A	472	LEU
1	A	474	MET
1	A	476	ARG
1	B	37	THR
1	B	42	ASP
1	B	59	ASP
1	B	61	ILE
1	B	76	LEU
1	B	81	THR
1	B	101	ASN
1	B	105	ILE
1	B	114	LEU
1	B	143	LYS
1	B	173	GLU
1	B	182	VAL
1	B	186	ASN
1	B	205	MET
1	B	234	SER
1	B	248	LEU
1	B	259	PHE

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Mol	Chain	Res	Type
1	B	279	GLU
1	B	289	GLU
1	B	296	LYS
1	B	310	GLU
1	B	368	HIS
1	B	370	PHE
1	B	374	GLU
1	B	375	MET
1	B	376	LEU
1	B	384	LEU
1	B	391	TYR
1	B	392	ASP
1	B	394	ARG
1	B	396	LEU
1	B	413	ARG
1	B	416	ASP
1	B	417	MET
1	B	418	HIS
1	B	421	LEU
1	B	426	ASP
1	B	430	THR
1	B	436	LYS
1	B	444	VAL
1	B	460	GLN
1	B	468	GLU
1	B	474	MET
1	C	3	ILE
1	C	4	GLU
1	C	16	LYS
1	C	29	GLU
1	C	42	ASP
1	C	44	LEU
1	C	46	GLU
1	C	51	VAL
1	C	61	ILE
1	C	76	LEU
1	C	104	LEU
1	C	114	LEU
1	C	123	LEU
1	C	128	LYS
1	C	129	THR
1	C	136	LEU

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Mol	Chain	Res	Type
1	C	141	LYS
1	C	146	SER
1	C	149	MET
1	C	153	GLN
1	C	176	LYS
1	C	179	ILE
1	C	199	LEU
1	C	201	LYS
1	C	206	ASN
1	C	252	LYS
1	C	259	PHE
1	C	309	GLU
1	C	312	LEU
1	C	323	GLU
1	C	330	ILE
1	C	366	GLN
1	C	368	HIS
1	C	369	ASN
1	C	374	GLU
1	C	376	LEU
1	C	382	GLU
1	C	383	GLN
1	C	385	THR
1	C	387	TYR
1	C	404	LEU
1	C	415	GLU
1	C	417	MET
1	C	426	ASP
1	C	432	LEU
1	C	442	ARG
1	C	445	LYS
1	C	458	LEU
1	C	459	MET
1	C	461	THR
1	C	462	ILE
1	C	464	THR
1	C	468	GLU
1	C	472	LEU
1	C	474	MET
1	D	8	LEU
1	D	15	ASP
1	D	30	LYS

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Mol	Chain	Res	Type
1	D	38	VAL
1	D	93	PHE
1	D	122	LEU
1	D	123	LEU
1	D	136	LEU
1	D	145	LYS
1	D	146	SER
1	D	171	LYS
1	D	176	LYS
1	D	194	THR
1	D	204	HIS
1	D	208	ASP
1	D	234	SER
1	D	252	LYS
1	D	259	PHE
1	D	296	LYS
1	D	309	GLU
1	D	323	GLU
1	D	329	GLU
1	D	355	ARG
1	D	356	GLN
1	D	357	THR
1	D	366	GLN
1	D	368	HIS
1	D	372	ASP
1	D	376	LEU
1	D	380	PHE
1	D	388	LEU
1	D	390	LYS
1	D	396	LEU
1	D	399	ILE
1	D	405	LYS
1	D	411	ASN
1	D	412	SER
1	D	413	ARG
1	D	414	HIS
1	D	416	ASP
1	D	420	MET
1	D	421	LEU
1	D	427	GLU
1	D	432	LEU
1	D	434	ARG

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Mol	Chain	Res	Type
1	D	436	LYS
1	D	437	LYS
1	D	442	ARG
1	D	450	THR
1	D	451	ILE
1	D	453	SER
1	D	458	LEU
1	D	460	GLN
1	D	461	THR
1	D	464	THR
1	D	468	GLU
1	D	472	LEU
1	D	474	MET
1	D	475	ARG
1	D	477	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	ASN
1	B	336	GLN
1	B	378	GLN
1	C	369	ASN
1	D	470	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	MLR	A	700	-	36,36,36	3.30	11 (30%)	53,53,53	2.50	16 (30%)
2	MLR	B	700	-	36,36,36	3.20	10 (27%)	53,53,53	1.90	8 (15%)
2	MLR	C	700	-	36,36,36	3.14	12 (33%)	53,53,53	2.18	13 (24%)
2	MLR	D	700	-	36,36,36	3.21	11 (30%)	53,53,53	1.68	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLR	A	700	-	-	0/14/74/74	0/3/3/3
2	MLR	B	700	-	-	0/14/74/74	0/3/3/3
2	MLR	C	700	-	-	0/14/74/74	0/3/3/3
2	MLR	D	700	-	-	0/14/74/74	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	MLR	C4C-C3C	-4.92	1.39	1.52
2	C	700	MLR	C4C-C3C	-4.26	1.41	1.52
2	D	700	MLR	C4C-C3C	-3.98	1.41	1.52
2	B	700	MLR	C4C-C3C	-3.97	1.42	1.52
2	A	700	MLR	C3C-C2C	-3.96	1.42	1.52
2	B	700	MLR	O4B-C1C	-3.83	1.31	1.41
2	B	700	MLR	C3C-C2C	-3.78	1.42	1.52
2	C	700	MLR	C3C-C2C	-3.69	1.42	1.52
2	C	700	MLR	O4B-C1C	-3.65	1.31	1.41
2	D	700	MLR	O4B-C1C	-3.40	1.32	1.41
2	D	700	MLR	C3C-C2C	-3.39	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	MLR	O4B-C1C	-3.00	1.33	1.41
2	C	700	MLR	C6C-C5C	-2.52	1.43	1.51
2	B	700	MLR	C6C-C5C	-2.45	1.43	1.51
2	A	700	MLR	C6C-C5C	-2.34	1.43	1.51
2	D	700	MLR	C6C-C5C	-2.33	1.43	1.51
2	A	700	MLR	O4B-C4B	2.09	1.49	1.43
2	C	700	MLR	O3A-C3A	2.11	1.48	1.43
2	C	700	MLR	O2A-C2A	2.15	1.48	1.43
2	B	700	MLR	O4C-C4C	2.47	1.48	1.43
2	C	700	MLR	O5A-C1A	2.54	1.47	1.43
2	B	700	MLR	O2C-C2C	2.59	1.49	1.43
2	D	700	MLR	O4C-C4C	2.68	1.49	1.43
2	C	700	MLR	O2C-C2C	2.78	1.49	1.43
2	D	700	MLR	O2C-C2C	2.85	1.49	1.43
2	D	700	MLR	O5A-C1A	2.85	1.48	1.43
2	A	700	MLR	O2C-C2C	2.92	1.50	1.43
2	B	700	MLR	O5B-C1B	3.03	1.49	1.41
2	D	700	MLR	O5B-C1B	3.08	1.49	1.41
2	C	700	MLR	O5B-C1B	3.09	1.49	1.41
2	A	700	MLR	O5B-C1B	3.10	1.49	1.41
2	A	700	MLR	O5A-C1A	3.44	1.49	1.43
2	C	700	MLR	O5C-C5C	7.64	1.63	1.44
2	A	700	MLR	O5C-C5C	7.84	1.64	1.44
2	C	700	MLR	O3C-C3C	7.85	1.61	1.43
2	B	700	MLR	O3C-C3C	8.04	1.62	1.43
2	B	700	MLR	O5C-C5C	8.04	1.64	1.44
2	A	700	MLR	O3C-C3C	8.05	1.62	1.43
2	D	700	MLR	O5C-C5C	8.14	1.64	1.44
2	D	700	MLR	O3C-C3C	8.15	1.62	1.43
2	D	700	MLR	O5C-C1C	11.58	1.71	1.41
2	C	700	MLR	O5C-C1C	11.59	1.71	1.41
2	B	700	MLR	O5C-C1C	11.76	1.72	1.41
2	A	700	MLR	O5C-C1C	12.30	1.73	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	MLR	C1C-O5C-C5C	-8.80	96.66	113.75
2	C	700	MLR	C1C-O5C-C5C	-7.64	98.92	113.75
2	B	700	MLR	C1C-O5C-C5C	-7.49	99.20	113.75
2	D	700	MLR	C1C-O5C-C5C	-6.10	101.90	113.75
2	C	700	MLR	O3C-C3C-C2C	-4.50	100.21	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	MLR	O3C-C3C-C2C	-3.92	101.50	110.34
2	B	700	MLR	O3C-C3C-C2C	-3.39	102.70	110.34
2	A	700	MLR	C6C-C5C-C4C	-3.24	105.03	113.02
2	A	700	MLR	O3B-C3B-C2B	-3.09	103.38	110.34
2	A	700	MLR	O3C-C3C-C4C	-2.96	103.67	110.34
2	C	700	MLR	C1A-O5A-C5A	-2.71	108.46	113.47
2	B	700	MLR	C1A-O5A-C5A	-2.60	108.66	113.47
2	D	700	MLR	O3C-C3C-C2C	-2.53	104.65	110.34
2	C	700	MLR	O4B-C4B-C5B	-2.51	102.73	109.32
2	B	700	MLR	O1X-C1A-O5A	-2.43	103.59	110.25
2	B	700	MLR	C1C-O4B-C4B	-2.35	111.87	118.01
2	A	700	MLR	O3A-C3A-C2A	-2.27	105.22	110.34
2	D	700	MLR	C6C-C5C-C4C	-2.05	107.95	113.02
2	A	700	MLR	C1C-C2C-C3C	2.00	113.92	109.97
2	A	700	MLR	O5B-C5B-C4B	2.02	114.01	109.75
2	C	700	MLR	C1B-C2B-C3B	2.03	113.98	109.97
2	A	700	MLR	C1A-O5A-C5A	2.09	117.33	113.47
2	C	700	MLR	O5A-C1A-C2A	2.09	113.12	109.80
2	C	700	MLR	C2B-C3B-C4B	2.11	114.22	109.60
2	C	700	MLR	O5A-C5A-C4A	2.17	114.34	109.75
2	C	700	MLR	O5C-C5C-C4C	2.19	113.80	109.68
2	A	700	MLR	O2C-C2C-C1C	2.21	114.87	110.02
2	B	700	MLR	O5B-C5B-C4B	2.29	114.58	109.75
2	D	700	MLR	O5A-C5A-C4A	2.40	114.81	109.75
2	A	700	MLR	O5A-C1A-C2A	2.51	113.81	109.80
2	A	700	MLR	O5A-C5A-C4A	2.59	115.23	109.75
2	A	700	MLR	C2B-C3B-C4B	2.60	115.31	109.60
2	D	700	MLR	C2A-C3A-C4A	2.65	115.42	109.60
2	D	700	MLR	O5B-C5B-C4B	2.90	115.87	109.75
2	A	700	MLR	C1A-C2A-C3A	3.27	115.29	110.43
2	C	700	MLR	C2A-C3A-C4A	3.36	116.98	109.60
2	D	700	MLR	O5C-C5C-C4C	3.58	116.41	109.68
2	C	700	MLR	O5B-C5B-C4B	3.67	117.50	109.75
2	B	700	MLR	O5C-C5C-C4C	3.81	116.83	109.68
2	C	700	MLR	C1A-C2A-C3A	3.88	116.20	110.43
2	A	700	MLR	O5C-C5C-C6C	4.74	118.34	106.36
2	D	700	MLR	C4C-C3C-C2C	6.18	122.32	110.79
2	B	700	MLR	C4C-C3C-C2C	6.79	123.46	110.79
2	C	700	MLR	C4C-C3C-C2C	8.06	125.83	110.79
2	A	700	MLR	C4C-C3C-C2C	9.52	128.55	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	MLR	7	0
2	B	700	MLR	7	0
2	C	700	MLR	5	0
2	D	700	MLR	6	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	478/487 (98%)	0.35	42 (8%) 12 12	31, 61, 95, 121	0
1	B	479/487 (98%)	0.37	35 (7%) 18 17	39, 66, 99, 135	0
1	C	476/487 (97%)	0.29	35 (7%) 17 17	41, 68, 105, 140	0
1	D	472/487 (96%)	0.34	39 (8%) 14 13	45, 73, 100, 138	0
All	All	1905/1948 (97%)	0.34	151 (7%) 15 14	31, 67, 101, 140	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	375	MET	6.1
1	C	380	PHE	6.1
1	C	372	ASP	6.0
1	C	173	GLU	6.0
1	B	386	ASN	5.9
1	C	382	GLU	5.6
1	B	143	LYS	5.5
1	B	417	MET	5.4
1	B	416	ASP	5.1
1	D	313	ALA	4.9
1	A	321	THR	4.9
1	D	125	ASN	4.9
1	C	404	LEU	4.8
1	B	449	GLU	4.8
1	B	59	ASP	4.5
1	C	4	GLU	4.3
1	A	167	GLY	4.2
1	D	256	SER	4.2
1	A	384	LEU	4.1
1	C	59	ASP	4.1
1	B	380	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	322	MET	3.9
1	C	379	GLU	3.9
1	A	146	SER	3.9
1	D	320	ALA	3.9
1	C	174	ASN	3.9
1	A	399	ILE	3.8
1	D	466	LEU	3.7
1	C	384	LEU	3.7
1	A	391	TYR	3.7
1	C	161	LEU	3.7
1	A	147	ALA	3.7
1	A	388	LEU	3.6
1	D	321	THR	3.6
1	C	60	ILE	3.6
1	A	145	LYS	3.5
1	A	224	ALA	3.5
1	A	415	GLU	3.5
1	C	136	LEU	3.5
1	C	137	ASP	3.4
1	C	147	ALA	3.2
1	B	8	LEU	3.2
1	A	383	GLN	3.2
1	A	370	PHE	3.2
1	C	165	ASP	3.2
1	B	480	LYS	3.1
1	B	18	TYR	3.0
1	D	370	PHE	3.0
1	D	393	TYR	3.0
1	D	425	GLU	3.0
1	A	398	ILE	3.0
1	A	182	VAL	3.0
1	A	166	GLY	3.0
1	A	179	ILE	2.9
1	A	394	ARG	2.9
1	B	371	ASP	2.9
1	C	416	ASP	2.9
1	D	123	LEU	2.9
1	C	135	ALA	2.9
1	B	116	LEU	2.9
1	D	389	LEU	2.9
1	C	403	ILE	2.8
1	B	139	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	169	ALA	2.8
1	C	266	GLY	2.8
1	D	323	GLU	2.8
1	D	399	ILE	2.8
1	A	403	ILE	2.8
1	D	281	LEU	2.8
1	D	300	LEU	2.7
1	C	301	GLY	2.7
1	A	162	ILE	2.7
1	D	340	PHE	2.7
1	A	373	LYS	2.6
1	B	376	LEU	2.6
1	A	264	SER	2.6
1	D	107	TYR	2.5
1	B	138	LYS	2.5
1	C	164	ALA	2.5
1	A	221	GLY	2.5
1	A	400	LYS	2.5
1	D	386	ASN	2.5
1	D	435	LEU	2.5
1	B	6	GLY	2.5
1	D	148	LEU	2.5
1	D	339	ALA	2.5
1	D	109	ILE	2.5
1	D	372	ASP	2.5
1	A	393	TYR	2.5
1	C	205	MET	2.5
1	A	275	GLU	2.4
1	B	424	ILE	2.4
1	C	196	LEU	2.4
1	D	286	LEU	2.4
1	A	244	GLY	2.4
1	B	36	VAL	2.4
1	D	463	LEU	2.4
1	C	130	TRP	2.4
1	A	365	ALA	2.4
1	A	416	ASP	2.4
1	A	120	LYS	2.4
1	B	268	ASN	2.4
1	B	210	ASP	2.4
1	C	409	SER	2.4
1	B	324	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	323	GLU	2.4
1	B	148	LEU	2.4
1	C	150	PHE	2.4
1	D	257	LYS	2.4
1	C	381	PRO	2.3
1	D	267	ILE	2.3
1	D	365	ALA	2.3
1	A	150	PHE	2.3
1	A	136	LEU	2.3
1	D	113	ALA	2.3
1	B	28	PHE	2.3
1	A	164	ALA	2.3
1	D	170	PHE	2.3
1	D	246	THR	2.3
1	D	403	ILE	2.3
1	A	222	GLU	2.2
1	A	323	GLU	2.2
1	B	365	ALA	2.2
1	B	418	HIS	2.2
1	B	375	MET	2.1
1	B	421	LEU	2.1
1	B	347	ALA	2.1
1	D	390	LYS	2.1
1	A	376	LEU	2.1
1	C	187	ALA	2.1
1	C	133	ILE	2.1
1	B	112	GLU	2.1
1	C	61	ILE	2.1
1	C	184	VAL	2.1
1	B	349	ILE	2.1
1	C	171	LYS	2.1
1	B	271	SER	2.1
1	A	152	LEU	2.1
1	B	193	LEU	2.1
1	B	164	ALA	2.1
1	D	459	MET	2.1
1	D	158	THR	2.1
1	A	396	LEU	2.0
1	B	419	TYR	2.0
1	A	27	LYS	2.0
1	A	286	LEU	2.0
1	C	300	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	152	LEU	2.0
1	A	223	THR	2.0
1	D	247	VAL	2.0
1	D	21	LEU	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
2	MLR	D	700	34/34	0.83	0.28	0.25	45,60,73,74	0
2	MLR	B	700	34/34	0.89	0.24	0.14	33,53,65,76	0
2	MLR	A	700	34/34	0.87	0.24	-0.05	30,42,62,76	0
2	MLR	C	700	34/34	0.95	0.20	-0.43	53,65,78,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.