Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:59 AM GMT

PDB ID	:	3QNQ
Title	:	Crystal structure of the transporter ChbC, the IIC component from the N,N'-diacetylchitobiose-specific phosphotransferase system
Authors	:	Cao, Y.; Jin, X.; Huang, H.; Levin, E.J.; Zhou, M.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on	:	2011-02-08
Resolution	:	3.29 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

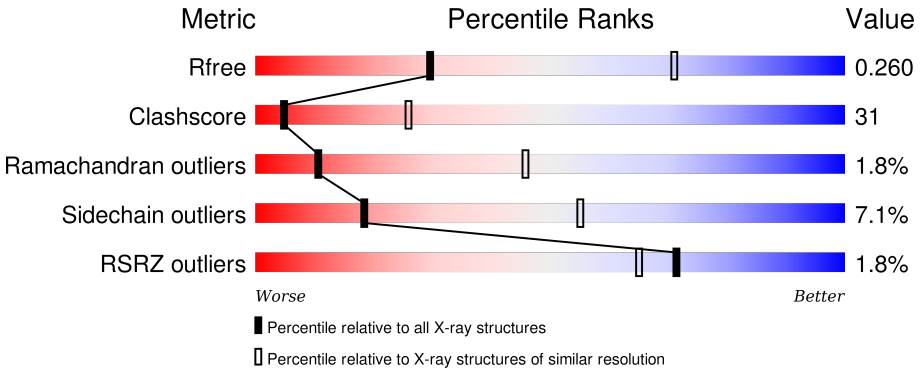
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 >=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 <=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	442	2% 50% 43% 5%
1	B	442	2% 50% 43% 5%
1	C	442	% 50% 43%
1	D	442	2% 44% 48% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13566 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 PTS system, cellobiose-specific IIC component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3272	2191	508	555	18			
1	B	432	Total	C	N	O	S	0	0	0
			3288	2201	516	553	18			
1	C	432	Total	C	N	O	S	0	0	0
			3280	2195	513	554	18			
1	D	436	Total	C	N	O	S	0	0	0
			3307	2211	520	558	18			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	ALA	-	EXPRESSION TAG	UNP Q72XQ0
A	435	ALA	-	EXPRESSION TAG	UNP Q72XQ0
A	436	ALA	-	EXPRESSION TAG	UNP Q72XQ0
A	437	GLU	-	EXPRESSION TAG	UNP Q72XQ0
A	438	ASN	-	EXPRESSION TAG	UNP Q72XQ0
A	439	LEU	-	EXPRESSION TAG	UNP Q72XQ0
A	440	TYR	-	EXPRESSION TAG	UNP Q72XQ0
A	441	PHE	-	EXPRESSION TAG	UNP Q72XQ0
A	442	GLN	-	EXPRESSION TAG	UNP Q72XQ0
B	434	ALA	-	EXPRESSION TAG	UNP Q72XQ0
B	435	ALA	-	EXPRESSION TAG	UNP Q72XQ0
B	436	ALA	-	EXPRESSION TAG	UNP Q72XQ0
B	437	GLU	-	EXPRESSION TAG	UNP Q72XQ0
B	438	ASN	-	EXPRESSION TAG	UNP Q72XQ0
B	439	LEU	-	EXPRESSION TAG	UNP Q72XQ0
B	440	TYR	-	EXPRESSION TAG	UNP Q72XQ0
B	441	PHE	-	EXPRESSION TAG	UNP Q72XQ0
B	442	GLN	-	EXPRESSION TAG	UNP Q72XQ0
C	434	ALA	-	EXPRESSION TAG	UNP Q72XQ0
C	435	ALA	-	EXPRESSION TAG	UNP Q72XQ0
C	436	ALA	-	EXPRESSION TAG	UNP Q72XQ0

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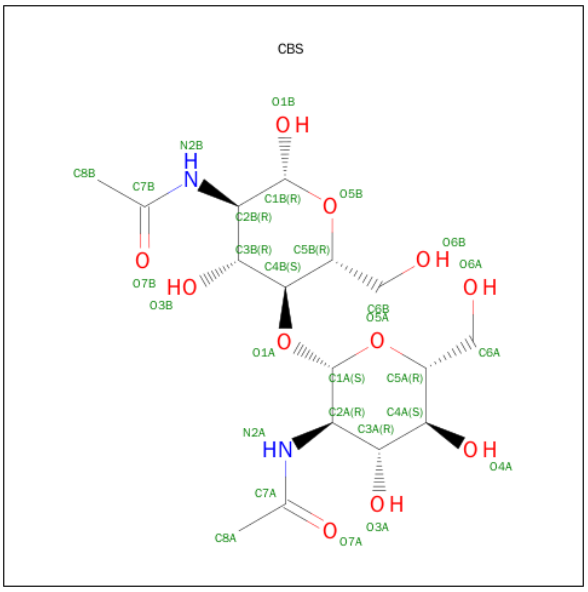
Chain	Residue	Modelled	Actual	Comment	Reference
C	437	GLU	-	EXPRESSION TAG	UNP Q72XQ0
C	438	ASN	-	EXPRESSION TAG	UNP Q72XQ0
C	439	LEU	-	EXPRESSION TAG	UNP Q72XQ0
C	440	TYR	-	EXPRESSION TAG	UNP Q72XQ0
C	441	PHE	-	EXPRESSION TAG	UNP Q72XQ0
C	442	GLN	-	EXPRESSION TAG	UNP Q72XQ0
D	434	ALA	-	EXPRESSION TAG	UNP Q72XQ0
D	435	ALA	-	EXPRESSION TAG	UNP Q72XQ0
D	436	ALA	-	EXPRESSION TAG	UNP Q72XQ0
D	437	GLU	-	EXPRESSION TAG	UNP Q72XQ0
D	438	ASN	-	EXPRESSION TAG	UNP Q72XQ0
D	439	LEU	-	EXPRESSION TAG	UNP Q72XQ0
D	440	TYR	-	EXPRESSION TAG	UNP Q72XQ0
D	441	PHE	-	EXPRESSION TAG	UNP Q72XQ0
D	442	GLN	-	EXPRESSION TAG	UNP Q72XQ0

- Molecule 2 is SUGAR (DI(N-ACETYL-D-GLUCOSAMINE)) (three-letter code: CBS) (formula: $C_{16}H_{28}N_2O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	16	2	11		
2	B	1	Total	C	N	O	0	0
			29	16	2	11		
2	C	1	Total	C	N	O	0	0
			29	16	2	11		

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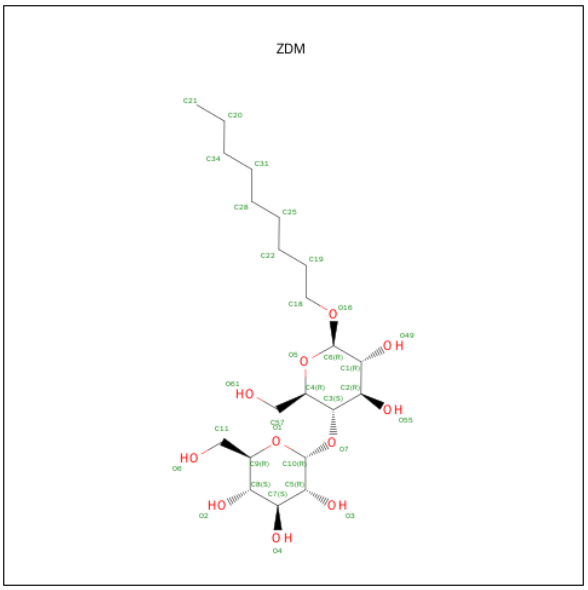
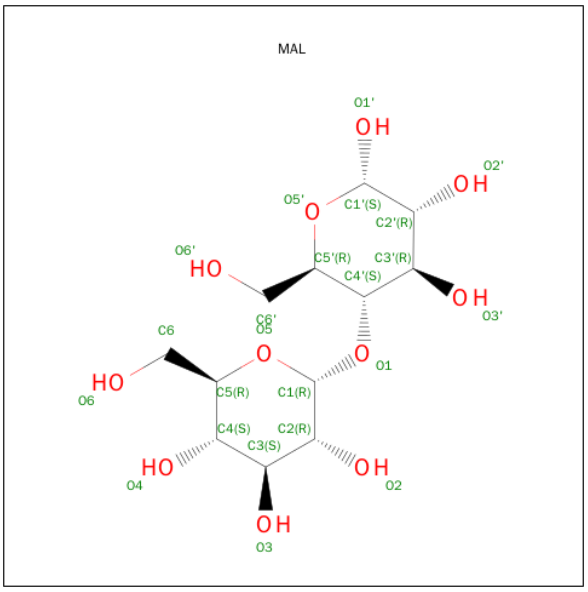
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			29	16	2	11		

- Molecule 3 is SUGAR (DECYL 4-O-ALPHA-D-GLUCOPYRANOSYL-BETA-D-GLUCOPYRANOSIDE) (three-letter code: ZDM) (formula: $C_{21}H_{40}O_{11}$).



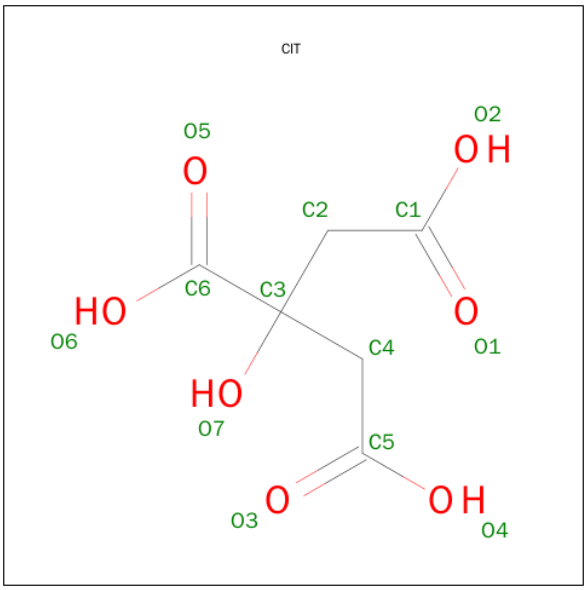
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			30	19	11		
3	A	1	Total	C	O	0	0
			30	19	11		
3	C	1	Total	C	O	0	0
			30	19	11		
3	C	1	Total	C	O	0	0
			30	19	11		

- Molecule 4 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 23 12 11	0	0
4	B	1	Total C O 23 12 11	0	0
4	C	1	Total C O 23 12 11	0	0
4	D	1	Total C O 23 12 11	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



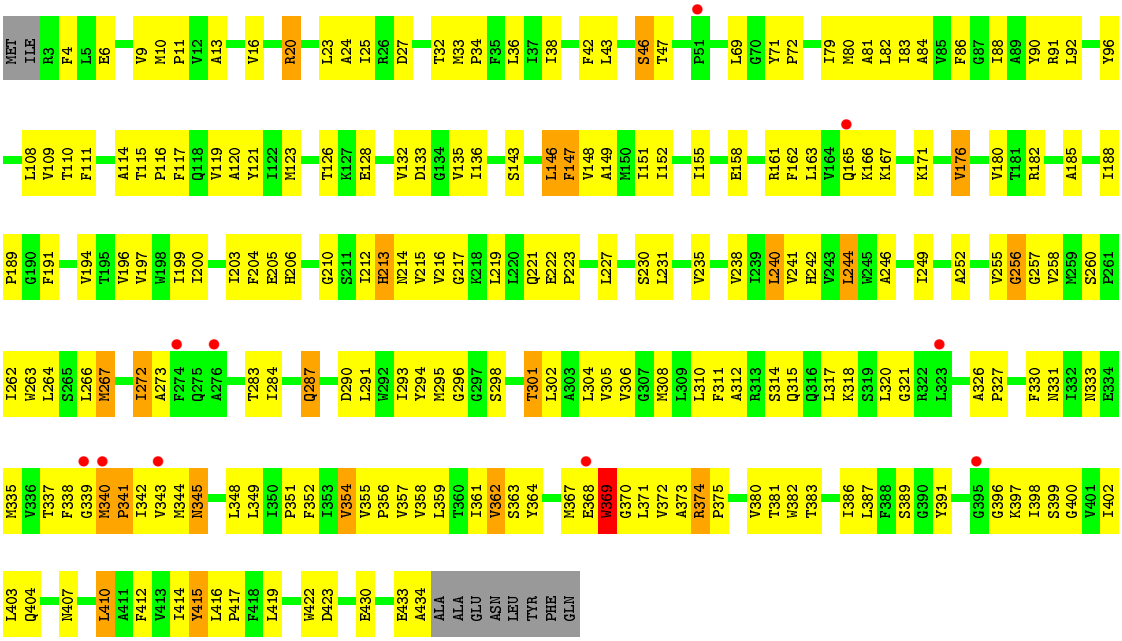
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 13 6 7	0	0
5	B	1	Total C O 13 6 7	0	0
5	C	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 7	0	0
5	A	1	Total C O 13 6 7	0	0
5	C	1	Total C O 13 6 7	0	0
5	C	1	Total C O 13 6 7	0	0

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.

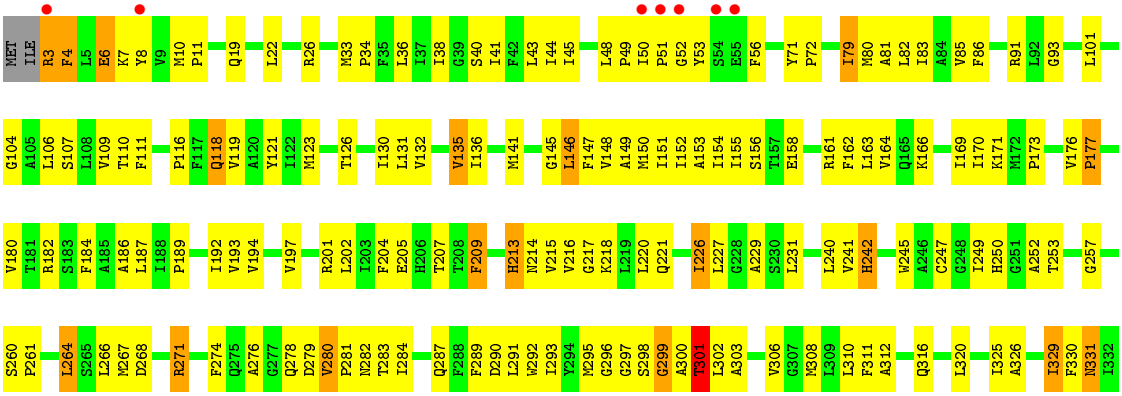
- Molecule 1: PTS system, cellobiose-specific IIC component

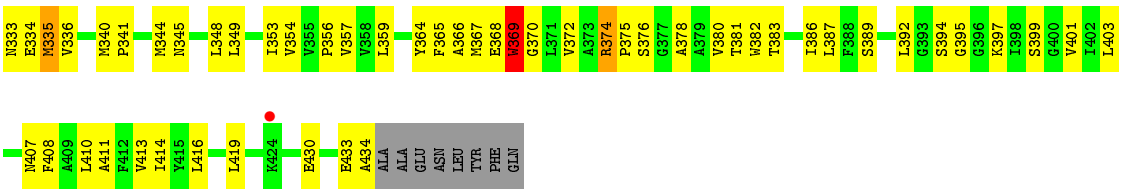
Chain A:



- Molecule 1: PTS system, cellobiose-specific IIC component

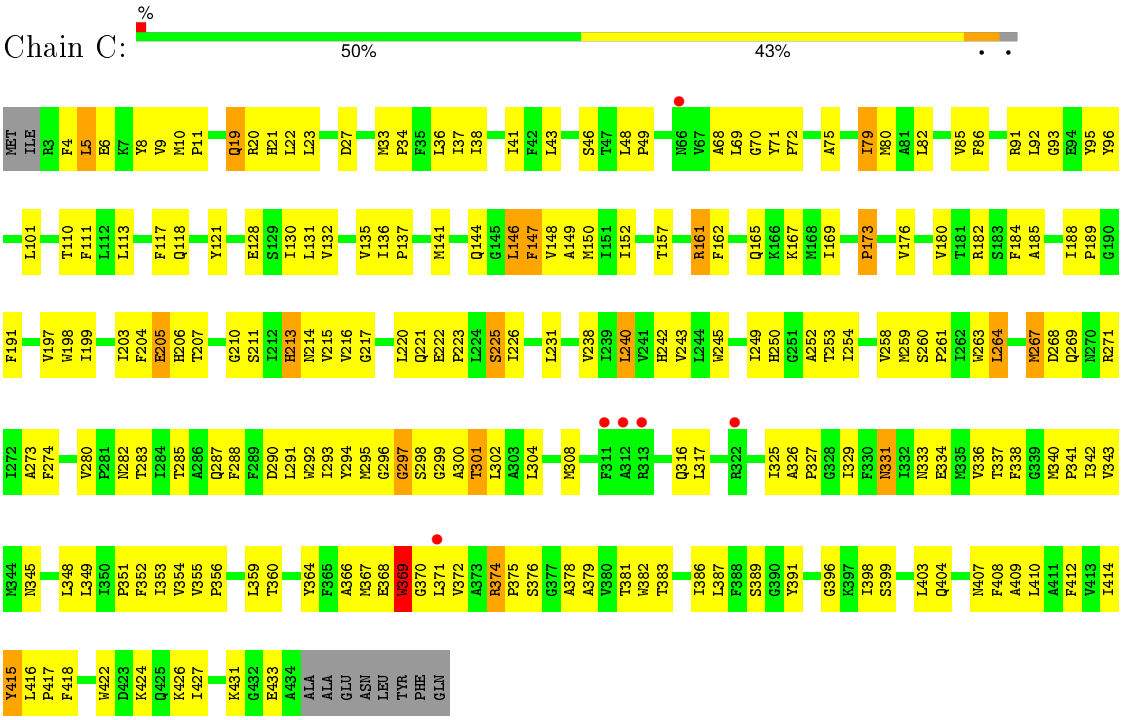
Chain B:





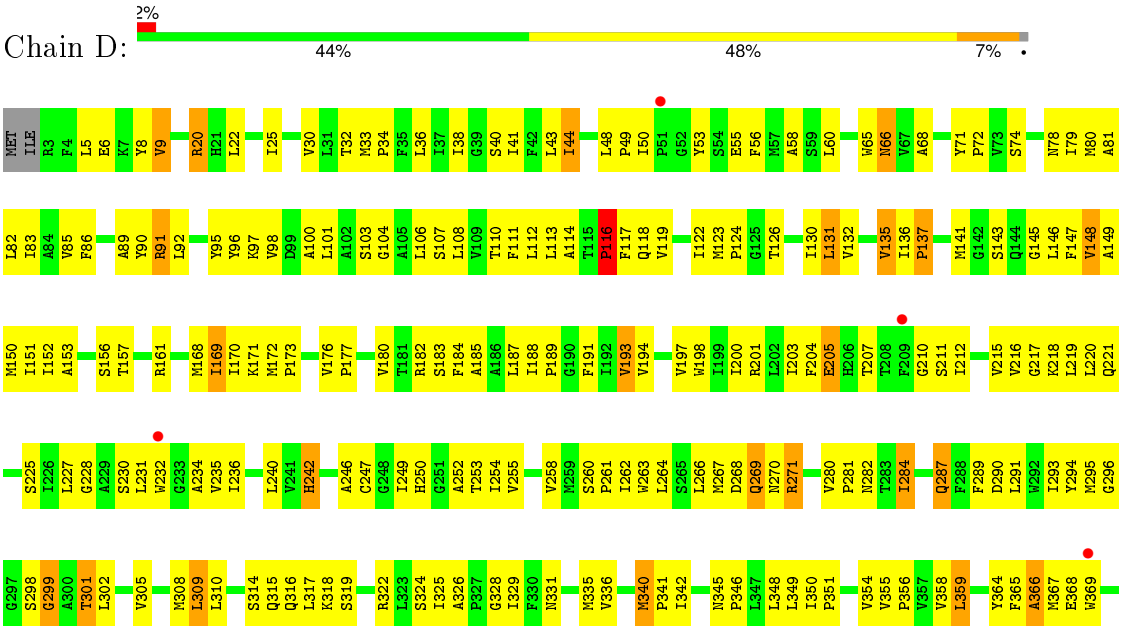
• Molecule 1: PTS system, cellobiose-specific IIC component

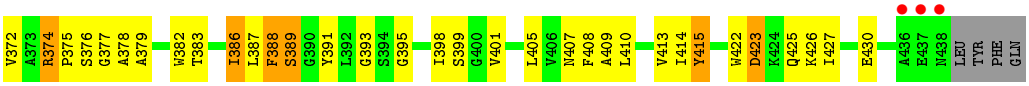
Chain C:



• Molecule 1: PTS system, cellobiose-specific IIC component

Chain D:




V372
A373
R374
P375
S376
G377
A378
A379
W382
T383
I386
L387
F388
S389
G390
Y391
L392
G393
S394
G395
I398
S399
G400
V401
L405
Y406
N407
F408
A409
L410
V413
I414
Y415
W422
D423
K424
Q425
K426
I427
E430
A436
E437
N438
LEU
TYR
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	132.81Å 132.81Å 452.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.29 46.68 – 3.29	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.97-3.29) 95.3 (46.68-3.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.228 , 0.264 0.226 , 0.260	Depositor DCC
R_{free} test set	3006 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	99.7	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 52.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	3 of 59461 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13566	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZDM, CBS, MAL, CIT

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	0.32	0/3356	0.53	0/4587
1	B	0.34	0/3372	0.55	1/4604 (0.0%)
1	C	0.32	0/3364	0.53	0/4596
1	D	0.34	0/3390	0.57	1/4628 (0.0%)
All	All	0.33	0/13482	0.55	2/18415 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	299	GLY	N-CA-C	-6.24	97.50	113.10
1	D	299	GLY	N-CA-C	-5.09	100.37	113.10

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	3272	0	3398	224	0
1	B	3288	0	3438	206	0
1	C	3280	0	3414	219	0
1	D	3307	0	3460	247	0
2	A	29	0	28	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	28	6	0
2	C	29	0	28	8	0
2	D	29	0	28	6	0
3	A	60	0	64	15	0
3	C	60	0	65	13	0
4	A	23	0	22	3	0
4	B	23	0	22	0	0
4	C	23	0	22	2	0
4	D	23	0	22	1	0
5	A	13	0	5	0	0
5	B	26	0	10	0	0
5	C	39	0	15	1	0
5	D	13	0	5	0	0
All	All	13566	0	14074	867	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 31.

All (867) 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:C:600:ZDM:O49	1:D:182:ARG:HD3	1.55	1.07
1:A:367:MET:HE3	1:A:375:PRO:HD3	1.42	1.01
1:C:252:ALA:HB1	2:C:500:CBS:H5B	1.45	0.98
1:C:182:ARG:HD3	3:C:443:ZDM:O49	1.63	0.98
1:B:345:ASN:ND2	1:B:348:LEU:HD12	1.83	0.93
1:D:296:GLY:HA3	1:D:302:LEU:H	1.34	0.92
1:D:324:SER:HB3	1:D:335:MET:HG2	1.51	0.90
1:C:298:SER:HB2	1:C:333:ASN:HD21	1.35	0.90
1:A:338:PHE:CD1	1:A:343:VAL:HG21	2.07	0.89
1:D:110:THR:HG22	1:D:152:ILE:HD13	1.54	0.89
1:B:164:VAL:HG12	1:B:169:ILE:HD11	1.53	0.89
1:C:111:PHE:HE1	1:C:148:VAL:HG23	1.37	0.89
1:B:4:PHE:H	1:B:4:PHE:HD2	1.21	0.88
1:A:264:LEU:HA	1:A:267:MET:HG2	1.53	0.88
1:D:173:PRO:O	1:D:176:VAL:HG12	1.74	0.86
1:C:342:ILE:O	1:C:342:ILE:HG22	1.73	0.86
1:B:345:ASN:HD21	1:B:348:LEU:HD12	1.39	0.86
1:B:295:MET:SD	1:B:386:ILE:HD11	2.16	0.85
1:C:338:PHE:CD1	1:C:343:VAL:HG21	2.12	0.85
1:D:388:PHE:HD2	1:D:388:PHE:H	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:HD23	1:D:197:VAL:HG12	1.60	0.84
1:B:82:LEU:O	1:B:85:VAL:HG12	1.79	0.82
1:C:132:VAL:HG21	1:D:132:VAL:HG11	1.61	0.82
3:A:600:ZDM:H18A	1:B:182:ARG:HD3	1.61	0.82
1:C:5:LEU:O	1:C:8:TYR:HB2	1.78	0.82
1:A:96:TYR:CD2	1:A:161:ARG:HG2	2.15	0.81
1:B:242:HIS:CD2	1:B:356:PRO:HG2	2.15	0.81
1:C:367:MET:HE3	1:C:375:PRO:HD3	1.63	0.81
1:A:298:SER:H	1:A:333:ASN:ND2	1.77	0.80
1:B:296:GLY:HA3	1:B:302:LEU:H	1.47	0.80
1:D:40:SER:O	1:D:44:ILE:HG23	1.80	0.79
1:D:252:ALA:HB1	2:D:500:CBS:H5B	1.64	0.78
1:B:52:GLY:O	1:B:56:PHE:HB2	1.83	0.78
1:C:337:THR:O	1:C:343:VAL:HG23	1.84	0.78
1:D:267:MET:HG3	1:D:287:GLN:HE22	1.49	0.76
1:A:244:LEU:HD23	1:A:249:ILE:HB	1.67	0.76
1:B:50:ILE:HG23	1:B:51:PRO:HD2	1.67	0.76
1:D:50:ILE:HB	1:D:53:TYR:HB3	1.66	0.76
1:C:161:ARG:HD2	1:C:162:PHE:N	2.01	0.76
1:B:217:GLY:HA2	1:B:221:GLN:HB3	1.66	0.76
1:D:267:MET:HG3	1:D:287:GLN:NE2	2.01	0.75
1:A:308:MET:O	1:A:312:ALA:HB2	1.86	0.75
1:C:19:GLN:HG3	1:C:22:LEU:HB2	1.69	0.75
1:C:38:ILE:HG21	1:D:194:VAL:HG21	1.68	0.75
1:D:367:MET:CE	1:D:375:PRO:HD3	2.17	0.74
1:D:242:HIS:CD2	1:D:356:PRO:HG2	2.22	0.74
1:D:266:LEU:HD12	1:D:284:ILE:HG22	1.69	0.74
1:D:287:GLN:H	1:D:287:GLN:CD	1.91	0.73
1:C:96:TYR:CD2	1:C:161:ARG:HG2	2.23	0.73
1:C:317:LEU:HD11	1:C:422:TRP:HD1	1.52	0.73
1:C:298:SER:H	1:C:333:ASN:ND2	1.86	0.73
2:A:500:CBS:H62A	1:B:176:VAL:HG23	1.70	0.73
1:B:19:GLN:HG2	1:B:22:LEU:HD13	1.71	0.73
1:D:340:MET:HG2	1:D:348:LEU:HD12	1.70	0.73
1:C:27:ASP:HB3	3:C:600:ZDM:O61	1.88	0.73
1:A:126:THR:HG23	1:A:128:GLU:HB2	1.68	0.73
1:D:231:LEU:HD13	1:D:364:TYR:CD1	2.23	0.73
1:B:367:MET:HE1	1:B:375:PRO:HD3	1.71	0.73
1:A:182:ARG:HD2	3:A:443:ZDM:O49	1.88	0.73
1:C:9:VAL:C	1:C:11:PRO:HD2	2.08	0.73
1:B:367:MET:CE	1:B:375:PRO:HD3	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:443:ZDM:H31	1:B:34:PRO:HG2	1.70	0.72
1:C:136:ILE:HB	1:D:136:ILE:HB	1.70	0.72
1:A:182:ARG:HH11	3:A:443:ZDM:H6	1.53	0.72
1:D:324:SER:HB3	1:D:335:MET:CG	2.20	0.72
1:B:359:LEU:HD22	1:B:407:ASN:HB3	1.71	0.72
1:C:296:GLY:O	1:C:331:ASN:HA	1.89	0.72
1:C:111:PHE:CE1	1:C:148:VAL:HG23	2.24	0.71
1:A:111:PHE:HE1	1:A:148:VAL:HG22	1.53	0.71
1:D:358:VAL:O	1:D:358:VAL:HG12	1.90	0.71
1:B:36:LEU:HD21	1:B:80:MET:HG2	1.72	0.71
1:B:204:PHE:HE1	1:B:215:VAL:HG21	1.55	0.71
1:A:79:ILE:HG22	1:A:79:ILE:O	1.91	0.71
1:A:80:MET:HE2	1:A:143:SER:HA	1.73	0.70
1:A:182:ARG:NH1	3:A:443:ZDM:H6	2.06	0.70
1:C:269:GLN:HE21	1:C:282:ASN:HD21	1.39	0.70
1:D:367:MET:HE1	1:D:375:PRO:HD3	1.74	0.70
1:C:345:ASN:HD21	1:C:348:LEU:H	1.36	0.70
1:A:337:THR:O	1:A:343:VAL:HG23	1.90	0.70
1:D:111:PHE:HE1	1:D:148:VAL:HG22	1.56	0.70
1:B:173:PRO:O	1:B:176:VAL:HG12	1.91	0.69
1:D:388:PHE:CD2	1:D:388:PHE:N	2.60	0.69
1:D:231:LEU:HD13	1:D:364:TYR:CG	2.27	0.69
1:C:213:HIS:HD2	1:C:214:ASN:H	1.40	0.69
1:B:130:ILE:HD11	1:C:130:ILE:HD13	1.73	0.69
1:A:387:LEU:HA	1:A:404:GLN:HE22	1.56	0.69
3:C:600:ZDM:O49	1:D:182:ARG:CD	2.37	0.69
1:C:148:VAL:HG12	1:C:216:VAL:HG21	1.73	0.69
1:B:71:TYR:HB2	1:B:72:PRO:HD3	1.75	0.69
1:A:96:TYR:HD2	1:A:161:ARG:HG2	1.55	0.68
1:A:13:ALA:O	1:A:16:VAL:HG12	1.93	0.68
1:B:151:ILE:O	1:B:155:ILE:HG13	1.92	0.68
1:A:27:ASP:HB3	3:A:600:ZDM:O61	1.94	0.68
1:B:250:HIS:CE1	1:B:253:THR:HG23	2.28	0.68
1:D:376:SER:HB3	1:D:395:GLY:N	2.08	0.68
1:C:86:PHE:CE2	1:D:86:PHE:CZ	2.81	0.68
1:A:295:MET:SD	1:A:386:ILE:HD11	2.34	0.68
1:C:204:PHE:CD1	1:C:215:VAL:HG21	2.29	0.68
1:C:182:ARG:CD	3:C:443:ZDM:O49	2.39	0.68
1:D:146:LEU:HD11	1:D:264:LEU:HD11	1.75	0.68
1:A:136:ILE:HB	1:B:136:ILE:HB	1.75	0.68
1:D:299:GLY:C	1:D:301:THR:H	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:SER:HB3	1:C:352:PHE:CZ	2.29	0.68
1:A:345:ASN:HD21	1:A:348:LEU:H	1.40	0.68
1:B:296:GLY:HA2	1:B:302:LEU:HB2	1.76	0.67
1:A:182:ARG:CD	3:A:443:ZDM:O49	2.42	0.67
1:C:342:ILE:O	1:C:342:ILE:CG2	2.43	0.67
1:A:351:PRO:HB2	1:A:415:TYR:CE1	2.30	0.67
1:D:345:ASN:O	1:D:349:LEU:HB2	1.94	0.67
1:A:264:LEU:HA	1:A:267:MET:CG	2.25	0.67
1:B:410:LEU:O	1:B:414:ILE:HG13	1.95	0.67
1:C:213:HIS:CD2	1:C:214:ASN:N	2.62	0.67
1:B:176:VAL:HG21	1:B:180:VAL:HG11	1.77	0.67
1:A:213:HIS:HD2	1:A:214:ASN:N	1.93	0.67
1:B:204:PHE:HA	1:B:207:THR:HG23	1.76	0.67
1:A:246:ALA:HB1	1:A:349:LEU:HD21	1.77	0.66
1:B:110:THR:HG23	1:B:197:VAL:HG11	1.77	0.66
1:A:301:THR:HG21	1:A:333:ASN:HB2	1.77	0.66
1:D:382:TRP:CZ3	1:D:383:THR:HG22	2.31	0.66
1:C:242:HIS:NE2	1:C:298:SER:O	2.29	0.66
1:C:204:PHE:CE1	1:C:215:VAL:HG11	2.30	0.66
1:B:4:PHE:CD2	1:B:4:PHE:N	2.59	0.66
1:B:33:MET:HB2	1:B:34:PRO:HD3	1.78	0.66
1:B:296:GLY:HA3	1:B:302:LEU:N	2.10	0.66
1:C:345:ASN:O	1:C:349:LEU:HB2	1.96	0.66
1:D:116:PRO:O	1:D:117:PHE:HB2	1.96	0.66
1:A:345:ASN:O	1:A:349:LEU:HB2	1.94	0.65
1:A:80:MET:CE	1:A:143:SER:HA	2.25	0.65
1:A:260:SER:O	1:A:264:LEU:HG	1.95	0.65
1:C:188:ILE:HB	1:C:189:PRO:HD3	1.79	0.65
1:C:34:PRO:HA	1:C:37:ILE:HD12	1.77	0.65
1:B:252:ALA:HB1	2:B:500:CBS:H5B	1.78	0.65
1:A:119:VAL:HG22	1:A:132:VAL:HB	1.78	0.65
1:C:381:THR:C	1:C:383:THR:H	2.00	0.65
1:C:316:GLN:HE22	1:C:426:LYS:HD2	1.61	0.65
1:B:213:HIS:CD2	1:B:214:ASN:N	2.64	0.65
1:A:33:MET:HB2	1:A:34:PRO:HD3	1.80	0.64
1:C:110:THR:HG23	1:C:197:VAL:HG11	1.78	0.64
1:A:296:GLY:HA3	1:A:302:LEU:H	1.62	0.64
1:A:252:ALA:HB1	2:A:500:CBS:H5B	1.79	0.64
1:D:316:GLN:HG3	1:D:430:GLU:OE2	1.98	0.64
1:C:412:PHE:HE2	1:C:416:LEU:HD22	1.63	0.64
1:C:41:ILE:HD12	1:D:191:PHE:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:THR:CG2	1:A:128:GLU:HB2	2.27	0.63
1:C:191:PHE:CE1	1:D:41:ILE:HD12	2.34	0.63
1:D:36:LEU:HD21	1:D:80:MET:HG2	1.79	0.63
1:A:235:VAL:HA	1:A:238:VAL:HG12	1.79	0.63
1:B:296:GLY:O	1:B:331:ASN:HA	1.99	0.63
1:C:38:ILE:CG2	1:D:194:VAL:HG21	2.28	0.63
1:A:109:VAL:CG2	1:B:83:ILE:HD11	2.29	0.63
1:D:296:GLY:HA3	1:D:302:LEU:N	2.10	0.63
1:D:43:LEU:HD12	1:D:378:ALA:HB2	1.80	0.63
1:D:55:GLU:HA	1:D:58:ALA:HB3	1.79	0.62
1:D:89:ALA:HB3	1:D:104:GLY:HA2	1.80	0.62
1:A:71:TYR:HB2	1:A:72:PRO:HD3	1.81	0.62
3:A:600:ZDM:O49	1:B:182:ARG:HD3	1.99	0.62
1:D:358:VAL:O	1:D:359:LEU:HD23	1.99	0.62
1:A:46:SER:HB3	1:A:69:LEU:HD12	1.82	0.62
1:C:340:MET:HG2	1:C:342:ILE:HG13	1.79	0.62
1:D:267:MET:SD	1:D:379:ALA:HB2	2.40	0.62
1:B:10:MET:HG3	1:B:247:CYS:HB3	1.82	0.62
1:C:295:MET:HG2	1:C:386:ILE:CD1	2.30	0.62
1:B:249:ILE:HG22	1:B:250:HIS:H	1.65	0.62
3:C:443:ZDM:H28A	1:D:34:PRO:HG2	1.81	0.62
1:B:130:ILE:HG21	1:D:132:VAL:HG12	1.80	0.62
1:C:410:LEU:O	1:C:414:ILE:HG13	1.99	0.62
1:A:110:THR:CG2	1:A:197:VAL:HG21	2.30	0.62
1:D:296:GLY:O	1:D:331:ASN:HA	2.00	0.61
1:C:211:SER:HB2	1:C:213:HIS:CD2	2.34	0.61
1:D:103:SER:HB2	1:D:157:THR:HG23	1.80	0.61
1:A:188:ILE:HB	1:A:189:PRO:HD3	1.80	0.61
1:B:26:ARG:HG3	1:B:257:GLY:HA3	1.82	0.61
1:C:253:THR:HG22	2:C:500:CBS:H1B	1.81	0.61
1:D:252:ALA:HB2	2:D:500:CBS:C7A	2.30	0.61
1:D:295:MET:HE1	1:D:407:ASN:HB2	1.81	0.61
1:A:135:VAL:HB	1:B:135:VAL:HG22	1.83	0.61
3:C:600:ZDM:HO49	1:D:182:ARG:HD3	1.61	0.61
1:D:71:TYR:HB2	1:D:72:PRO:HD3	1.82	0.61
1:C:351:PRO:HB2	1:C:415:TYR:CD1	2.35	0.61
1:C:250:HIS:CE1	1:C:253:THR:HG23	2.36	0.61
1:A:123:MET:O	1:A:126:THR:HG22	2.00	0.61
1:A:369:TRP:HB2	1:A:371:LEU:HD12	1.82	0.61
1:C:254:ILE:O	1:C:258:VAL:HG23	2.00	0.61
1:B:202:LEU:O	1:B:205:GLU:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:MET:HB2	1:D:34:PRO:HD3	1.83	0.61
1:B:331:ASN:N	1:B:331:ASN:HD22	1.98	0.61
1:B:264:LEU:HA	1:B:267:MET:HB3	1.83	0.61
1:B:131:LEU:O	1:B:131:LEU:HD12	2.01	0.61
1:C:298:SER:CB	1:C:333:ASN:HD21	2.12	0.61
1:B:80:MET:HE1	1:B:264:LEU:HD13	1.83	0.61
1:C:252:ALA:HB2	2:C:500:CBS:C7A	2.31	0.60
1:A:362:VAL:HG12	1:A:362:VAL:O	2.00	0.60
1:D:359:LEU:CD1	1:D:407:ASN:HB3	2.30	0.60
1:D:204:PHE:HA	1:D:207:THR:HG23	1.82	0.60
1:B:43:LEU:HD12	1:B:44:ILE:HG22	1.83	0.60
1:A:110:THR:HG21	1:A:197:VAL:HG21	1.84	0.60
1:C:408:PHE:CG	1:C:408:PHE:O	2.54	0.60
1:C:33:MET:HB2	1:C:34:PRO:HD3	1.84	0.60
1:A:126:THR:HG23	1:A:128:GLU:H	1.66	0.60
3:C:443:ZDM:H5	3:C:443:ZDM:O55	2.02	0.60
1:B:204:PHE:CE1	1:B:215:VAL:HG21	2.37	0.60
1:D:188:ILE:HB	1:D:189:PRO:HD3	1.84	0.60
1:D:172:MET:HG3	1:D:176:VAL:HG11	1.82	0.60
1:A:91:ARG:HE	3:A:600:ZDM:C57	2.14	0.60
1:D:249:ILE:HG22	1:D:250:HIS:N	2.16	0.60
1:D:147:PHE:O	1:D:151:ILE:HG13	2.02	0.60
1:B:252:ALA:HB2	2:B:500:CBS:C7A	2.32	0.59
1:A:298:SER:CB	1:A:333:ASN:HD21	2.14	0.59
1:A:338:PHE:CE1	1:A:343:VAL:HG21	2.36	0.59
1:A:86:PHE:CE2	1:B:86:PHE:CZ	2.90	0.59
1:C:147:PHE:HA	1:C:150:MET:HE3	1.84	0.59
1:A:146:LEU:HD21	1:A:264:LEU:HD11	1.83	0.59
1:D:364:TYR:CE2	1:D:368:GLU:HG3	2.38	0.59
1:C:79:ILE:CD1	1:D:112:LEU:HD12	2.33	0.59
1:A:38:ILE:HG21	1:B:194:VAL:HG21	1.84	0.59
1:B:34:PRO:O	1:B:38:ILE:HG13	2.02	0.59
1:B:216:VAL:O	1:B:220:LEU:HB2	2.02	0.59
1:D:41:ILE:O	1:D:44:ILE:HG13	2.02	0.59
1:D:293:ILE:N	1:D:293:ILE:HD12	2.18	0.59
1:A:359:LEU:HD22	1:A:407:ASN:OD1	2.03	0.58
1:C:79:ILE:HD11	1:D:112:LEU:CD1	2.33	0.58
1:B:382:TRP:CZ3	1:B:383:THR:HG22	2.38	0.58
1:B:249:ILE:HG22	1:B:250:HIS:N	2.17	0.58
1:B:325:ILE:HD12	1:B:326:ALA:N	2.18	0.58
1:D:260:SER:O	1:D:264:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:700:MAL:O3'	4:A:700:MAL:O5	2.20	0.58
1:B:359:LEU:HD22	1:B:407:ASN:CB	2.33	0.58
1:D:409:ALA:O	1:D:413:VAL:HG13	2.03	0.58
1:A:317:LEU:HD11	1:A:422:TRP:HD1	1.66	0.58
1:D:110:THR:HG23	1:D:197:VAL:HG21	1.85	0.58
1:B:130:ILE:CD1	1:C:130:ILE:HD13	2.32	0.58
1:C:91:ARG:HE	3:C:600:ZDM:H57A	1.67	0.58
1:C:213:HIS:HD2	1:C:214:ASN:N	2.01	0.58
1:A:304:LEU:HB2	1:A:415:TYR:CD2	2.39	0.58
1:A:351:PRO:HB2	1:A:415:TYR:CD1	2.38	0.58
1:A:416:LEU:N	1:A:417:PRO:HD2	2.19	0.58
3:A:443:ZDM:C57	1:B:91:ARG:HE	2.17	0.58
1:C:86:PHE:CZ	1:D:86:PHE:CZ	2.92	0.58
1:B:268:ASP:OD1	1:B:271:ARG:HD3	2.04	0.58
1:C:71:TYR:HB2	1:C:72:PRO:HD3	1.84	0.58
1:C:283:THR:HA	1:C:374:ARG:HG3	1.86	0.58
1:D:50:ILE:HB	1:D:53:TYR:CB	2.34	0.58
1:B:296:GLY:CA	1:B:302:LEU:HB2	2.34	0.58
1:C:182:ARG:NH1	3:C:443:ZDM:H6	2.19	0.57
1:A:298:SER:HB2	1:A:333:ASN:HD21	1.69	0.57
1:B:335:MET:HA	1:B:335:MET:CE	2.34	0.57
1:B:353:ILE:O	1:B:356:PRO:HD2	2.04	0.57
1:A:42:PHE:CD1	1:A:72:PRO:HG2	2.39	0.57
1:B:119:VAL:HG22	1:B:135:VAL:HG11	1.86	0.57
1:A:146:LEU:HD21	1:A:264:LEU:CD1	2.34	0.57
1:A:295:MET:HE1	1:A:407:ASN:HB3	1.86	0.57
1:B:340:MET:N	1:B:341:PRO:HA	2.20	0.57
1:D:386:ILE:HG23	1:D:387:LEU:N	2.19	0.57
1:C:268:ASP:O	1:C:271:ARG:HB3	2.04	0.57
1:B:299:GLY:C	1:B:301:THR:H	2.08	0.57
1:B:282:ASN:O	1:B:374:ARG:HG2	2.04	0.57
3:A:443:ZDM:H5	3:A:443:ZDM:O55	2.04	0.57
1:C:351:PRO:HB2	1:C:415:TYR:CE1	2.40	0.57
1:C:369:TRP:HB3	1:C:371:LEU:HD12	1.86	0.57
1:D:367:MET:CE	1:D:374:ARG:HA	2.35	0.57
1:C:10:MET:N	1:C:11:PRO:HD2	2.20	0.57
1:A:295:MET:CE	1:A:407:ASN:HB3	2.35	0.57
1:A:204:PHE:CE1	1:A:215:VAL:HG11	2.40	0.57
1:A:311:PHE:N	1:A:311:PHE:CD2	2.72	0.57
1:D:53:TYR:HA	1:D:56:PHE:HB3	1.87	0.57
1:D:250:HIS:CE1	1:D:253:THR:HG23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:VAL:CG1	1:D:107:SER:HB3	2.35	0.56
1:A:80:MET:HE3	1:A:146:LEU:HD23	1.86	0.56
1:A:382:TRP:CZ3	1:A:383:THR:HG22	2.40	0.56
1:C:217:GLY:HA2	1:C:221:GLN:HB3	1.86	0.56
1:A:291:LEU:HD22	1:A:389:SER:OG	2.05	0.56
1:A:310:LEU:C	1:A:311:PHE:HD2	2.08	0.56
1:D:249:ILE:HG22	1:D:250:HIS:H	1.71	0.56
1:A:252:ALA:CB	2:A:500:CBS:H5B	2.36	0.56
1:A:213:HIS:CD2	1:A:214:ASN:N	2.71	0.56
1:A:311:PHE:HE1	1:A:416:LEU:HD21	1.71	0.56
1:D:250:HIS:ND1	1:D:253:THR:HG23	2.21	0.56
1:B:146:LEU:HA	1:B:149:ALA:HB3	1.88	0.56
1:A:221:GLN:O	1:A:221:GLN:HG3	2.03	0.56
1:D:119:VAL:HG23	1:D:132:VAL:CG2	2.36	0.56
1:C:331:ASN:N	1:C:331:ASN:HD22	2.04	0.56
1:B:287:GLN:HA	1:B:290:ASP:HB2	1.87	0.56
1:D:221:GLN:O	1:D:225:SER:HB2	2.05	0.56
1:C:110:THR:CG2	1:C:197:VAL:HG11	2.36	0.56
1:B:44:ILE:O	1:B:44:ILE:HG13	2.05	0.56
1:A:20:ARG:HH11	1:A:20:ARG:HB3	1.71	0.56
1:A:382:TRP:HE1	2:A:500:CBS:HN2B	1.54	0.56
1:B:367:MET:HB3	1:B:374:ARG:HD2	1.88	0.55
1:A:372:VAL:HG13	1:A:399:SER:O	2.07	0.55
1:A:315:GLN:HB2	1:A:430:GLU:OE1	2.07	0.55
1:D:146:LEU:O	1:D:149:ALA:HB3	2.06	0.55
1:A:302:LEU:O	1:A:306:VAL:HG23	2.06	0.55
1:A:373:ALA:HB2	1:A:397:LYS:HD3	1.89	0.55
1:C:91:ARG:HE	3:C:600:ZDM:C57	2.18	0.55
1:B:250:HIS:ND1	1:B:253:THR:HG23	2.21	0.55
1:D:295:MET:CE	1:D:407:ASN:HB2	2.37	0.55
1:A:240:LEU:O	1:A:244:LEU:HB2	2.06	0.55
1:D:246:ALA:HB1	1:D:349:LEU:HD21	1.88	0.55
1:B:161:ARG:HD2	1:B:162:PHE:N	2.22	0.55
1:C:19:GLN:CG	1:C:22:LEU:HB2	2.35	0.55
2:A:500:CBS:C6A	1:B:176:VAL:HG23	2.35	0.55
1:D:5:LEU:O	1:D:8:TYR:HB2	2.07	0.55
1:C:334:GLU:OE2	2:C:500:CBS:H61A	2.06	0.55
1:D:113:LEU:HD21	1:D:198:TRP:HB2	1.87	0.55
1:C:340:MET:HB3	1:C:342:ILE:N	2.22	0.55
1:D:359:LEU:HD11	1:D:407:ASN:HB3	1.89	0.55
1:A:354:VAL:HG12	1:A:355:VAL:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLU:HA	1:A:210:GLY:O	2.07	0.55
1:D:169:ILE:HG12	1:D:185:ALA:O	2.07	0.55
1:B:345:ASN:O	1:B:349:LEU:HB2	2.07	0.55
1:C:211:SER:HB2	1:C:213:HIS:NE2	2.21	0.55
1:A:311:PHE:HD1	1:A:416:LEU:HD11	1.72	0.55
1:B:121:TYR:CD1	1:C:130:ILE:HG22	2.42	0.54
1:A:301:THR:O	1:A:305:VAL:HG23	2.07	0.54
1:D:80:MET:CE	1:D:143:SER:HA	2.37	0.54
1:B:292:TRP:C	1:B:293:ILE:HD12	2.28	0.54
1:C:79:ILE:CD1	1:D:112:LEU:CD1	2.85	0.54
1:D:317:LEU:HD11	1:D:422:TRP:HD1	1.72	0.54
1:A:264:LEU:CA	1:A:267:MET:HG2	2.32	0.54
1:A:391:TYR:CE1	1:A:396:GLY:HA2	2.42	0.54
1:B:372:VAL:HG13	1:B:399:SER:O	2.07	0.54
1:D:299:GLY:C	1:D:301:THR:N	2.61	0.54
1:A:196:VAL:O	1:A:200:ILE:HG13	2.08	0.54
1:A:326:ALA:HB3	1:A:327:PRO:HD3	1.89	0.54
1:D:172:MET:CG	1:D:176:VAL:HG11	2.38	0.54
1:A:342:ILE:O	1:A:349:LEU:HD13	2.07	0.54
1:C:285:THR:O	1:C:288:PHE:HB3	2.08	0.54
1:D:340:MET:HG2	1:D:348:LEU:CD1	2.37	0.54
1:C:345:ASN:ND2	1:C:348:LEU:H	2.05	0.54
1:A:320:LEU:CD2	1:A:340:MET:HB3	2.37	0.54
1:A:4:PHE:C	1:A:6:GLU:H	2.11	0.54
1:A:191:PHE:HD1	1:B:38:ILE:HG23	1.72	0.54
1:D:189:PRO:O	1:D:193:VAL:HG23	2.08	0.54
1:D:227:LEU:O	1:D:230:SER:HB3	2.08	0.54
1:D:367:MET:HB3	1:D:374:ARG:HD2	1.89	0.54
1:D:289:PHE:HA	1:D:293:ILE:HD13	1.90	0.54
1:A:91:ARG:NE	3:A:600:ZDM:O61	2.37	0.53
1:A:119:VAL:HB	1:D:123:MET:CE	2.37	0.53
1:D:170:ILE:HG13	1:D:188:ILE:HG12	1.91	0.53
1:A:241:VAL:HG12	1:A:242:HIS:ND1	2.24	0.53
1:C:101:LEU:HD13	1:D:90:TYR:CD2	2.44	0.53
1:B:44:ILE:HD12	1:B:392:LEU:HD22	1.89	0.53
1:B:284:ILE:O	1:B:284:ILE:HG22	2.09	0.53
1:B:152:ILE:HD12	1:B:153:ALA:N	2.23	0.53
1:A:355:VAL:HG22	1:A:414:ILE:HD12	1.90	0.53
1:D:204:PHE:CD2	1:D:215:VAL:HG21	2.44	0.53
1:D:110:THR:CG2	1:D:197:VAL:HG21	2.37	0.53
1:D:319:SER:HB2	1:D:322:ARG:NH2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:GLN:NE2	1:C:379:ALA:HA	2.24	0.53
1:B:81:ALA:HB3	1:B:141:MET:O	2.09	0.53
1:B:19:GLN:CG	1:B:22:LEU:HD13	2.39	0.53
1:D:423:ASP:O	1:D:427:ILE:HG13	2.08	0.53
1:D:176:VAL:HG21	1:D:180:VAL:HG11	1.91	0.53
1:C:381:THR:C	1:C:383:THR:N	2.62	0.53
1:D:372:VAL:HG13	1:D:399:SER:O	2.09	0.53
1:D:111:PHE:CE1	1:D:148:VAL:HG22	2.40	0.53
1:A:296:GLY:HA3	1:A:302:LEU:N	2.24	0.53
1:B:289:PHE:HA	1:B:293:ILE:HD13	1.90	0.53
1:D:114:ALA:HB1	1:D:212:ILE:HD12	1.90	0.53
1:C:412:PHE:CE2	1:C:416:LEU:HD22	2.44	0.52
1:C:424:LYS:O	1:C:427:ILE:HG13	2.09	0.52
1:C:355:VAL:HB	1:C:356:PRO:HD3	1.90	0.52
1:C:416:LEU:N	1:C:417:PRO:HD2	2.24	0.52
1:C:367:MET:HB3	1:C:374:ARG:HD2	1.91	0.52
1:C:176:VAL:HG13	1:C:180:VAL:HB	1.91	0.52
1:D:340:MET:HB3	1:D:341:PRO:C	2.29	0.52
1:A:341:PRO:O	1:A:345:ASN:HB3	2.10	0.52
1:C:369:TRP:CB	1:C:371:LEU:HD12	2.39	0.52
1:A:33:MET:SD	2:A:500:CBS:H83B	2.49	0.52
1:C:376:SER:HB2	1:C:378:ALA:H	1.75	0.52
1:B:301:THR:HG21	1:B:333:ASN:HB2	1.91	0.52
1:D:22:LEU:HD21	1:D:258:VAL:CG2	2.39	0.52
3:C:600:ZDM:O55	3:C:600:ZDM:H10	2.10	0.52
1:D:296:GLY:HA2	1:D:302:LEU:HB2	1.90	0.52
1:D:106:LEU:HD21	1:D:193:VAL:HG21	1.91	0.52
1:D:410:LEU:O	1:D:414:ILE:HG13	2.10	0.52
1:C:367:MET:CE	1:C:374:ARG:HA	2.39	0.52
1:D:118:GLN:NE2	1:D:131:LEU:HD12	2.25	0.52
1:C:367:MET:HE3	1:C:374:ARG:HA	1.91	0.52
1:B:367:MET:HE2	1:B:374:ARG:HA	1.92	0.52
1:D:314:SER:O	1:D:318:LYS:HB2	2.10	0.52
1:A:199:ILE:O	1:A:203:ILE:HG13	2.10	0.52
1:D:89:ALA:HB1	1:D:103:SER:O	2.09	0.52
1:B:433:GLU:O	1:B:434:ALA:HB3	2.10	0.52
1:A:111:PHE:HE1	1:A:148:VAL:CG2	2.23	0.51
1:B:245:TRP:HA	1:B:249:ILE:O	2.10	0.51
1:C:398:ILE:HG22	1:C:398:ILE:O	2.10	0.51
1:B:123:MET:HB3	1:B:126:THR:OG1	2.10	0.51
1:D:6:GLU:OE2	1:D:9:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:VAL:HG11	1:C:213:HIS:HA	1.91	0.51
1:A:204:PHE:C	1:A:206:HIS:H	2.13	0.51
1:D:375:PRO:HA	1:D:393:GLY:O	2.10	0.51
1:B:334:GLU:OE1	2:B:500:CBS:H61A	2.10	0.51
1:D:124:PRO:O	1:D:126:THR:HG23	2.11	0.51
1:D:240:LEU:HB3	1:D:255:VAL:HG21	1.92	0.51
1:D:382:TRP:HE1	2:D:500:CBS:HN2B	1.58	0.51
1:D:317:LEU:HD11	1:D:422:TRP:CD1	2.45	0.51
1:C:20:ARG:HB3	1:C:95:TYR:CZ	2.46	0.51
1:D:131:LEU:H	1:D:131:LEU:HD23	1.75	0.51
1:D:287:GLN:HA	1:D:290:ASP:HB2	1.93	0.51
1:D:367:MET:HE2	1:D:374:ARG:HA	1.93	0.51
1:B:154:ILE:O	1:B:158:GLU:HB2	2.10	0.51
1:C:297:GLY:O	2:C:500:CBS:H83A	2.10	0.51
1:D:302:LEU:HG	1:D:302:LEU:O	2.10	0.51
1:C:338:PHE:CE1	1:C:343:VAL:HG21	2.45	0.51
1:C:10:MET:N	1:C:11:PRO:CD	2.74	0.51
1:C:222:GLU:N	1:C:223:PRO:HD2	2.26	0.51
1:C:231:LEU:HD13	1:C:364:TYR:CG	2.46	0.51
1:A:27:ASP:CB	3:A:600:ZDM:O61	2.59	0.50
1:D:228:GLY:O	1:D:284:ILE:HG21	2.10	0.50
1:A:132:VAL:HG21	1:B:132:VAL:HG21	1.93	0.50
1:D:123:MET:HB3	1:D:126:THR:OG1	2.11	0.50
1:C:300:ALA:O	1:C:302:LEU:N	2.45	0.50
1:D:96:TYR:O	1:D:97:LYS:HB2	2.11	0.50
1:A:114:ALA:HB1	1:A:212:ILE:HD12	1.93	0.50
1:A:146:LEU:CD2	1:A:264:LEU:HD11	2.41	0.50
1:B:367:MET:CE	1:B:374:ARG:HA	2.40	0.50
1:D:116:PRO:HA	1:D:201:ARG:NH2	2.27	0.50
1:A:320:LEU:HD21	1:A:340:MET:HB3	1.94	0.50
1:A:256:GLY:C	1:A:258:VAL:H	2.15	0.50
1:D:25:ILE:HD13	1:D:150:MET:SD	2.52	0.50
1:A:33:MET:CB	1:A:34:PRO:HD3	2.40	0.50
1:B:213:HIS:HD2	1:B:214:ASN:N	2.07	0.50
1:A:46:SER:CB	1:A:69:LEU:HD12	2.41	0.50
1:D:81:ALA:O	1:D:85:VAL:HG23	2.11	0.50
1:D:284:ILE:HG22	1:D:284:ILE:O	2.12	0.50
1:B:381:THR:HG23	1:B:383:THR:H	1.76	0.50
1:A:133:ASP:HB2	1:C:128:GLU:OE2	2.12	0.50
1:C:299:GLY:C	1:C:301:THR:H	2.14	0.50
1:C:43:LEU:HD12	1:C:378:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LEU:O	1:A:414:ILE:HG13	2.11	0.50
1:D:131:LEU:N	1:D:131:LEU:HD23	2.27	0.50
1:D:205:GLU:HA	1:D:210:GLY:O	2.11	0.50
1:C:43:LEU:HD13	1:C:43:LEU:O	2.12	0.50
1:D:242:HIS:HD2	1:D:356:PRO:HG2	1.77	0.50
1:B:186:ALA:O	1:B:189:PRO:HD2	2.11	0.50
3:A:600:ZDM:O49	1:B:182:ARG:CD	2.59	0.49
1:C:316:GLN:NE2	1:C:426:LYS:HD2	2.26	0.49
1:D:319:SER:O	1:D:322:ARG:HB2	2.12	0.49
1:D:22:LEU:HD23	1:D:22:LEU:O	2.12	0.49
1:A:367:MET:CE	1:A:375:PRO:HD3	2.30	0.49
1:C:340:MET:CB	1:C:342:ILE:HG13	2.42	0.49
1:C:117:PHE:CE1	1:C:136:ILE:HG12	2.47	0.49
1:D:316:GLN:OE1	1:D:426:LYS:HD2	2.12	0.49
1:C:101:LEU:HD13	1:D:90:TYR:CE2	2.46	0.49
5:C:444:CIT:O5	5:C:444:CIT:C1	2.60	0.49
1:D:44:ILE:HD12	1:D:44:ILE:C	2.32	0.49
1:B:213:HIS:C	1:B:213:HIS:CD2	2.85	0.49
1:A:176:VAL:HG13	1:A:180:VAL:HB	1.93	0.49
1:B:336:VAL:HG13	1:B:340:MET:HG3	1.94	0.49
1:B:231:LEU:HD13	1:B:364:TYR:CG	2.48	0.49
1:D:218:LYS:O	1:D:219:LEU:HD23	2.10	0.49
1:C:249:ILE:HG22	1:C:250:HIS:N	2.27	0.49
1:A:310:LEU:C	1:A:311:PHE:CD2	2.85	0.49
1:D:80:MET:HE1	1:D:146:LEU:HD11	1.94	0.49
1:A:231:LEU:HD13	1:A:364:TYR:CG	2.47	0.49
1:D:346:PRO:O	1:D:350:ILE:HD13	2.12	0.49
3:C:443:ZDM:C57	1:D:91:ARG:HE	2.25	0.49
1:D:359:LEU:HD13	1:D:407:ASN:HB3	1.95	0.49
1:B:252:ALA:HB2	2:B:500:CBS:O7A	2.13	0.49
1:C:325:ILE:HG23	1:C:326:ALA:H	1.77	0.49
1:B:3:ARG:O	1:B:6:GLU:HB3	2.13	0.49
1:A:335:MET:O	1:A:339:GLY:HA3	2.11	0.49
1:C:269:GLN:HE21	1:C:282:ASN:ND2	2.08	0.49
1:B:86:PHE:CD1	1:B:104:GLY:O	2.66	0.49
1:D:216:VAL:HG13	1:D:220:LEU:HD12	1.94	0.49
1:B:145:GLY:O	1:B:148:VAL:HG12	2.13	0.49
1:B:10:MET:N	1:B:11:PRO:HD2	2.27	0.49
1:C:386:ILE:O	1:C:389:SER:HB3	2.13	0.49
1:D:225:SER:HA	1:D:262:ILE:HG23	1.93	0.49
1:A:10:MET:N	1:A:11:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:HG21	1:B:38:ILE:HG21	1.94	0.49
1:A:386:ILE:HG23	1:A:387:LEU:N	2.27	0.49
1:A:326:ALA:HB3	1:A:327:PRO:CD	2.42	0.49
1:C:165:GLN:C	1:C:167:LYS:H	2.15	0.49
2:C:500:CBS:C6A	1:D:176:VAL:HG23	2.43	0.48
1:A:415:TYR:C	1:A:417:PRO:HD2	2.33	0.48
1:C:340:MET:CG	1:C:342:ILE:HG13	2.43	0.48
1:B:242:HIS:HD2	1:B:356:PRO:HG2	1.76	0.48
1:C:293:ILE:HG12	1:C:360:THR:OG1	2.12	0.48
1:D:426:LYS:O	1:D:430:GLU:HG3	2.13	0.48
4:C:700:MAL:O3'	4:C:700:MAL:O5	2.18	0.48
1:B:287:GLN:HB3	1:B:291:LEU:CD1	2.44	0.48
1:A:345:ASN:HD21	1:A:348:LEU:N	2.10	0.48
1:B:310:LEU:HB3	1:B:311:PHE:CD2	2.48	0.48
1:A:242:HIS:NE2	1:A:298:SER:O	2.47	0.48
1:D:242:HIS:NE2	1:D:298:SER:O	2.46	0.48
1:D:117:PHE:HA	1:D:135:VAL:O	2.14	0.48
1:D:43:LEU:CD1	1:D:378:ALA:HB2	2.41	0.48
1:C:408:PHE:O	1:C:408:PHE:CD1	2.66	0.48
1:C:367:MET:CE	1:C:375:PRO:HD3	2.37	0.48
1:D:264:LEU:HA	1:D:267:MET:CB	2.44	0.48
1:A:256:GLY:O	1:A:258:VAL:N	2.47	0.48
1:A:10:MET:N	1:A:11:PRO:HD2	2.29	0.48
1:D:74:SER:O	1:D:78:ASN:HB2	2.13	0.48
1:B:48:LEU:HB3	1:B:53:TYR:CE2	2.48	0.48
1:D:112:LEU:O	1:D:117:PHE:HE2	1.97	0.48
1:D:184:PHE:HD2	1:D:184:PHE:H	1.61	0.48
1:D:287:GLN:CD	1:D:287:GLN:N	2.64	0.48
1:A:386:ILE:HG23	1:A:387:LEU:HG	1.96	0.48
1:C:368:GLU:C	1:C:370:GLY:H	2.16	0.48
1:A:227:LEU:O	1:A:230:SER:HB3	2.13	0.48
1:C:316:GLN:NE2	1:C:426:LYS:HB3	2.29	0.47
1:C:240:LEU:HA	1:C:243:VAL:HG22	1.95	0.47
1:A:222:GLU:N	1:A:223:PRO:HD2	2.29	0.47
1:D:48:LEU:HA	1:D:49:PRO:HD3	1.62	0.47
1:A:298:SER:HB3	1:A:352:PHE:CZ	2.49	0.47
1:B:366:ALA:HB1	1:B:372:VAL:CG2	2.44	0.47
1:A:368:GLU:C	1:A:370:GLY:H	2.18	0.47
1:B:242:HIS:NE2	1:B:298:SER:O	2.47	0.47
1:A:79:ILE:O	1:A:79:ILE:CG2	2.62	0.47
1:C:231:LEU:HD13	1:C:364:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:ASP:OD1	1:D:271:ARG:NH1	2.44	0.47
1:C:372:VAL:HA	1:C:399:SER:HB2	1.96	0.47
1:A:38:ILE:CG2	1:B:194:VAL:HG21	2.44	0.47
1:A:311:PHE:CD1	1:A:416:LEU:HD11	2.50	0.47
1:B:325:ILE:HD12	1:B:326:ALA:H	1.79	0.47
1:D:269:GLN:H	1:D:269:GLN:HG2	1.56	0.47
1:B:163:LEU:HD11	1:B:192:ILE:HG21	1.96	0.47
1:D:336:VAL:HG12	1:D:342:ILE:CD1	2.44	0.47
1:C:176:VAL:HG12	1:C:176:VAL:O	2.15	0.47
1:B:79:ILE:O	1:B:80:MET:C	2.52	0.47
1:B:204:PHE:CE1	1:B:215:VAL:HG11	2.49	0.47
1:C:386:ILE:HG23	1:C:387:LEU:N	2.29	0.47
1:A:163:LEU:HD13	1:A:189:PRO:HA	1.96	0.47
1:C:274:PHE:HB2	1:C:280:VAL:CG1	2.45	0.47
1:A:80:MET:HE2	1:A:143:SER:CA	2.43	0.47
1:A:241:VAL:HG23	1:A:255:VAL:HG21	1.96	0.47
1:D:295:MET:SD	1:D:386:ILE:HD11	2.55	0.47
1:B:106:LEU:HD21	1:B:193:VAL:HG11	1.95	0.47
1:C:295:MET:HG2	1:C:386:ILE:HG13	1.96	0.47
1:D:204:PHE:HA	1:D:207:THR:CG2	2.44	0.47
1:A:171:LYS:O	1:A:171:LYS:HG3	2.14	0.47
1:D:253:THR:HG22	2:D:500:CBS:H1B	1.97	0.47
1:C:176:VAL:HG22	2:D:500:CBS:H62A	1.97	0.47
1:C:110:THR:HG22	1:C:152:ILE:HD13	1.97	0.47
1:C:293:ILE:HG22	1:C:294:TYR:CD1	2.50	0.47
1:A:83:ILE:HD11	1:B:109:VAL:CG2	2.44	0.47
1:C:245:TRP:HA	1:C:249:ILE:O	2.15	0.47
1:B:50:ILE:HA	1:B:51:PRO:HD3	1.78	0.47
1:A:312:ALA:HB1	1:A:318:LYS:HB2	1.97	0.47
1:D:68:ALA:HA	1:D:71:TYR:CE2	2.49	0.47
1:C:259:MET:C	1:C:261:PRO:HD2	2.34	0.47
1:D:91:ARG:HD2	1:D:91:ARG:O	2.15	0.47
1:D:345:ASN:ND2	1:D:348:LEU:HB2	2.30	0.47
1:A:182:ARG:O	1:A:185:ALA:HB3	2.15	0.47
1:B:110:THR:HG23	1:B:197:VAL:HG21	1.96	0.47
1:C:79:ILE:HD11	1:D:112:LEU:HD12	1.96	0.47
1:C:292:TRP:HA	1:C:295:MET:HE3	1.97	0.47
1:C:46:SER:HB2	1:C:69:LEU:HB3	1.95	0.47
1:B:193:VAL:O	1:B:197:VAL:HG23	2.16	0.46
1:C:20:ARG:HD3	1:C:95:TYR:CE2	2.50	0.46
1:D:351:PRO:HB2	1:D:415:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ILE:HG22	1:D:398:ILE:O	2.14	0.46
1:B:226:ILE:HA	1:B:226:ILE:HD12	1.73	0.46
1:D:264:LEU:HA	1:D:267:MET:HB3	1.97	0.46
1:C:295:MET:HE2	1:C:404:GLN:HG2	1.98	0.46
1:B:287:GLN:HB3	1:B:291:LEU:HD11	1.97	0.46
1:C:267:MET:HE2	1:C:267:MET:HB3	1.77	0.46
1:C:298:SER:HB3	1:C:352:PHE:HZ	1.80	0.46
1:B:148:VAL:O	1:B:152:ILE:HG13	2.16	0.46
1:D:340:MET:N	1:D:341:PRO:HA	2.29	0.46
1:A:296:GLY:CA	1:A:302:LEU:HB2	2.44	0.46
1:C:291:LEU:HD22	1:C:389:SER:OG	2.15	0.46
1:A:86:PHE:CZ	1:B:86:PHE:CZ	3.04	0.46
1:D:9:VAL:HG22	1:D:247:CYS:SG	2.56	0.46
1:B:310:LEU:HB3	1:B:311:PHE:HD2	1.79	0.46
1:A:398:ILE:HD12	1:A:398:ILE:N	2.31	0.46
1:A:298:SER:N	1:A:333:ASN:ND2	2.57	0.46
1:B:40:SER:O	1:B:44:ILE:HG23	2.16	0.46
1:D:145:GLY:O	1:D:148:VAL:HG13	2.15	0.46
1:C:383:THR:HG22	1:C:383:THR:O	2.14	0.46
1:B:10:MET:N	1:B:11:PRO:CD	2.79	0.46
1:C:326:ALA:N	1:C:327:PRO:HD2	2.31	0.46
4:D:700:MAL:O5	4:D:700:MAL:O3'	2.31	0.46
1:B:303:ALA:HA	1:B:408:PHE:HE1	1.80	0.46
1:D:110:THR:HG23	1:D:197:VAL:HG11	1.97	0.46
1:A:146:LEU:HD12	1:A:147:PHE:N	2.31	0.46
1:B:111:PHE:HE1	1:B:148:VAL:HG13	1.81	0.46
1:D:80:MET:CE	1:D:146:LEU:HD11	2.46	0.46
1:C:325:ILE:HG23	1:C:326:ALA:N	2.31	0.46
1:C:146:LEU:HA	1:C:149:ALA:CB	2.46	0.46
1:A:357:VAL:O	1:A:361:ILE:HG13	2.15	0.46
1:C:220:LEU:HA	1:C:220:LEU:HD23	1.72	0.46
1:C:222:GLU:O	1:C:226:ILE:HG12	2.16	0.46
1:C:146:LEU:HA	1:C:149:ALA:HB2	1.98	0.46
1:A:402:ILE:HG13	1:A:403:LEU:N	2.30	0.46
1:C:264:LEU:HA	1:C:267:MET:HB3	1.97	0.46
1:C:118:GLN:HE21	1:C:131:LEU:HD11	1.81	0.46
1:A:262:ILE:O	1:A:266:LEU:HG	2.15	0.46
1:C:37:ILE:HG21	1:D:187:LEU:HD21	1.98	0.45
1:D:100:ALA:O	1:D:101:LEU:C	2.54	0.45
1:C:242:HIS:CD2	1:C:298:SER:O	2.70	0.45
1:C:6:GLU:OE2	1:C:9:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:C	1:B:8:TYR:CD2	2.90	0.45
1:D:354:VAL:HG12	1:D:355:VAL:N	2.31	0.45
1:C:121:TYR:HB2	1:C:130:ILE:HG23	1.98	0.45
1:A:291:LEU:HD11	1:A:380:VAL:CG1	2.47	0.45
1:D:270:ASN:OD1	1:D:282:ASN:OD1	2.34	0.45
1:B:410:LEU:O	1:B:413:VAL:HG22	2.16	0.45
1:A:204:PHE:HE1	1:A:215:VAL:HG21	1.80	0.45
1:B:316:GLN:HB2	1:B:430:GLU:OE2	2.16	0.45
1:C:71:TYR:HB2	1:C:72:PRO:CD	2.45	0.45
1:D:367:MET:HE3	1:D:375:PRO:HD3	1.98	0.45
1:D:200:ILE:HG22	1:D:212:ILE:HD11	1.97	0.45
1:C:398:ILE:CG2	1:C:398:ILE:O	2.65	0.45
1:D:391:TYR:HB2	1:D:401:VAL:CG2	2.47	0.45
1:B:394:SER:HB3	1:B:397:LYS:HB2	1.97	0.45
1:B:365:PHE:O	1:B:366:ALA:C	2.55	0.45
1:C:85:VAL:HG12	1:C:149:ALA:HA	1.98	0.45
1:A:290:ASP:OD2	1:A:382:TRP:HB3	2.16	0.45
1:A:121:TYR:CE1	1:D:123:MET:HB2	2.52	0.45
1:D:43:LEU:HD12	1:D:378:ALA:CB	2.47	0.45
1:B:170:ILE:HB	1:B:184:PHE:O	2.16	0.45
1:D:325:ILE:HG13	1:D:326:ALA:H	1.82	0.45
1:A:161:ARG:HD2	1:A:162:PHE:N	2.32	0.45
1:B:36:LEU:HD21	1:B:80:MET:CG	2.45	0.45
1:B:340:MET:HB2	1:B:341:PRO:C	2.37	0.45
1:D:6:GLU:HA	1:D:6:GLU:OE2	2.17	0.45
1:B:152:ILE:C	1:B:152:ILE:HD12	2.37	0.45
1:A:386:ILE:O	1:A:404:GLN:NE2	2.50	0.45
1:B:253:THR:HG22	2:B:500:CBS:H1B	1.98	0.45
4:A:700:MAL:H6'2	4:A:700:MAL:O2	2.17	0.45
1:C:407:ASN:C	1:C:409:ALA:H	2.19	0.45
1:A:96:TYR:CD2	1:A:161:ARG:CG	2.94	0.45
1:A:284:ILE:HD11	1:A:364:TYR:CD1	2.51	0.45
1:B:308:MET:HB2	1:B:308:MET:HE2	1.91	0.45
1:C:213:HIS:CD2	1:C:214:ASN:H	2.21	0.44
1:B:146:LEU:HA	1:B:149:ALA:CB	2.47	0.44
1:B:146:LEU:HD21	1:B:264:LEU:HD13	1.99	0.44
1:C:110:THR:HG21	1:C:197:VAL:HG21	2.00	0.44
1:C:20:ARG:HG3	1:C:21:HIS:H	1.81	0.44
1:C:368:GLU:C	1:C:370:GLY:N	2.71	0.44
1:C:146:LEU:HD21	1:C:264:LEU:CD1	2.46	0.44
1:D:182:ARG:O	1:D:185:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:SER:N	1:C:333:ASN:ND2	2.60	0.44
1:D:80:MET:HE2	1:D:80:MET:HB2	1.55	0.44
1:D:203:ILE:O	1:D:207:THR:HG23	2.17	0.44
1:B:382:TRP:CE3	1:B:383:THR:HG22	2.52	0.44
1:C:260:SER:HA	1:C:263:TRP:HB2	2.00	0.44
1:A:115:THR:HA	1:A:116:PRO:HD3	1.76	0.44
1:C:72:PRO:HD3	1:D:198:TRP:CD1	2.52	0.44
1:D:410:LEU:O	1:D:413:VAL:HG22	2.16	0.44
1:B:226:ILE:HG22	1:B:227:LEU:N	2.31	0.44
1:B:260:SER:N	1:B:261:PRO:CD	2.80	0.44
1:C:340:MET:HB3	1:C:341:PRO:C	2.37	0.44
1:D:348:LEU:HA	1:D:348:LEU:HD23	1.74	0.44
1:B:372:VAL:HG11	1:B:403:LEU:HD22	1.99	0.44
1:C:48:LEU:HA	1:C:49:PRO:HD3	1.77	0.44
1:C:206:HIS:O	1:C:207:THR:HG23	2.17	0.44
1:C:91:ARG:C	1:C:93:GLY:N	2.70	0.44
1:C:290:ASP:OD2	1:C:382:TRP:HB3	2.17	0.44
1:A:119:VAL:HB	1:D:123:MET:HE3	1.99	0.44
1:A:284:ILE:HD11	1:A:364:TYR:HD1	1.83	0.44
1:D:309:LEU:O	1:D:310:LEU:HD23	2.17	0.44
1:B:376:SER:HB3	1:B:395:GLY:HA3	1.99	0.44
1:B:85:VAL:HG21	1:B:152:ILE:HD11	1.99	0.44
1:B:331:ASN:ND2	1:B:331:ASN:N	2.65	0.44
1:C:169:ILE:HG23	1:C:185:ALA:HA	1.99	0.44
1:A:36:LEU:HD23	1:A:36:LEU:N	2.32	0.44
1:A:81:ALA:HB2	1:A:146:LEU:N	2.32	0.44
1:A:96:TYR:CE2	1:A:161:ARG:NE	2.85	0.44
1:C:173:PRO:O	1:C:176:VAL:HB	2.17	0.44
1:D:252:ALA:HB2	2:D:500:CBS:O7A	2.17	0.44
1:A:382:TRP:CH2	1:A:383:THR:HG22	2.52	0.44
1:B:367:MET:HA	1:B:372:VAL:O	2.18	0.44
1:D:131:LEU:N	1:D:131:LEU:CD2	2.80	0.44
1:B:306:VAL:O	1:B:310:LEU:HB2	2.17	0.44
1:D:382:TRP:CE3	1:D:383:THR:HG22	2.52	0.44
1:A:176:VAL:HG22	2:B:500:CBS:H62A	1.99	0.44
1:B:368:GLU:C	1:B:370:GLY:N	2.70	0.44
1:C:238:VAL:O	1:C:242:HIS:ND1	2.51	0.44
1:A:96:TYR:CE2	1:A:161:ARG:HG2	2.52	0.44
1:A:293:ILE:O	1:A:295:MET:N	2.50	0.44
1:D:268:ASP:O	1:D:269:GLN:C	2.55	0.44
1:C:46:SER:HB2	1:C:69:LEU:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:HA	1:A:88:ILE:HG12	1.98	0.44
1:A:314:SER:HB3	1:A:423:ASP:OD2	2.18	0.44
1:A:352:PHE:HA	1:A:415:TYR:OH	2.17	0.43
1:A:79:ILE:HG23	1:A:82:LEU:HB3	2.00	0.43
1:C:110:THR:CG2	1:C:197:VAL:HG21	2.48	0.43
1:A:215:VAL:HG13	1:A:216:VAL:N	2.33	0.43
1:A:222:GLU:H	1:A:223:PRO:HD2	1.83	0.43
1:A:361:ILE:C	1:A:363:SER:H	2.21	0.43
1:A:165:GLN:C	1:A:167:LYS:H	2.22	0.43
1:B:349:LEU:HD12	1:B:349:LEU:HA	1.78	0.43
1:B:48:LEU:O	1:B:53:TYR:HD2	2.01	0.43
1:B:207:THR:OG1	1:B:209:PHE:HD2	2.01	0.43
1:B:274:PHE:C	1:B:276:ALA:H	2.22	0.43
1:B:278:GLN:HG2	1:B:279:ASP:H	1.82	0.43
1:A:330:PHE:O	1:A:331:ASN:HB2	2.18	0.43
1:B:10:MET:SD	1:B:247:CYS:HB3	2.58	0.43
1:B:118:GLN:HA	1:B:135:VAL:HG12	2.01	0.43
1:C:147:PHE:HA	1:C:150:MET:CE	2.47	0.43
1:C:391:TYR:CE1	1:C:396:GLY:O	2.72	0.43
1:B:229:ALA:HB2	1:B:266:LEU:CD1	2.48	0.43
1:B:386:ILE:HG23	1:B:387:LEU:HG	2.00	0.43
1:C:375:PRO:O	1:C:376:SER:C	2.57	0.43
1:D:85:VAL:HG12	1:D:107:SER:HB3	1.99	0.43
1:D:56:PHE:CE2	1:D:60:LEU:HD11	2.53	0.43
1:D:32:THR:HG22	1:D:83:ILE:HB	2.01	0.43
1:C:431:LYS:HE2	1:C:433:GLU:CD	2.39	0.43
1:C:113:LEU:HD21	1:C:198:TRP:HB2	2.00	0.43
1:A:310:LEU:HB3	1:A:311:PHE:CE2	2.54	0.43
1:D:146:LEU:O	1:D:150:MET:HG3	2.18	0.43
1:D:260:SER:HA	1:D:263:TRP:HB2	1.99	0.43
1:A:387:LEU:HA	1:A:404:GLN:NE2	2.26	0.43
1:A:246:ALA:CB	1:A:349:LEU:HD21	2.45	0.43
1:C:79:ILE:HG12	1:C:82:LEU:HB3	2.01	0.43
1:A:9:VAL:C	1:A:11:PRO:HD2	2.39	0.43
1:A:146:LEU:HA	1:A:149:ALA:CB	2.49	0.43
1:C:336:VAL:O	1:C:340:MET:HB2	2.18	0.43
1:A:349:LEU:HA	1:A:349:LEU:HD12	1.90	0.43
1:D:291:LEU:HB3	1:D:389:SER:OG	2.18	0.43
1:D:81:ALA:HB3	1:D:141:MET:O	2.18	0.43
1:C:79:ILE:HA	1:C:141:MET:O	2.18	0.43
1:D:65:TRP:CG	1:D:66:ASN:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:VAL:HA	1:D:308:MET:HE2	2.01	0.43
1:D:232:TRP:O	1:D:236:ILE:HG13	2.19	0.43
1:A:219:LEU:N	1:A:219:LEU:HD23	2.34	0.43
1:C:43:LEU:C	1:C:43:LEU:HD13	2.39	0.43
1:C:369:TRP:HB3	1:C:371:LEU:CD1	2.49	0.43
1:C:80:MET:HE1	1:C:264:LEU:HD13	2.00	0.43
1:B:387:LEU:HD22	1:B:401:VAL:HG13	1.99	0.43
1:D:82:LEU:HA	1:D:82:LEU:HD12	1.69	0.43
1:B:3:ARG:HG3	1:B:344:MET:HG3	2.00	0.43
1:B:280:VAL:HA	1:B:281:PRO:HD2	1.86	0.43
1:C:199:ILE:O	1:C:203:ILE:HG13	2.18	0.43
1:D:79:ILE:O	1:D:80:MET:C	2.56	0.42
1:B:320:LEU:CD2	1:B:340:MET:HG2	2.49	0.42
1:D:184:PHE:CD2	1:D:184:PHE:N	2.87	0.42
1:B:354:VAL:O	1:B:357:VAL:HG22	2.19	0.42
1:B:241:VAL:HG12	1:B:242:HIS:ND1	2.34	0.42
1:A:79:ILE:HD12	1:A:79:ILE:HG23	1.77	0.42
1:C:204:PHE:HE1	1:C:215:VAL:HG11	1.83	0.42
1:D:316:GLN:O	1:D:319:SER:HB3	2.19	0.42
1:C:416:LEU:HA	1:C:416:LEU:HD12	1.69	0.42
1:B:325:ILE:HG13	1:B:325:ILE:H	1.70	0.42
1:A:317:LEU:HD11	1:A:422:TRP:CD1	2.51	0.42
1:A:217:GLY:HA2	1:A:221:GLN:HB3	2.01	0.42
1:B:229:ALA:HB2	1:B:266:LEU:HD13	2.02	0.42
1:D:171:LYS:HG3	1:D:171:LYS:O	2.20	0.42
1:A:151:ILE:O	1:A:155:ILE:HB	2.19	0.42
1:A:146:LEU:HA	1:A:149:ALA:HB3	2.00	0.42
1:B:48:LEU:HA	1:B:49:PRO:HD3	1.72	0.42
1:D:426:LYS:HD3	1:D:426:LYS:HA	1.87	0.42
1:A:43:LEU:O	1:A:47:THR:HG23	2.18	0.42
1:B:116:PRO:HB3	1:B:201:ARG:HH21	1.85	0.42
1:C:304:LEU:O	1:C:308:MET:HG3	2.18	0.42
1:C:292:TRP:CD1	1:C:403:LEU:HD23	2.55	0.42
1:B:166:LYS:HA	1:B:166:LYS:HD3	1.50	0.42
1:A:308:MET:HG2	1:A:419:LEU:HD11	2.02	0.42
1:C:369:TRP:CZ3	4:C:700:MAL:H2'	2.55	0.42
1:D:240:LEU:HA	1:D:240:LEU:HD23	1.67	0.42
1:D:98:VAL:HG11	1:D:161:ARG:HA	2.02	0.42
1:A:283:THR:HA	1:A:374:ARG:HG3	2.02	0.42
2:C:500:CBS:H62A	1:D:176:VAL:HG23	2.02	0.42
1:A:381:THR:HG23	1:A:383:THR:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:ILE:O	1:D:328:GLY:N	2.52	0.42
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.76	0.42
1:B:71:TYR:CB	1:B:72:PRO:HD3	2.48	0.42
1:B:110:THR:HG21	1:B:156:SER:OG	2.19	0.42
1:C:383:THR:CG2	1:C:383:THR:O	2.68	0.42
1:B:293:ILE:N	1:B:293:ILE:HD12	2.34	0.42
1:C:36:LEU:HD21	1:C:80:MET:HG2	2.02	0.42
1:A:158:GLU:O	1:A:161:ARG:HG3	2.18	0.42
1:A:312:ALA:HB1	1:A:318:LYS:CB	2.49	0.42
1:A:272:ILE:HG22	1:A:273:ALA:N	2.34	0.42
1:B:300:ALA:HB3	1:B:411:ALA:HB1	2.01	0.42
1:A:163:LEU:CD1	1:A:189:PRO:HA	2.50	0.42
1:C:221:GLN:O	1:C:225:SER:HB2	2.19	0.42
1:C:46:SER:HB2	1:C:69:LEU:HD12	2.02	0.42
1:D:119:VAL:HG13	1:D:137:PRO:HB3	2.01	0.42
1:D:79:ILE:O	1:D:79:ILE:HG22	2.20	0.42
1:D:242:HIS:N	1:D:242:HIS:ND1	2.65	0.42
1:A:205:GLU:HG2	1:A:210:GLY:O	2.20	0.42
1:B:329:ILE:HG22	1:B:330:PHE:CD1	2.55	0.42
1:C:92:LEU:HD23	1:C:157:THR:HB	2.02	0.42
1:B:218:LYS:HD3	1:B:218:LYS:HA	1.90	0.42
1:D:315:GLN:OE1	1:D:315:GLN:HA	2.19	0.42
1:A:287:GLN:H	1:A:287:GLN:NE2	2.18	0.42
1:C:68:ALA:C	1:C:70:GLY:H	2.22	0.42
1:D:34:PRO:O	1:D:38:ILE:HG13	2.19	0.41
1:C:298:SER:HB3	1:C:352:PHE:CE1	2.55	0.41
1:B:176:VAL:HG13	1:B:176:VAL:O	2.20	0.41
1:B:176:VAL:CG2	1:B:177:PRO:HD2	2.50	0.41
1:D:386:ILE:CG2	1:D:387:LEU:N	2.83	0.41
1:D:85:VAL:HG13	1:D:153:ALA:HB2	2.01	0.41
1:D:365:PHE:O	1:D:367:MET:N	2.53	0.41
1:D:375:PRO:C	1:D:377:GLY:H	2.24	0.41
1:B:283:THR:HG23	1:B:367:MET:SD	2.60	0.41
1:A:110:THR:HG22	1:A:152:ILE:HG23	2.02	0.41
1:A:398:ILE:C	1:A:400:GLY:H	2.24	0.41
1:B:416:LEU:HA	1:B:416:LEU:HD12	1.84	0.41
1:B:240:LEU:HA	1:B:240:LEU:HD23	1.86	0.41
1:A:182:ARG:HD3	3:A:443:ZDM:O49	2.18	0.41
1:A:358:VAL:HG12	1:A:359:LEU:N	2.36	0.41
1:B:291:LEU:HD11	1:B:380:VAL:CG1	2.50	0.41
1:A:4:PHE:C	1:A:6:GLU:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:HD13	1:A:364:TYR:CD2	2.55	0.41
1:B:50:ILE:HB	1:B:53:TYR:HB2	2.01	0.41
1:B:107:SER:HA	1:B:110:THR:HB	2.02	0.41
1:A:296:GLY:HA2	1:A:302:LEU:HB2	2.02	0.41
1:B:287:GLN:H	1:B:287:GLN:CD	2.24	0.41
1:B:278:GLN:HG2	1:B:279:ASP:N	2.35	0.41
1:D:20:ARG:HB3	1:D:95:TYR:CZ	2.56	0.41
1:C:336:VAL:O	1:C:337:THR:C	2.59	0.41
1:D:92:LEU:HD23	1:D:157:THR:HB	2.02	0.41
1:A:344:MET:O	1:A:344:MET:HG3	2.20	0.41
1:C:205:GLU:HA	1:C:210:GLY:O	2.21	0.41
1:A:242:HIS:CD2	1:A:356:PRO:HG2	2.55	0.41
1:C:117:PHE:CE1	1:C:136:ILE:CG1	3.02	0.41
1:B:10:MET:CG	1:B:247:CYS:HB3	2.48	0.41
1:A:369:TRP:CB	1:A:371:LEU:HD12	2.49	0.41
1:A:24:ALA:HB1	1:A:92:LEU:HB2	2.01	0.41
1:C:184:PHE:HD2	1:C:184:PHE:H	1.67	0.41
1:D:80:MET:HE1	1:D:143:SER:HA	2.02	0.41
1:A:369:TRP:CZ3	4:A:700:MAL:H2'	2.55	0.41
1:D:309:LEU:CD1	1:D:325:ILE:HG21	2.51	0.41
1:A:412:PHE:O	1:A:416:LEU:HB2	2.20	0.41
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.73	0.41
1:B:43:LEU:HD12	1:B:378:ALA:HB2	2.02	0.41
1:D:217:GLY:HA2	1:D:221:GLN:HB3	2.02	0.41
1:C:382:TRP:HE1	2:C:500:CBS:HN2B	1.69	0.41
1:C:340:MET:HB3	1:C:342:ILE:HG13	2.02	0.41
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.83	0.41
1:A:308:MET:HE3	1:A:321:GLY:N	2.36	0.41
1:B:204:PHE:HA	1:B:207:THR:CG2	2.48	0.41
1:C:37:ILE:HG12	1:C:381:THR:HG23	2.03	0.41
1:A:71:TYR:CB	1:A:72:PRO:HD3	2.50	0.41
1:B:308:MET:HA	1:B:312:ALA:HB2	2.03	0.41
1:A:24:ALA:CB	1:A:92:LEU:HB2	2.51	0.41
1:B:369:TRP:CE3	1:B:369:TRP:N	2.89	0.41
1:D:119:VAL:O	1:D:132:VAL:HG22	2.21	0.41
1:D:376:SER:HB3	1:D:395:GLY:CA	2.51	0.41
1:C:355:VAL:O	1:C:359:LEU:HB2	2.21	0.41
1:B:91:ARG:C	1:B:93:GLY:N	2.73	0.40
1:C:4:PHE:C	1:C:6:GLU:H	2.25	0.40
1:A:117:PHE:HA	1:A:135:VAL:O	2.20	0.40
1:B:335:MET:HE3	1:B:335:MET:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ALA:HB3	1:C:355:VAL:HG11	2.03	0.40
1:A:32:THR:HG21	1:A:84:ALA:HB2	2.01	0.40
1:A:162:PHE:CE2	1:A:166:LYS:HD2	2.56	0.40
1:C:136:ILE:HA	1:C:137:PRO:HD3	1.90	0.40
1:A:120:ALA:O	1:D:123:MET:HG3	2.21	0.40
1:C:417:PRO:HG2	1:C:418:PHE:CD2	2.56	0.40
1:D:122:ILE:HD12	1:D:122:ILE:HA	1.91	0.40
1:D:365:PHE:O	1:D:366:ALA:C	2.59	0.40
1:C:353:ILE:HG22	1:C:353:ILE:O	2.21	0.40
1:D:254:ILE:N	1:D:254:ILE:HD13	2.34	0.40
1:D:30:VAL:HA	1:D:33:MET:HG3	2.03	0.40
1:C:75:ALA:O	1:C:79:ILE:HG21	2.21	0.40
1:C:316:GLN:HE21	1:C:426:LYS:HB3	1.85	0.40
1:C:295:MET:HG2	1:C:386:ILE:HD11	2.03	0.40
1:A:110:THR:HG23	1:A:197:VAL:HG21	2.03	0.40
1:A:331:ASN:N	1:A:331:ASN:HD22	2.19	0.40
1:A:90:TYR:CE2	1:B:101:LEU:HD13	2.55	0.40
1:A:260:SER:HA	1:A:263:TRP:HB2	2.03	0.40
1:B:242:HIS:CD2	1:B:298:SER:O	2.75	0.40
1:D:79:ILE:O	1:D:82:LEU:N	2.52	0.40
1:D:85:VAL:CG2	1:D:149:ALA:HB1	2.51	0.40
1:D:366:ALA:HB1	1:D:372:VAL:CG2	2.51	0.40
1:D:234:ALA:HB2	1:D:284:ILE:CG1	2.52	0.40
1:D:387:LEU:HD21	1:D:405:LEU:HD21	2.03	0.40
1:B:186:ALA:O	1:B:187:LEU:C	2.60	0.40
1:A:433:GLU:HG2	1:A:434:ALA:H	1.87	0.40
1:B:41:ILE:O	1:B:45:ILE:HB	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	430/442 (97%)	339 (79%)	84 (20%)	7 (2%)	12 48
1	B	430/442 (97%)	365 (85%)	60 (14%)	5 (1%)	16 54
1	C	430/442 (97%)	355 (83%)	67 (16%)	8 (2%)	10 45
1	D	434/442 (98%)	353 (81%)	70 (16%)	11 (2%)	7 37
All	All	1724/1768 (98%)	1412 (82%)	281 (16%)	31 (2%)	11 46

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	PRO
1	C	301	THR
1	D	301	THR
1	B	301	THR
1	B	369	TRP
1	A	257	GLY
1	B	150	MET
1	B	177	PRO
1	A	294	TYR
1	C	273	ALA
1	D	177	PRO
1	D	366	ALA
1	A	369	TRP
1	C	5	LEU
1	D	183	SER
1	D	261	PRO
1	D	294	TYR
1	D	386	ILE
1	A	362	VAL
1	C	366	ALA
1	C	369	TRP
1	D	423	ASP
1	D	116	PRO
1	D	137	PRO
1	D	281	PRO
1	B	297	GLY
1	A	256	GLY
1	A	340	MET
1	C	173	PRO
1	C	79	ILE
1	C	297	GLY

5.3.2 Protein sidechains (i)

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	345/361 (96%)	325 (94%)	20 (6%)	25 64
1	B	348/361 (96%)	324 (93%)	24 (7%)	19 57
1	C	346/361 (96%)	327 (94%)	19 (6%)	27 66
1	D	349/361 (97%)	314 (90%)	35 (10%)	9 36
All	All	1388/1444 (96%)	1290 (93%)	98 (7%)	18 55

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	23	LEU
1	A	46	SER
1	A	108	LEU
1	A	146	LEU
1	A	147	PHE
1	A	176	VAL
1	A	213	HIS
1	A	240	LEU
1	A	244	LEU
1	A	267	MET
1	A	272	ILE
1	A	287	GLN
1	A	301	THR
1	A	345	ASN
1	A	354	VAL
1	A	369	TRP
1	A	374	ARG
1	A	410	LEU
1	A	415	TYR
1	B	3	ARG
1	B	4	PHE
1	B	6	GLU
1	B	79	ILE

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Mol	Chain	Res	Type
1	B	118	GLN
1	B	135	VAL
1	B	146	LEU
1	B	147	PHE
1	B	171	LYS
1	B	209	PHE
1	B	213	HIS
1	B	226	ILE
1	B	242	HIS
1	B	264	LEU
1	B	271	ARG
1	B	280	VAL
1	B	301	THR
1	B	329	ILE
1	B	331	ASN
1	B	335	MET
1	B	369	TRP
1	B	374	ARG
1	B	389	SER
1	B	419	LEU
1	C	19	GLN
1	C	23	LEU
1	C	135	VAL
1	C	144	GLN
1	C	146	LEU
1	C	147	PHE
1	C	161	ARG
1	C	205	GLU
1	C	213	HIS
1	C	225	SER
1	C	240	LEU
1	C	264	LEU
1	C	267	MET
1	C	329	ILE
1	C	331	ASN
1	C	354	VAL
1	C	369	TRP
1	C	374	ARG
1	C	415	TYR
1	D	9	VAL
1	D	20	ARG
1	D	44	ILE

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Mol	Chain	Res	Type
1	D	66	ASN
1	D	91	ARG
1	D	108	LEU
1	D	116	PRO
1	D	130	ILE
1	D	131	LEU
1	D	135	VAL
1	D	148	VAL
1	D	156	SER
1	D	168	MET
1	D	169	ILE
1	D	193	VAL
1	D	205	GLU
1	D	211	SER
1	D	235	VAL
1	D	242	HIS
1	D	269	GLN
1	D	271	ARG
1	D	280	VAL
1	D	284	ILE
1	D	287	GLN
1	D	309	LEU
1	D	329	ILE
1	D	340	MET
1	D	359	LEU
1	D	369	TRP
1	D	374	ARG
1	D	388	PHE
1	D	389	SER
1	D	408	PHE
1	D	415	TYR
1	D	425	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	206	HIS
1	A	287	GLN
1	A	316	GLN
1	A	331	ASN
1	A	333	ASN

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Mol	Chain	Res	Type
1	A	345	ASN
1	A	404	GLN
1	B	213	HIS
1	B	221	GLN
1	B	316	GLN
1	B	331	ASN
1	C	118	GLN
1	C	213	HIS
1	C	282	ASN
1	C	316	GLN
1	C	331	ASN
1	C	333	ASN
1	D	66	ASN
1	D	118	GLN
1	D	287	GLN
1	D	331	ASN
1	D	404	GLN

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

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ZDM	A	443	-	31,31,33	1.63	7 (22%)	42,42,44	1.97	14 (33%)
5	CIT	A	444	-	3,12,12	1.24	1 (33%)	3,17,17	2.35	1 (33%)
2	CBS	A	500	-	30,30,30	2.08	10 (33%)	36,43,43	1.44	6 (16%)
3	ZDM	A	600	-	31,31,33	1.65	8 (25%)	42,42,44	1.49	6 (14%)
4	MAL	A	700	-	24,24,24	1.71	4 (16%)	35,35,35	1.31	4 (11%)
5	CIT	B	443	-	3,12,12	1.03	0	3,17,17	1.04	0
2	CBS	B	500	-	30,30,30	2.15	10 (33%)	36,43,43	1.46	7 (19%)
4	MAL	B	700	-	24,24,24	1.74	5 (20%)	35,35,35	1.20	2 (5%)
5	CIT	B	800	-	3,12,12	1.08	0	3,17,17	1.83	1 (33%)
3	ZDM	C	443	-	31,31,33	1.57	6 (19%)	42,42,44	1.78	14 (33%)
5	CIT	C	444	-	3,12,12	1.08	0	3,17,17	0.73	0
5	CIT	C	445	-	3,12,12	1.08	0	3,17,17	1.66	1 (33%)
2	CBS	C	500	-	30,30,30	2.06	9 (30%)	36,43,43	1.40	7 (19%)
3	ZDM	C	600	-	31,31,33	1.57	6 (19%)	42,42,44	1.57	10 (23%)
4	MAL	C	700	-	24,24,24	1.76	4 (16%)	35,35,35	1.22	2 (5%)
5	CIT	C	800	-	3,12,12	1.15	0	3,17,17	1.20	1 (33%)
2	CBS	D	500	-	30,30,30	2.08	10 (33%)	36,43,43	1.43	8 (22%)
4	MAL	D	700	-	24,24,24	1.74	5 (20%)	35,35,35	1.18	3 (8%)
5	CIT	D	800	-	3,12,12	1.07	0	3,17,17	1.57	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZDM	A	443	-	-	0/16/56/58	0/2/2/2
5	CIT	A	444	-	-	0/6/16/16	0/0/0/0
2	CBS	A	500	-	-	0/16/56/56	0/2/2/2
3	ZDM	A	600	-	-	0/16/56/58	0/2/2/2
4	MAL	A	700	-	-	0/8/48/48	0/2/2/2
5	CIT	B	443	-	-	0/6/16/16	0/0/0/0
2	CBS	B	500	-	-	0/16/56/56	0/2/2/2
4	MAL	B	700	-	-	0/8/48/48	0/2/2/2
5	CIT	B	800	-	-	0/6/16/16	0/0/0/0
3	ZDM	C	443	-	-	0/16/56/58	0/2/2/2
5	CIT	C	444	-	-	0/6/16/16	0/0/0/0
5	CIT	C	445	-	-	0/6/16/16	0/0/0/0
2	CBS	C	500	-	-	0/16/56/56	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZDM	C	600	-	-	0/16/56/58	0/2/2/2
4	MAL	C	700	-	-	0/8/48/48	0/2/2/2
5	CIT	C	800	-	-	0/6/16/16	0/0/0/0
2	CBS	D	500	-	-	0/16/56/56	0/2/2/2
4	MAL	D	700	-	-	0/8/48/48	0/2/2/2
5	CIT	D	800	-	-	0/6/16/16	0/0/0/0

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	CBS	C3A-C2A	-5.20	1.42	1.53
2	B	500	CBS	C3A-C2A	-5.18	1.42	1.53
2	C	500	CBS	C3A-C2A	-5.10	1.42	1.53
2	D	500	CBS	C3A-C2A	-4.97	1.43	1.53
3	A	443	ZDM	C7-C8	-4.64	1.40	1.52
3	C	443	ZDM	C7-C8	-4.50	1.40	1.52
3	A	600	ZDM	C7-C8	-4.47	1.40	1.52
3	C	600	ZDM	C7-C8	-4.40	1.40	1.52
4	C	700	MAL	C3'-C2'	-4.38	1.40	1.52
4	B	700	MAL	C3'-C2'	-4.23	1.41	1.52
4	D	700	MAL	C3'-C2'	-4.05	1.41	1.52
2	B	500	CBS	C3B-C2B	-4.05	1.44	1.53
4	A	700	MAL	C3'-C2'	-3.98	1.41	1.52
2	D	500	CBS	C3B-C2B	-3.94	1.45	1.53
2	A	500	CBS	C3B-C2B	-3.91	1.45	1.53
3	A	600	ZDM	C2-C3	-3.76	1.41	1.52
3	C	600	ZDM	C2-C3	-3.76	1.41	1.52
2	A	500	CBS	C3B-C4B	-3.71	1.42	1.52
2	C	500	CBS	C3B-C2B	-3.68	1.45	1.53
3	C	443	ZDM	C2-C3	-3.66	1.42	1.52
2	B	500	CBS	C3B-C4B	-3.64	1.42	1.52
3	A	443	ZDM	C2-C3	-3.60	1.42	1.52
2	D	500	CBS	C3B-C4B	-3.59	1.42	1.52
2	C	500	CBS	C3B-C4B	-3.56	1.42	1.52
4	B	700	MAL	C4-C3	-3.49	1.43	1.52
4	D	700	MAL	C4-C3	-3.46	1.43	1.52
4	B	700	MAL	C3'-C4'	-3.46	1.42	1.52
4	C	700	MAL	C3'-C4'	-3.44	1.42	1.52
4	D	700	MAL	C3'-C4'	-3.41	1.42	1.52
4	A	700	MAL	C4-C3	-3.40	1.43	1.52
4	C	700	MAL	C4-C3	-3.38	1.43	1.52
4	A	700	MAL	C3'-C4'	-3.32	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	CBS	C1B-C2B	-3.30	1.49	1.53
2	D	500	CBS	C1B-C2B	-3.24	1.49	1.53
2	C	500	CBS	C1B-C2B	-2.97	1.49	1.53
2	A	500	CBS	C1B-C2B	-2.89	1.49	1.53
3	A	600	ZDM	C7-C5	-2.62	1.45	1.52
3	A	443	ZDM	C7-C5	-2.57	1.45	1.52
3	C	600	ZDM	C7-C5	-2.54	1.45	1.52
3	C	443	ZDM	C7-C5	-2.54	1.45	1.52
3	A	443	ZDM	C8-C9	-2.46	1.47	1.53
3	A	600	ZDM	C8-C9	-2.41	1.48	1.53
2	D	500	CBS	C1A-C2A	-2.17	1.49	1.53
2	B	500	CBS	O5A-C5A	-2.16	1.38	1.44
2	A	500	CBS	C1A-C2A	-2.11	1.49	1.53
3	A	600	ZDM	C2-C1	-2.07	1.47	1.52
2	A	500	CBS	O3B-C3B	2.00	1.47	1.43
4	D	700	MAL	O3-C3	2.02	1.47	1.43
3	A	600	ZDM	O4-C7	2.02	1.47	1.43
3	A	443	ZDM	O5-C4	2.03	1.49	1.44
2	D	500	CBS	O3B-C3B	2.03	1.47	1.43
4	C	700	MAL	O3'-C3'	2.05	1.47	1.43
4	B	700	MAL	O3-C3	2.06	1.47	1.43
5	A	444	CIT	O7-C3	2.06	1.46	1.43
3	C	443	ZDM	O7-C3	2.07	1.49	1.43
3	C	600	ZDM	O5-C4	2.08	1.49	1.44
3	A	443	ZDM	O4-C7	2.09	1.48	1.43
4	D	700	MAL	O3'-C3'	2.11	1.48	1.43
2	D	500	CBS	C2A-N2A	2.16	1.49	1.45
4	B	700	MAL	O3'-C3'	2.16	1.48	1.43
3	C	600	ZDM	O4-C7	2.18	1.48	1.43
2	B	500	CBS	O3B-C3B	2.19	1.48	1.43
4	A	700	MAL	O3'-C3'	2.19	1.48	1.43
2	C	500	CBS	C2A-N2A	2.20	1.49	1.45
3	A	443	ZDM	O7-C3	2.21	1.49	1.43
3	A	600	ZDM	O5-C4	2.22	1.49	1.44
3	C	600	ZDM	O7-C3	2.24	1.49	1.43
3	C	443	ZDM	O4-C7	2.29	1.48	1.43
2	A	500	CBS	C2A-N2A	2.34	1.49	1.45
3	C	443	ZDM	O5-C4	2.34	1.50	1.44
2	C	500	CBS	O3B-C3B	2.38	1.48	1.43
2	B	500	CBS	C2A-N2A	2.45	1.49	1.45
3	A	600	ZDM	O7-C3	2.47	1.50	1.43
2	C	500	CBS	C7A-N2A	2.63	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	CBS	O5A-C1A	2.65	1.48	1.41
2	A	500	CBS	C7A-N2A	2.69	1.44	1.34
2	D	500	CBS	O5A-C1A	2.77	1.48	1.41
2	B	500	CBS	O5A-C1A	2.79	1.49	1.41
2	D	500	CBS	C7A-N2A	2.81	1.45	1.34
2	C	500	CBS	O5A-C1A	2.85	1.49	1.41
2	B	500	CBS	C7A-N2A	2.92	1.45	1.34
2	A	500	CBS	C7B-N2B	3.37	1.47	1.34
2	D	500	CBS	C7B-N2B	3.40	1.47	1.34
2	C	500	CBS	C7B-N2B	3.41	1.47	1.34
2	B	500	CBS	C7B-N2B	3.51	1.47	1.34

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	800	CIT	C3-C4-C5	-3.13	109.95	114.96
2	A	500	CBS	C6A-C5A-C4A	-2.87	105.94	113.02
2	A	500	CBS	C1A-O1A-C4B	-2.65	111.09	118.01
5	D	800	CIT	C3-C4-C5	-2.64	110.75	114.96
3	A	443	ZDM	O49-C1-C2	-2.63	104.41	110.34
5	C	445	CIT	C3-C2-C1	-2.47	111.01	114.96
3	A	443	ZDM	C10-O7-C3	-2.36	111.84	118.01
2	C	500	CBS	C6A-C5A-C4A	-2.33	107.26	113.02
2	D	500	CBS	C2A-N2A-C7A	-2.30	117.19	123.10
3	C	600	ZDM	C10-O7-C3	-2.26	112.11	118.01
3	C	443	ZDM	C6-O5-C4	-2.22	109.44	113.75
2	D	500	CBS	C1A-O1A-C4B	-2.18	112.31	118.01
3	C	443	ZDM	C2-C3-C4	-2.14	106.01	110.84
4	A	700	MAL	C1-O1-C4'	-2.12	112.46	118.01
2	C	500	CBS	C1A-O1A-C4B	-2.10	112.51	118.01
2	D	500	CBS	C6A-C5A-C4A	-2.08	107.89	113.02
3	A	443	ZDM	O55-C2-C1	-2.06	105.70	110.34
2	B	500	CBS	C1A-O1A-C4B	-2.02	112.74	118.01
5	C	800	CIT	C3-C4-C5	-2.01	111.75	114.96
3	C	600	ZDM	O7-C3-C2	2.00	112.34	107.17
2	C	500	CBS	O6A-C6A-C5A	2.00	117.95	111.33
3	C	443	ZDM	O5-C4-C3	2.01	114.00	109.75
2	D	500	CBS	O6B-C6B-C5B	2.02	117.99	111.33
4	B	700	MAL	O6'-C6'-C5'	2.04	118.07	111.33
3	C	443	ZDM	O55-C2-C3	2.04	114.70	109.87
3	A	600	ZDM	O6-C11-C9	2.04	118.08	111.33
2	A	500	CBS	O5A-C5A-C4A	2.04	113.52	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	600	ZDM	C10-C5-C7	2.05	114.02	109.97
2	A	500	CBS	C1A-O5A-C5A	2.06	117.75	113.75
2	C	500	CBS	C1B-O5B-C5B	2.07	117.29	113.47
4	C	700	MAL	O3'-C3'-C4'	2.07	114.77	109.87
4	D	700	MAL	C2'-C3'-C4'	2.07	114.15	109.60
3	C	600	ZDM	O16-C18-C19	2.08	118.15	109.88
2	B	500	CBS	O6B-C6B-C5B	2.10	118.27	111.33
3	C	600	ZDM	C6-C1-C2	2.10	114.12	109.97
3	C	443	ZDM	O16-C18-C19	2.10	118.25	109.88
4	D	700	MAL	O6-C6-C5	2.11	118.29	111.33
3	C	600	ZDM	O1-C9-C11	2.11	111.68	106.36
2	C	500	CBS	C8A-C7A-N2A	2.11	120.14	116.11
3	C	443	ZDM	O6-C11-C9	2.12	118.32	111.33
2	A	500	CBS	C8A-C7A-N2A	2.15	120.21	116.11
2	B	500	CBS	O6A-C6A-C5A	2.15	118.42	111.33
3	A	600	ZDM	O16-C18-C19	2.17	118.50	109.88
2	D	500	CBS	O6A-C6A-C5A	2.17	118.50	111.33
2	D	500	CBS	C8A-C7A-N2A	2.17	120.27	116.11
2	C	500	CBS	O6B-C6B-C5B	2.19	118.56	111.33
2	B	500	CBS	O1A-C4B-C3B	2.19	112.82	107.17
3	A	443	ZDM	O2-C8-C7	2.19	115.27	110.34
4	A	700	MAL	C3-C4-C5	2.20	114.03	110.20
3	A	600	ZDM	O16-C6-C1	2.20	110.81	108.04
4	A	700	MAL	O6'-C6'-C5'	2.24	118.72	111.33
3	A	443	ZDM	O7-C10-C5	2.25	113.58	108.10
3	C	443	ZDM	O2-C8-C9	2.31	115.37	109.24
2	B	500	CBS	C8A-C7A-N2A	2.32	120.56	116.11
4	D	700	MAL	O1-C1-C2	2.33	113.77	108.10
3	C	443	ZDM	O7-C10-C5	2.33	113.77	108.10
3	A	443	ZDM	O1-C9-C11	2.34	112.26	106.36
2	D	500	CBS	C3B-C2B-N2B	2.34	115.51	110.66
3	A	443	ZDM	O16-C18-C19	2.36	119.27	109.88
3	C	600	ZDM	O16-C6-C1	2.36	111.02	108.04
3	C	443	ZDM	C10-C5-C7	2.38	114.66	109.97
4	B	700	MAL	O1-C1-C2	2.40	113.95	108.10
4	C	700	MAL	O1-C1-C2	2.43	114.02	108.10
3	A	443	ZDM	O3-C5-C10	2.45	115.38	110.02
3	C	443	ZDM	O3-C5-C10	2.47	115.43	110.02
3	A	443	ZDM	O7-C3-C2	2.53	113.69	107.17
2	B	500	CBS	C3B-C2B-N2B	2.55	115.95	110.66
4	A	700	MAL	C2'-C3'-C4'	2.63	115.36	109.60
3	A	443	ZDM	O49-C1-C6	2.67	115.86	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	600	ZDM	O5-C4-C3	2.69	115.42	109.75
3	C	443	ZDM	O7-C3-C2	2.77	114.32	107.17
3	C	600	ZDM	O1-C10-C5	2.82	116.06	110.28
3	C	600	ZDM	O5-C4-C3	2.83	115.72	109.75
3	C	443	ZDM	O1-C10-C5	2.85	116.12	110.28
3	A	443	ZDM	C10-C5-C7	2.86	115.61	109.97
5	A	444	CIT	C3-C2-C1	3.64	120.78	114.96
2	A	500	CBS	O5B-C5B-C4B	3.68	117.51	109.75
3	A	443	ZDM	O1-C10-C5	3.75	117.96	110.28
3	A	600	ZDM	O7-C3-C2	3.82	117.02	107.17
2	B	500	CBS	O5B-C5B-C4B	3.84	117.86	109.75
3	C	443	ZDM	O16-C6-C1	3.94	113.01	108.04
2	D	500	CBS	O5B-C5B-C4B	3.99	118.17	109.75
3	A	600	ZDM	C18-O16-C6	4.33	121.51	113.94
2	C	500	CBS	O5B-C5B-C4B	4.47	119.18	109.75
3	C	443	ZDM	C18-O16-C6	4.52	121.84	113.94
3	A	443	ZDM	O16-C6-C1	4.63	113.89	108.04
3	C	600	ZDM	C18-O16-C6	5.15	122.95	113.94
3	A	443	ZDM	C18-O16-C6	5.26	123.14	113.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	443	ZDM	8	0
2	A	500	CBS	6	0
3	A	600	ZDM	7	0
4	A	700	MAL	3	0
2	B	500	CBS	6	0
3	C	443	ZDM	6	0
5	C	444	CIT	1	0
2	C	500	CBS	8	0
3	C	600	ZDM	7	0
4	C	700	MAL	2	0
2	D	500	CBS	6	0
4	D	700	MAL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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^2)	Q<0.9
1	A	432/442 (97%)	-0.21	10 (2%)	64	57	79, 105, 141, 172	0
1	B	432/442 (97%)	-0.20	8 (1%)	70	63	77, 101, 146, 207	0
1	C	432/442 (97%)	-0.24	6 (1%)	78	73	77, 103, 138, 161	0
1	D	436/442 (98%)	-0.29	7 (1%)	74	69	76, 98, 148, 196	0
All	All	1732/1768 (97%)	-0.24	31 (1%)	71	65	76, 102, 144, 207	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	PRO	7.6
1	D	438	ASN	4.0
1	B	54	SER	3.9
1	A	51	PRO	3.9
1	C	313	ARG	3.3
1	C	311	PHE	3.3
1	A	323	LEU	3.2
1	A	395	GLY	3.0
1	D	209	PHE	3.0
1	B	52	GLY	3.0
1	A	368	GLU	2.7
1	D	51	PRO	2.7
1	A	274	PHE	2.7
1	C	312	ALA	2.6
1	D	436	ALA	2.6
1	B	3	ARG	2.5
1	A	340	MET	2.5
1	D	437	GLU	2.4
1	C	322	ARG	2.3
1	B	55	GLU	2.3
1	D	232	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	276	ALA	2.2
1	A	343	VAL	2.2
1	B	50	ILE	2.1
1	B	8	TYR	2.1
1	A	339	GLY	2.1
1	A	165	GLN	2.1
1	B	424	LYS	2.1
1	C	371	LEU	2.1
1	D	369	TRP	2.0
1	C	66	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	CIT	C	800	13/13	0.76	0.34	1.15	98,116,131,131	0
2	CBS	C	500	29/29	0.95	0.23	1.10	91,104,110,116	0
2	CBS	B	500	29/29	0.95	0.23	0.95	84,99,106,115	0
3	ZDM	C	443	30/32	0.92	0.23	0.85	63,89,101,107	0
2	CBS	A	500	29/29	0.94	0.25	0.84	95,103,112,117	0
5	CIT	C	444	13/13	0.91	0.16	0.77	95,117,125,128	0
5	CIT	A	444	13/13	0.84	0.24	0.72	84,105,124,128	0
3	ZDM	C	600	30/32	0.93	0.23	0.66	72,88,100,105	0
3	ZDM	A	600	30/32	0.89	0.23	0.52	77,92,107,114	0
5	CIT	D	800	13/13	0.87	0.16	0.22	120,131,139,140	0
2	CBS	D	500	29/29	0.95	0.20	0.22	81,97,103,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZDM	A	443	30/32	0.92	0.20	0.16	67,90,99,106	0
5	CIT	B	443	13/13	0.81	0.19	-0.08	120,141,148,148	0
5	CIT	B	800	13/13	0.83	0.18	-0.14	100,114,127,127	0
4	MAL	C	700	23/23	0.87	0.22	-	119,133,147,150	0
5	CIT	C	445	13/13	0.82	0.21	-	151,165,175,176	0
4	MAL	D	700	23/23	0.84	0.49	-	115,129,135,136	0
4	MAL	A	700	23/23	0.78	0.29	-	114,132,138,141	0
4	MAL	B	700	23/23	0.85	0.38	-	123,137,142,144	0

6.5 Other polymers

There are no such residues in this entry.