Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:37 AM GMT

PDB ID	:	2RFY
Title	:	Crystal structure of cellobiohydrolase from Melanocarpus albomyces complexed with cellobiose
Authors	:	Parkkinen, T.; Koivula, A.; Vehmaanper, J.; Rouvinen, J.
Deposited on	:	2007-10-02
Resolution	:	1.70 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 ⓘ symbol.

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

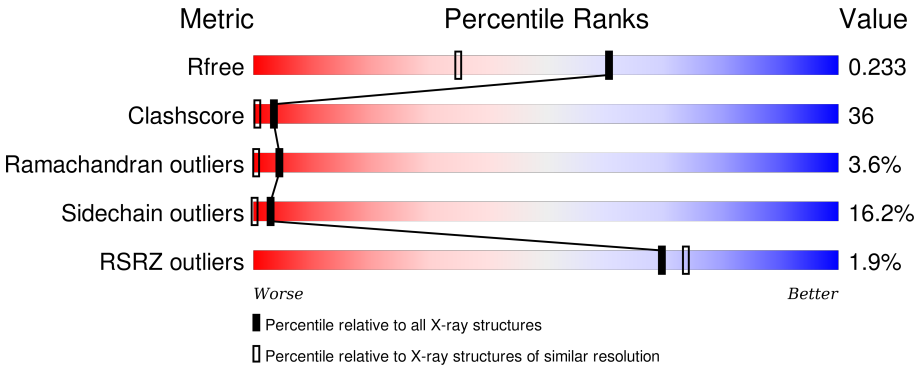
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	430	3% 27% 55% 17%
1	B	430	3% 27% 53% 17%
1	C	430	57% 36% 7%
1	D	430	% 60% 33% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14561 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.

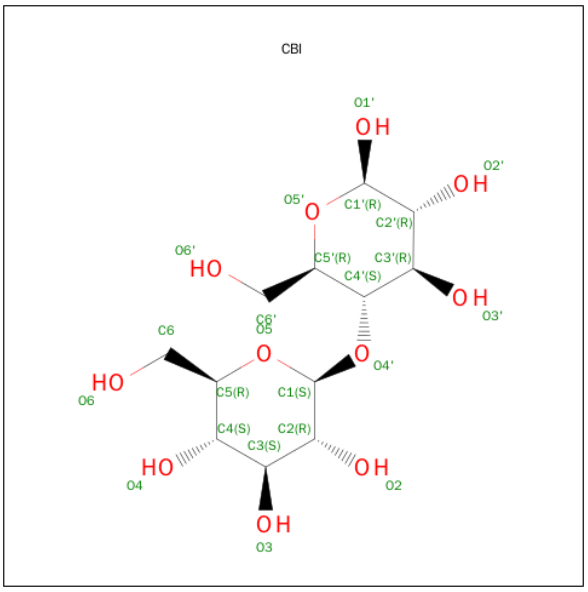
- Molecule 1 is a protein called Cellulose 1,4-beta-cellobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	B	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	C	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	D	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
B	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
C	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
D	1	PCA	GLN	ENGINEERED	UNP Q8J0K6

- Molecule 2 is SUGAR (CELLOBIOSE) (three-letter code: CBI) (formula: $C_{12}H_{22}O_{11}$).



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

- Molecule 3 is water.

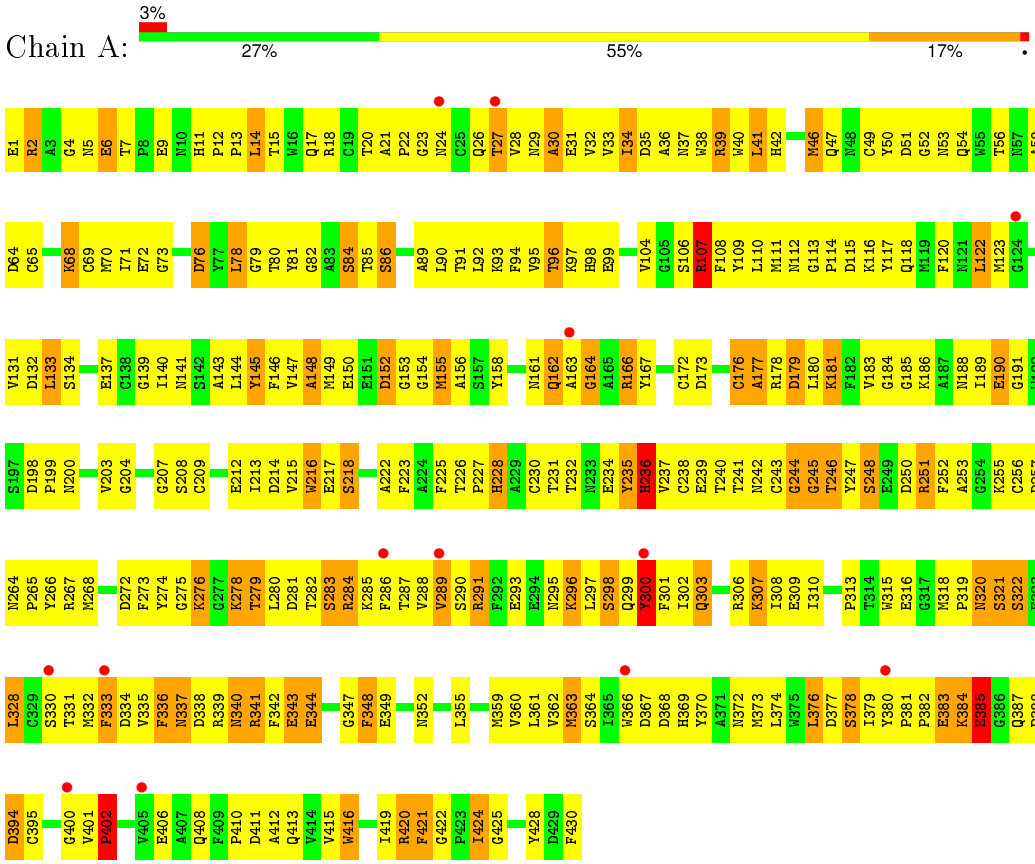
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	224	Total O 224 224	0	0
3	B	255	Total O 255 255	0	0
3	C	319	Total O 319 319	0	0
3	D	339	Total O 339 339	0	0

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.

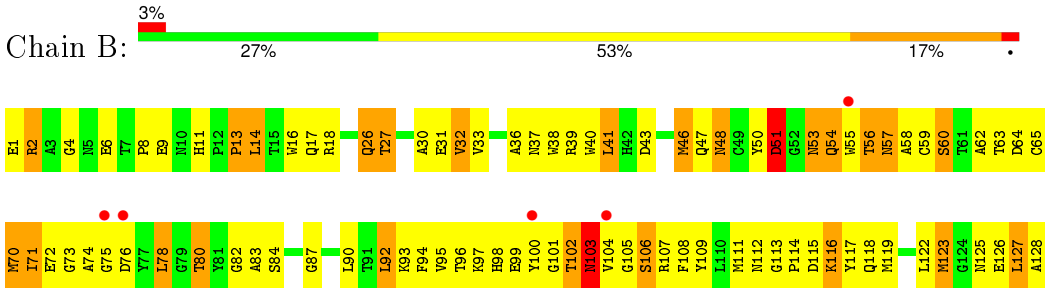
- Molecule 1: Cellulose 1,4-beta-cellobiosidase

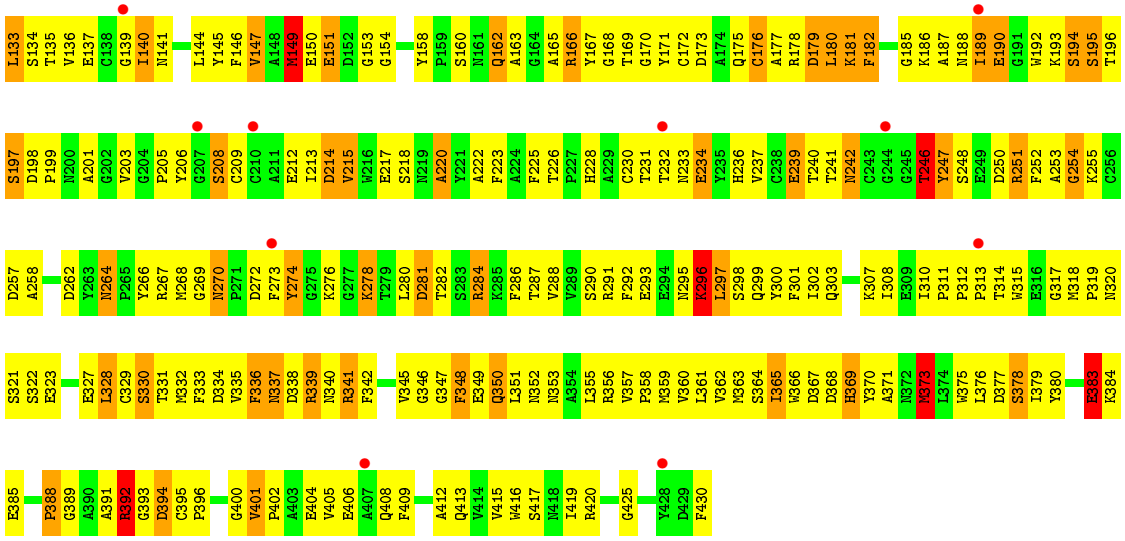
Chain A:



- Molecule 1: Cellulose 1,4-beta-cellobiosidase

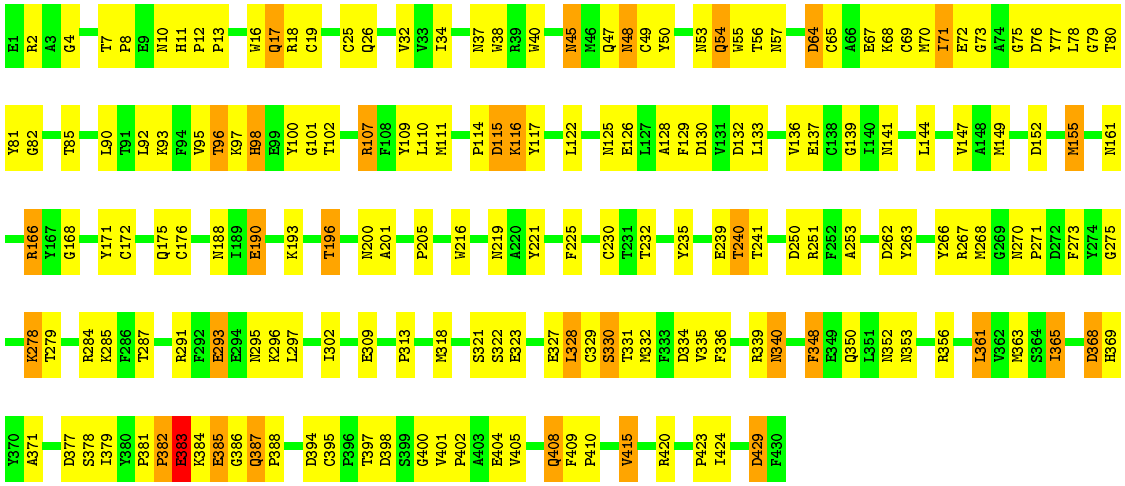
Chain B:





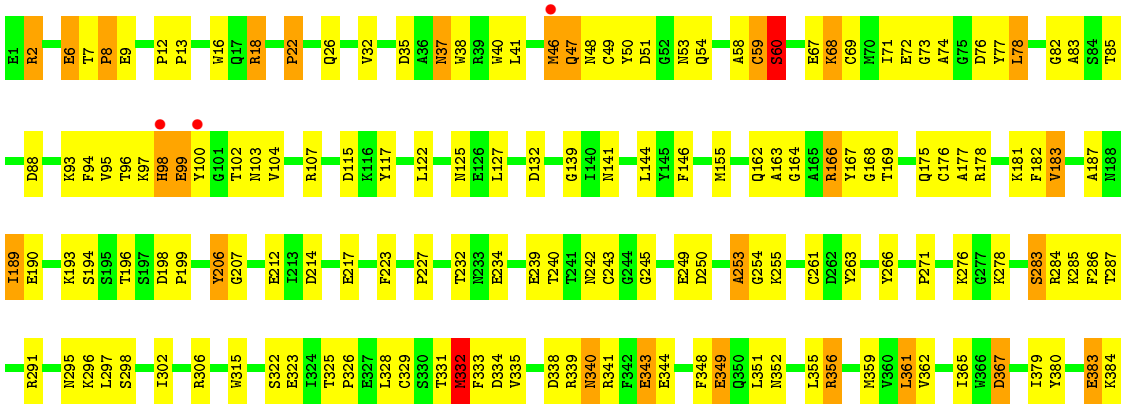
• Molecule 1: Cellulose 1,4-beta-cellobiosidase

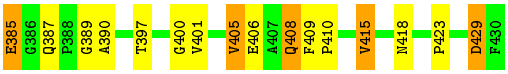
Chain C:



• Molecule 1: Cellulose 1,4-beta-cellobiosidase

Chain D:




E385
G386
Q387
P388
G389
A390
T397
G400
V401
V405
E406
A407
Q408
F409
P410
V415
N418
P423
D429
F430

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.92Å 94.66Å 189.96Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.71 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-1.70) 99.4 (19.71-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.40 (at 1.70Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.185 , 0.238 0.187 , 0.233	Depositor DCC
R_{free} test set	9838 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	9.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 90.4	EDS
Estimated twinning fraction	0.440 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 197103 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14561	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.84% 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: PCA, CBI

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	0.38	0/3416	1.16	15/4648 (0.3%)
1	B	0.38	0/3416	1.16	8/4648 (0.2%)
1	C	0.41	0/3416	1.24	15/4648 (0.3%)
1	D	0.42	0/3416	1.25	14/4648 (0.3%)
All	All	0.40	0/13664	1.20	52/18592 (0.3%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	253	ALA	C-N-CA	-10.42	100.41	122.30
1	D	284	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	C	356	ARG	CD-NE-CZ	9.81	137.34	123.60
1	C	356	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	420	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	B	341	ARG	CD-NE-CZ	8.84	135.97	123.60
1	A	107	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	C	361	LEU	CA-CB-CG	7.80	133.23	115.30
1	C	267	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	336	PHE	C-N-CA	7.50	140.44	121.70
1	D	291	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	C	166	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	D	166	ARG	CD-NE-CZ	7.21	133.69	123.60
1	C	267	ARG	CD-NE-CZ	7.17	133.64	123.60
1	A	251	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	D	284	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	163	ALA	C-N-CA	6.96	136.92	122.30
1	D	253	ALA	O-C-N	-6.77	111.70	123.20
1	A	107	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	239	GLU	C-N-CA	6.57	138.11	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	420	ARG	CD-NE-CZ	6.38	132.53	123.60
1	A	244	GLY	C-N-CA	6.16	135.23	122.30
1	D	339	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	C	77	TYR	CA-CB-CG	6.04	124.87	113.40
1	A	216	TRP	C-N-CA	5.97	136.63	121.70
1	A	235	TYR	CB-CG-CD2	5.95	124.57	121.00
1	B	179	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	300	TYR	CB-CG-CD2	5.88	124.53	121.00
1	D	107	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	D	88	ASP	CB-CG-OD1	5.82	123.53	118.30
1	C	166	ARG	CD-NE-CZ	5.76	131.67	123.60
1	C	107	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	C	339	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	50	TYR	CB-CG-CD2	5.70	124.42	121.00
1	A	39	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	B	336	PHE	C-N-CA	5.56	135.60	121.70
1	D	284	ARG	CD-NE-CZ	5.51	131.32	123.60
1	D	356	ARG	CD-NE-CZ	5.37	131.12	123.60
1	D	367	ASP	CB-CG-OD1	5.33	123.10	118.30
1	D	8	PRO	C-N-CA	5.32	135.01	121.70
1	C	98	HIS	CA-CB-CG	5.32	122.64	113.60
1	B	341	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	77	TYR	CB-CG-CD1	5.26	124.16	121.00
1	B	400	GLY	N-CA-C	5.21	126.13	113.10
1	B	274	TYR	CA-CB-CG	5.21	123.30	113.40
1	A	236	HIS	CA-CB-CG	5.16	122.38	113.60
1	C	235	TYR	CB-CG-CD2	5.16	124.10	121.00
1	A	152	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	329	CYS	C-N-CA	5.10	134.45	121.70
1	D	359	MET	CA-CB-CG	5.06	121.90	113.30
1	B	392	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	195	SER	C-N-CA	5.03	134.28	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3333	0	3028	341	0
1	B	3333	0	3028	357	0
1	C	3333	0	3028	126	0
1	D	3333	0	3028	125	0
2	A	23	0	22	4	0
2	B	23	0	22	5	0
2	C	23	0	22	1	0
2	D	23	0	22	0	0
3	A	224	0	0	22	0
3	B	255	0	0	29	0
3	C	319	0	0	16	0
3	D	339	0	0	16	0
All	All	14561	0	12200	931	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 36.

All (931) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLY:HA2	1:A:70:MET:CE	1.80	1.10
1:A:4:GLY:HA2	1:A:70:MET:HE2	1.37	1.06
1:A:5:ASN:N	1:A:70:MET:CE	2.19	1.04
1:A:286:PHE:HB3	1:A:303:GLN:HG3	1.44	0.97
1:A:4:GLY:CA	1:A:70:MET:HE2	1.95	0.96
1:B:300:TYR:HH	1:B:430:PHE:HD1	1.07	0.95
1:B:53:ASN:HD22	1:B:195:SER:H	1.14	0.94
1:A:34:ILE:HD11	1:A:106:SER:HB2	1.46	0.94
1:A:4:GLY:CA	1:A:70:MET:CE	2.46	0.93
1:D:47:GLN:HG2	1:D:58:ALA:HB2	1.52	0.91
1:A:4:GLY:C	1:A:70:MET:HE3	1.91	0.90
1:A:268:MET:HB3	1:A:313:PRO:HB3	1.53	0.90
1:B:292:PHE:HA	1:B:297:LEU:HD12	1.54	0.88
1:A:296:LYS:HG2	1:A:325:THR:HG22	1.52	0.88
1:B:292:PHE:HB3	1:B:355:LEU:HD22	1.56	0.88
1:A:4:GLY:C	1:A:70:MET:CE	2.43	0.87
1:A:91:THR:HG23	1:A:415:VAL:HG12	1.57	0.86
1:B:233:ASN:HD21	1:B:350:GLN:HE22	1.19	0.86
1:C:295:ASN:H	1:C:352:ASN:HD21	1.19	0.85
1:B:267:ARG:HD2	1:B:392:ARG:HG2	1.59	0.85
1:A:263:TYR:HB2	1:A:324:ILE:HD11	1.59	0.84
1:A:295:ASN:HD22	1:A:326:PRO:HG3	1.38	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:HG22	1:B:103:ASN:HD22	1.43	0.83
1:A:5:ASN:N	1:A:70:MET:HE2	1.94	0.83
1:D:250:ASP:HB3	1:D:253:ALA:HB2	1.59	0.83
1:D:379:ILE:HG21	1:D:385:GLU:HB2	1.61	0.81
1:B:111:MET:HA	1:B:118:GLN:H	1.44	0.80
1:A:372:ASN:HB3	1:A:400:GLY:HA3	1.61	0.80
1:A:287:THR:HB	1:A:302:ILE:HB	1.61	0.80
1:B:31:GLU:HG3	1:B:111:MET:HE3	1.64	0.80
1:B:76:ASP:HB3	1:C:76:ASP:HB2	1.64	0.79
1:B:105:GLY:HA2	1:B:365:ILE:HG23	1.65	0.78
1:B:18:ARG:HD2	1:B:26:GLN:HE22	1.46	0.77
1:B:132:ASP:HB3	1:B:415:VAL:HG22	1.67	0.77
1:D:408:GLN:HG3	3:D:602:HOH:O	1.84	0.77
1:A:22:PRO:HG3	1:A:425:GLY:O	1.83	0.77
1:B:149:MET:SD	1:B:171:TYR:HA	2.23	0.77
1:C:132:ASP:HB3	1:C:415:VAL:HG22	1.67	0.77
1:B:341:ARG:O	1:B:345:VAL:HG13	1.85	0.76
1:A:381:PRO:HB2	1:A:383:GLU:HG2	1.68	0.76
1:A:295:ASN:H	1:A:352:ASN:HD21	1.34	0.76
1:B:290:SER:OG	1:B:299:GLN:HG3	1.85	0.76
1:C:155:MET:HG2	1:C:161:ASN:O	1.85	0.76
1:D:96:THR:OG1	1:D:103:ASN:HB3	1.85	0.76
1:B:63:THR:HA	3:B:576:HOH:O	1.86	0.76
1:B:252:PHE:HA	3:B:462:HOH:O	1.85	0.76
1:D:125:ASN:HD22	1:D:423:PRO:HA	1.50	0.76
1:A:227:PRO:HD2	1:A:261:CYS:O	1.85	0.76
1:A:251:ARG:HD2	3:A:546:HOH:O	1.84	0.75
1:B:267:ARG:HA	1:B:391:ALA:O	1.86	0.75
1:A:131:VAL:O	1:A:285:LYS:HA	1.85	0.75
1:D:295:ASN:H	1:D:352:ASN:HD21	1.34	0.75
1:B:107:ARG:HA	1:B:364:SER:HB3	1.68	0.75
1:C:17:GLN:HG3	1:C:420:ARG:HG2	1.67	0.75
1:C:76:ASP:OD1	1:C:79:GLY:HA3	1.87	0.75
1:B:254:GLY:HA3	3:B:666:HOH:O	1.84	0.75
1:A:132:ASP:HB2	1:A:285:LYS:HG3	1.67	0.74
1:A:137:GLU:O	1:A:140:ILE:HD12	1.86	0.74
1:B:32:VAL:HG12	1:B:109:TYR:O	1.86	0.74
1:A:340:ASN:ND2	1:A:343:GLU:H	1.85	0.74
1:B:233:ASN:HD21	1:B:350:GLN:NE2	1.86	0.73
1:B:154:GLY:O	1:B:158:TYR:HB2	1.87	0.73
1:C:321:SER:OG	1:C:323:GLU:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:TRP:O	1:B:392:ARG:HD3	1.87	0.73
1:A:244:GLY:O	1:A:248:SER:HB2	1.87	0.73
1:B:123:MET:HB3	3:B:498:HOH:O	1.89	0.72
1:A:340:ASN:O	1:A:344:GLU:HG2	1.88	0.72
1:B:198:ASP:HB3	1:B:201:ALA:HB3	1.71	0.72
1:B:297:LEU:HD21	1:B:351:LEU:HD21	1.71	0.72
1:A:321:SER:HA	3:A:478:HOH:O	1.87	0.72
1:C:382:PRO:HG2	1:C:383:GLU:OE1	1.89	0.72
1:A:238:CYS:HB2	1:A:242:ASN:O	1.89	0.72
1:B:272:ASP:O	1:B:278:LYS:HG2	1.90	0.72
1:A:21:ALA:HB3	1:A:24:ASN:HB2	1.71	0.72
1:B:17:GLN:HB2	1:B:420:ARG:HG2	1.70	0.72
1:B:80:THR:O	1:B:96:THR:HG21	1.88	0.72
1:A:42:HIS:ND1	1:A:46:MET:HG3	2.05	0.72
1:A:145:TYR:HB2	1:A:213:ILE:O	1.90	0.71
3:B:669:HOH:O	1:C:8:PRO:HD2	1.88	0.71
1:D:58:ALA:O	1:D:68:LYS:HD2	1.90	0.71
1:A:84:SER:HB2	1:A:91:THR:HB	1.70	0.71
1:B:273:PHE:O	1:B:278:LYS:HB3	1.91	0.70
1:A:266:TYR:HB3	1:A:392:ARG:O	1.92	0.70
1:B:111:MET:HB2	1:B:116:LYS:O	1.90	0.70
1:B:384:LYS:HB2	3:B:564:HOH:O	1.90	0.70
1:A:5:ASN:H	1:A:70:MET:CE	2.05	0.70
1:C:327:GLU:O	1:C:330:SER:HB2	1.92	0.69
1:B:39:ARG:HD3	1:B:72:GLU:O	1.91	0.69
1:D:298:SER:HB3	1:D:323:GLU:HG2	1.72	0.69
1:B:4:GLY:HA2	1:B:70:MET:HE3	1.74	0.69
1:A:340:ASN:HD21	1:A:342:PHE:HB3	1.57	0.69
1:C:114:PRO:HG2	1:C:115:ASP:OD1	1.91	0.69
1:D:99:GLU:HG3	1:D:100:TYR:HD1	1.57	0.69
1:A:56:THR:OG1	1:A:58:ALA:HB3	1.93	0.69
1:B:59:CYS:HB3	1:B:189:ILE:HD13	1.72	0.69
1:A:36:ALA:O	1:A:39:ARG:HB2	1.93	0.69
1:B:182:PHE:HA	1:B:186:LYS:O	1.93	0.69
1:B:331:THR:O	1:B:335:VAL:HG23	1.93	0.69
1:B:109:TYR:OH	1:B:171:TYR:HB2	1.92	0.68
1:B:50:TYR:HA	1:B:55:TRP:HA	1.75	0.68
1:A:153:GLY:HA2	3:A:616:HOH:O	1.93	0.68
1:A:421:PHE:HD2	1:A:422:GLY:H	1.41	0.68
1:A:5:ASN:N	1:A:70:MET:HE3	2.04	0.68
1:B:122:LEU:HD13	1:B:359:MET:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HD2	1:B:26:GLN:NE2	2.07	0.67
1:A:41:LEU:HD23	1:A:71:ILE:HG22	1.76	0.67
1:D:249:GLU:HG2	3:D:723:HOH:O	1.93	0.67
1:B:218:SER:HB2	1:B:222:ALA:O	1.94	0.67
1:B:226:THR:HG21	2:B:431:CBI:O2	1.94	0.67
1:B:144:LEU:HG	1:B:363:MET:HG2	1.76	0.67
1:A:37:ASN:ND2	1:A:180:LEU:HA	2.09	0.67
1:B:160:SER:O	1:B:162:GLN:HG2	1.94	0.67
1:C:11:HIS:HB3	1:C:32:VAL:O	1.94	0.67
1:A:178:ARG:NH1	1:A:243:CYS:HB2	2.09	0.67
1:A:63:THR:HA	1:A:186:LYS:HG2	1.77	0.67
1:A:349:GLU:O	1:A:352:ASN:HB2	1.95	0.66
1:D:22:PRO:HB3	1:D:429:ASP:OD1	1.95	0.66
1:B:239:GLU:HG2	3:B:605:HOH:O	1.96	0.66
1:B:99:GLU:HG3	1:C:40:TRP:HB3	1.77	0.66
1:D:239:GLU:O	1:D:242:ASN:HB2	1.96	0.66
1:D:356:ARG:HG2	1:D:356:ARG:HH11	1.59	0.66
1:C:18:ARG:HD2	3:C:478:HOH:O	1.95	0.66
1:B:195:SER:HB3	1:B:198:ASP:O	1.95	0.66
1:A:319:PRO:HD2	1:A:328:LEU:HD23	1.76	0.66
1:A:5:ASN:H	1:A:70:MET:HE2	1.58	0.65
1:A:291:ARG:O	1:A:297:LEU:HA	1.96	0.65
1:C:387:GLN:HG2	1:C:388:PRO:HD2	1.78	0.65
1:B:378:SER:HA	1:B:393:GLY:O	1.96	0.65
1:B:53:ASN:ND2	1:B:194:SER:HB3	2.10	0.65
1:A:158:TYR:HB3	1:A:184:GLY:O	1.97	0.65
1:B:40:TRP:HB3	1:B:72:GLU:HB2	1.78	0.65
1:B:197:SER:O	1:B:199:PRO:HD3	1.96	0.65
1:B:190:GLU:O	1:B:205:PRO:HD3	1.97	0.65
1:B:286:PHE:HB3	1:B:303:GLN:NE2	2.11	0.65
1:B:177:ALA:HB1	1:B:180:LEU:HG	1.77	0.65
1:B:176:CYS:HA	1:B:208:SER:O	1.97	0.65
1:A:30:ALA:HB1	1:A:111:MET:O	1.97	0.65
1:A:128:ALA:HB3	1:A:420:ARG:HB2	1.78	0.65
1:C:295:ASN:H	1:C:352:ASN:ND2	1.93	0.65
1:B:146:PHE:HA	1:B:360:VAL:O	1.96	0.65
1:A:250:ASP:OD2	1:A:253:ALA:HB2	1.97	0.65
1:D:406:GLU:O	1:D:410:PRO:HD3	1.95	0.65
1:A:99:GLU:HG3	1:D:48:ASN:HD21	1.60	0.65
1:D:178:ARG:HG2	1:D:206:TYR:O	1.96	0.65
1:D:401:VAL:O	1:D:405:VAL:HG22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASP:HB2	1:A:226:THR:O	1.97	0.64
1:B:111:MET:HA	1:B:118:GLN:N	2.11	0.64
1:C:144:LEU:HD12	1:C:363:MET:HG2	1.79	0.64
1:C:293:GLU:HG3	3:C:433:HOH:O	1.98	0.64
1:B:312:PRO:HB3	1:B:321:SER:N	2.13	0.64
1:C:13:PRO:O	1:C:85:THR:HG21	1.98	0.64
1:C:398:ASP:HA	3:C:736:HOH:O	1.97	0.64
1:B:39:ARG:HD2	1:B:71:ILE:HG13	1.79	0.64
1:C:96:THR:HG23	3:C:633:HOH:O	1.96	0.64
1:B:209:CYS:HB2	1:B:236:HIS:NE2	2.13	0.64
1:D:41:LEU:HD12	1:D:181:LYS:HE2	1.80	0.63
1:C:377:ASP:O	1:C:395:CYS:HB2	1.98	0.63
1:A:109:TYR:CD1	1:A:362:VAL:HG22	2.33	0.63
1:B:50:TYR:O	1:B:56:THR:HG23	1.98	0.63
1:A:92:LEU:HD22	1:A:106:SER:OG	1.97	0.63
1:B:175:GLN:HE22	2:B:431:CBI:H4	1.64	0.63
1:A:333:PHE:CE2	1:A:338:ASP:HB3	2.34	0.63
1:B:50:TYR:O	1:B:51:ASP:HB2	1.99	0.63
1:D:132:ASP:HB3	1:D:415:VAL:HG13	1.80	0.63
1:A:251:ARG:HH22	2:A:431:CBI:H61	1.63	0.63
1:A:394:ASP:OD2	3:A:534:HOH:O	2.16	0.63
1:B:33:VAL:HB	1:B:111:MET:HE1	1.80	0.63
1:B:38:TRP:CE2	1:B:106:SER:HA	2.34	0.63
1:A:263:TYR:OH	1:A:322:SER:HA	1.99	0.62
1:B:296:LYS:HE2	1:B:323:GLU:OE2	1.99	0.62
1:B:144:LEU:HD21	1:B:361:LEU:HD11	1.81	0.62
1:B:78:LEU:HD13	1:C:10:ASN:ND2	2.14	0.62
1:B:8:PRO:HG2	1:C:78:LEU:HD21	1.82	0.62
1:A:272:ASP:O	1:A:278:LYS:HG3	2.00	0.62
1:B:349:GLU:O	1:B:352:ASN:HB2	1.99	0.62
1:A:9:GLU:HA	3:A:544:HOH:O	1.98	0.62
1:C:328:LEU:HD22	1:C:332:MET:HG3	1.82	0.62
1:A:21:ALA:HB3	1:A:24:ASN:HD22	1.64	0.62
1:B:11:HIS:HB2	1:B:31:GLU:OE2	2.00	0.62
1:C:190:GLU:HB3	3:C:505:HOH:O	1.99	0.62
1:D:139:GLY:HA3	1:D:400:GLY:HA2	1.81	0.62
1:B:230:CYS:HB2	1:B:232:THR:O	1.99	0.61
1:A:49:CYS:HA	1:A:56:THR:OG1	1.99	0.61
1:B:348:PHE:CE2	1:B:351:LEU:HD23	2.36	0.61
1:B:331:THR:O	1:B:334:ASP:HB2	2.00	0.61
1:D:232:THR:HG22	1:D:234:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LYS:HD2	1:B:430:PHE:CG	2.36	0.61
1:A:37:ASN:HA	1:A:181:LYS:HD2	1.82	0.61
1:B:96:THR:HG22	1:B:103:ASN:HB3	1.82	0.61
1:B:367:ASP:HA	1:B:373:MET:HE2	1.81	0.61
1:D:41:LEU:HB3	1:D:49:CYS:HB2	1.83	0.61
1:A:155:MET:HG3	1:A:164:GLY:HA3	1.83	0.61
1:C:266:TYR:CD2	1:C:271:PRO:HA	2.35	0.61
1:B:108:PHE:O	1:B:362:VAL:HG13	2.01	0.61
1:B:209:CYS:HB2	1:B:236:HIS:CE1	2.36	0.61
1:B:126:GLU:OE1	1:B:291:ARG:HG2	2.01	0.60
1:B:36:ALA:HA	1:B:39:ARG:HG3	1.84	0.60
1:D:99:GLU:HG3	1:D:100:TYR:CD1	2.36	0.60
1:C:429:ASP:HB2	3:C:526:HOH:O	2.00	0.60
1:A:275:GLY:H	1:A:282:THR:HG23	1.67	0.60
1:B:40:TRP:CE3	1:B:72:GLU:HG3	2.37	0.60
1:D:53:ASN:ND2	1:D:194:SER:HB3	2.15	0.60
1:A:4:GLY:CA	1:A:70:MET:HE3	2.24	0.60
1:A:384:LYS:O	1:A:385:GLU:HB3	2.01	0.60
1:B:269:GLY:HA3	1:B:314:THR:HG23	1.83	0.60
1:A:37:ASN:OD1	1:A:181:LYS:HG3	2.02	0.60
1:D:8:PRO:HA	3:D:753:HOH:O	2.01	0.60
1:B:36:ALA:HB1	1:B:71:ILE:HD12	1.84	0.60
1:B:327:GLU:O	1:B:331:THR:HG23	2.02	0.59
1:A:177:ALA:HB1	1:A:180:LEU:HG	1.84	0.59
1:B:408:GLN:HG2	1:B:409:PHE:CD1	2.37	0.59
1:A:333:PHE:HE2	1:A:338:ASP:HB3	1.67	0.59
1:C:2:ARG:HB2	1:C:70:MET:HG2	1.84	0.59
1:A:315:TRP:CH2	1:A:388:PRO:HA	2.36	0.59
1:B:38:TRP:NE1	1:B:106:SER:HA	2.18	0.59
1:A:154:GLY:O	1:A:158:TYR:HB2	2.02	0.59
1:D:276:LYS:NZ	1:D:283:SER:HB2	2.18	0.59
1:B:280:LEU:HD23	1:B:308:ILE:HD13	1.85	0.59
1:C:111:MET:HB3	1:C:116:LYS:O	2.03	0.59
1:A:15:THR:HG22	1:A:29:ASN:ND2	2.18	0.59
1:B:163:ALA:HB1	1:B:167:TYR:HB2	1.84	0.59
1:A:39:ARG:HH12	1:A:73:GLY:HA2	1.68	0.59
1:B:328:LEU:O	1:B:332:MET:HB2	2.03	0.59
1:B:1:PCA:HB3	1:B:182:PHE:CE2	2.37	0.59
1:A:209:CYS:HB2	1:A:236:HIS:CE1	2.37	0.59
1:D:329:CYS:O	1:D:332:MET:HB2	2.03	0.59
1:C:225:PHE:CZ	1:C:297:LEU:HD23	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:TYR:OH	1:C:171:TYR:HB2	2.02	0.58
1:B:41:LEU:HD12	1:B:181:LYS:NZ	2.18	0.58
1:A:108:PHE:O	1:A:362:VAL:HG13	2.03	0.58
1:C:188:ASN:OD1	1:C:205:PRO:HD2	2.02	0.58
1:B:178:ARG:HA	1:B:206:TYR:O	2.03	0.58
1:B:288:VAL:HG12	3:B:436:HOH:O	2.02	0.58
1:A:113:GLY:HA3	3:A:496:HOH:O	2.03	0.58
1:A:21:ALA:HB3	1:A:24:ASN:ND2	2.17	0.58
1:D:163:ALA:HB1	1:D:167:TYR:CD2	2.38	0.58
1:B:270:ASN:ND2	1:B:311:PRO:HB2	2.19	0.58
1:A:307:LYS:HE3	1:A:430:PHE:HB3	1.86	0.58
1:B:119:MET:HG3	1:B:151:GLU:HG2	1.86	0.58
1:B:11:HIS:HB3	1:B:32:VAL:O	2.03	0.58
1:A:363:MET:HB3	1:A:416:TRP:NE1	2.19	0.58
1:B:115:ASP:OD1	1:B:166:ARG:HG2	2.03	0.58
1:D:164:GLY:O	1:D:169:THR:HG23	2.04	0.58
1:A:250:ASP:HA	3:A:535:HOH:O	2.04	0.57
1:A:82:GLY:HA3	1:A:93:LYS:HB2	1.86	0.57
1:B:13:PRO:O	1:B:14:LEU:HB2	2.03	0.57
1:B:396:PRO:HG2	3:B:470:HOH:O	2.04	0.57
1:A:4:GLY:HA2	1:A:70:MET:HG3	1.86	0.57
1:D:132:ASP:HB3	1:D:415:VAL:CG1	2.34	0.57
1:A:39:ARG:NH1	1:A:73:GLY:HA2	2.20	0.57
1:D:266:TYR:CD2	1:D:271:PRO:HA	2.39	0.57
1:A:257:ASP:OD1	1:A:341:ARG:HB3	2.04	0.57
1:B:331:THR:HA	1:B:334:ASP:OD2	2.05	0.57
1:A:368:ASP:HB3	1:A:373:MET:H	1.68	0.57
1:D:349:GLU:OE2	1:D:349:GLU:HA	2.03	0.57
1:B:246:THR:HG22	1:B:370:TYR:CD2	2.40	0.57
1:A:214:ASP:HB2	1:A:226:THR:HB	1.86	0.57
1:D:183:VAL:HG11	1:D:206:TYR:HB3	1.86	0.57
1:B:203:VAL:HG22	1:B:247:TYR:HD1	1.70	0.57
1:C:17:GLN:CG	1:C:420:ARG:HG2	2.33	0.56
1:A:98:HIS:HE1	3:A:612:HOH:O	1.88	0.56
1:B:233:ASN:ND2	1:B:350:GLN:HE22	1.96	0.56
1:D:343:GLU:HG3	3:D:536:HOH:O	2.05	0.56
1:B:98:HIS:HE1	3:B:560:HOH:O	1.88	0.56
1:B:330:SER:HB3	3:B:587:HOH:O	2.04	0.56
1:D:379:ILE:CG2	1:D:385:GLU:HB2	2.34	0.56
1:B:251:ARG:HH11	1:B:251:ARG:HB2	1.68	0.56
1:B:425:GLY:HA2	3:B:671:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:LYS:HE3	3:D:462:HOH:O	2.05	0.56
1:A:195:SER:OG	1:A:198:ASP:HB3	2.05	0.56
1:B:98:HIS:CD2	1:B:101:GLY:H	2.24	0.56
1:A:37:ASN:HD21	1:A:180:LEU:HA	1.70	0.56
1:A:6:GLU:HB2	1:A:72:GLU:OE2	2.06	0.56
1:A:280:LEU:HD13	1:A:280:LEU:O	2.04	0.56
1:B:175:GLN:NE2	2:B:431:CBI:H4	2.20	0.56
1:B:139:GLY:O	1:B:140:ILE:O	2.24	0.56
1:D:16:TRP:CH2	1:D:18:ARG:HG3	2.41	0.56
1:A:109:TYR:HD1	1:A:362:VAL:HG22	1.70	0.56
1:B:274:TYR:CD1	1:B:280:LEU:HD12	2.41	0.55
1:A:47:GLN:NE2	1:A:58:ALA:HB2	2.21	0.55
1:D:340:ASN:ND2	1:D:343:GLU:H	2.04	0.55
1:C:350:GLN:O	1:C:353:ASN:HB2	2.06	0.55
1:B:66:ALA:HB2	1:B:182:PHE:CE1	2.41	0.55
1:D:50:TYR:CG	1:D:181:LYS:HE3	2.41	0.55
1:C:273:PHE:O	1:C:279:THR:HB	2.07	0.55
1:D:389:GLY:HA3	3:D:744:HOH:O	2.05	0.55
1:A:42:HIS:CE1	1:A:46:MET:HG3	2.42	0.55
1:A:145:TYR:O	1:A:361:LEU:HD12	2.06	0.55
1:B:112:ASN:HB2	1:B:118:GLN:OE1	2.07	0.55
1:B:220:ALA:HB1	1:B:282:THR:OG1	2.07	0.55
1:A:172:CYS:O	1:A:173:ASP:HB3	2.06	0.55
1:A:26:GLN:HG2	1:A:27:THR:H	1.72	0.55
1:A:307:LYS:HG3	1:A:430:PHE:CD2	2.42	0.55
1:A:132:ASP:HB3	1:A:415:VAL:CG2	2.37	0.55
1:A:307:LYS:CE	1:A:430:PHE:HB3	2.37	0.55
1:B:115:ASP:HA	1:B:166:ARG:HG2	1.88	0.55
1:B:237:VAL:HG23	3:B:655:HOH:O	2.06	0.54
1:A:50:TYR:OH	1:A:53:ASN:HA	2.06	0.54
1:C:415:VAL:HG23	3:C:592:HOH:O	2.07	0.54
1:B:37:ASN:OD1	1:B:181:LYS:HE3	2.08	0.54
1:B:16:TRP:HE1	1:B:30:ALA:HB2	1.72	0.54
1:B:257:ASP:HB2	1:B:345:VAL:HG11	1.89	0.54
1:A:1:PCA:OE	1:A:185:GLY:HA2	2.06	0.54
1:D:67:GLU:OE1	1:D:67:GLU:HA	2.07	0.54
1:A:5:ASN:HB2	1:A:70:MET:HE1	1.89	0.54
1:B:242:ASN:O	1:B:254:GLY:HA2	2.07	0.54
1:A:274:TYR:CE2	1:A:282:THR:HG21	2.43	0.54
1:B:225:PHE:HB3	3:B:650:HOH:O	2.08	0.54
1:A:2:ARG:O	1:A:70:MET:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:MET:HG3	1:B:113:GLY:O	2.08	0.54
1:A:143:ALA:HB3	1:A:364:SER:OG	2.08	0.54
1:A:128:ALA:HB1	1:A:428:TYR:HE1	1.73	0.54
1:A:128:ALA:HB2	1:A:289:VAL:HG13	1.90	0.54
1:B:375:TRP:HA	1:B:392:ARG:HH11	1.73	0.54
1:A:20:THR:HB	1:B:112:ASN:OD1	2.07	0.54
1:B:281:ASP:HB3	1:B:284:ARG:HG2	1.90	0.54
1:B:317:GLY:O	1:B:331:THR:HB	2.07	0.54
1:B:214:ASP:HB3	1:B:226:THR:HB	1.88	0.54
1:B:228:HIS:HE1	2:B:431:CBI:H2	1.73	0.54
1:A:94:PHE:HB2	1:A:412:ALA:HB3	1.90	0.54
1:A:319:PRO:HA	3:A:506:HOH:O	2.07	0.53
1:A:53:ASN:ND2	1:A:199:PRO:HA	2.23	0.53
1:B:83:ALA:HB1	1:B:92:LEU:HD23	1.88	0.53
1:C:136:VAL:HG12	1:C:219:ASN:HB2	1.90	0.53
1:A:408:GLN:O	1:A:408:GLN:HG2	2.07	0.53
1:A:245:GLY:O	1:A:251:ARG:HG3	2.08	0.53
1:B:175:GLN:OE1	1:B:258:ALA:HB1	2.08	0.53
1:A:147:VAL:HG12	1:A:212:GLU:HA	1.90	0.53
1:B:117:TYR:HD2	1:B:150:GLU:O	1.91	0.53
1:A:50:TYR:HE2	1:A:52:GLY:O	1.91	0.53
1:A:318:MET:HE2	1:A:332:MET:HA	1.90	0.53
1:A:128:ALA:O	1:A:419:ILE:HA	2.09	0.53
1:A:374:LEU:HA	1:A:378:SER:OG	2.09	0.53
1:B:40:TRP:HB3	1:B:72:GLU:CB	2.37	0.53
1:D:13:PRO:O	1:D:85:THR:HG21	2.08	0.53
1:B:117:TYR:HE2	1:B:153:GLY:HA2	1.74	0.53
1:A:372:ASN:HB3	1:A:400:GLY:CA	2.35	0.53
1:B:268:MET:HE3	1:B:328:LEU:HD21	1.90	0.53
1:A:307:LYS:HG3	1:A:430:PHE:CG	2.44	0.53
1:B:96:THR:HG22	1:B:103:ASN:ND2	2.17	0.53
1:B:352:ASN:O	1:B:356:ARG:HD2	2.09	0.53
1:A:373:MET:HG3	1:A:376:LEU:HD23	1.91	0.53
1:C:381:PRO:HG2	1:C:383:GLU:HG3	1.90	0.53
1:A:80:THR:O	1:A:96:THR:HG21	2.08	0.53
1:A:79:GLY:O	1:A:98:HIS:HB3	2.08	0.53
1:A:94:PHE:CD2	1:A:95:VAL:HG23	2.43	0.53
1:C:291:ARG:NE	1:C:424:ILE:HG23	2.23	0.53
1:D:227:PRO:HG3	1:D:297:LEU:HD22	1.91	0.53
1:A:27:THR:HG22	1:A:29:ASN:HD21	1.74	0.53
1:A:327:GLU:HG2	3:A:550:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASP:OD2	1:B:371:ALA:HB3	2.08	0.52
1:C:19:CYS:HA	1:C:25:CYS:HA	1.90	0.52
1:D:254:GLY:HA3	3:D:447:HOH:O	2.10	0.52
1:A:223:PHE:CE2	1:A:265:PRO:HG2	2.44	0.52
1:B:76:ASP:OD1	1:C:76:ASP:HA	2.09	0.52
1:B:90:LEU:HD21	1:B:92:LEU:HD21	1.90	0.52
1:A:114:PRO:O	1:A:166:ARG:HA	2.10	0.52
1:B:130:ASP:HA	1:B:287:THR:HA	1.89	0.52
1:A:127:LEU:HD13	1:A:421:PHE:CD1	2.45	0.52
1:B:179:ASP:HB3	1:B:247:TYR:HE1	1.75	0.52
1:B:246:THR:HB	1:B:247:TYR:CD2	2.44	0.52
1:A:274:TYR:CD1	1:A:280:LEU:HD12	2.44	0.52
1:C:48:ASN:O	1:C:56:THR:HG21	2.09	0.52
1:D:379:ILE:HD13	1:D:397:THR:CG2	2.40	0.52
1:C:166:ARG:HG3	3:C:594:HOH:O	2.08	0.52
1:A:94:PHE:CB	1:A:412:ALA:HB3	2.39	0.52
1:A:132:ASP:HB3	1:A:415:VAL:HG22	1.91	0.52
1:D:96:THR:HG23	3:D:455:HOH:O	2.09	0.52
1:B:55:TRP:CH2	1:B:187:ALA:HB1	2.44	0.52
1:B:377:ASP:O	1:B:395:CYS:HB2	2.10	0.52
1:D:380:TYR:O	1:D:390:ALA:HA	2.10	0.52
1:A:130:ASP:HA	1:A:286:PHE:O	2.09	0.52
1:A:188:ASN:HB3	1:A:204:GLY:HA3	1.91	0.52
1:D:189:ILE:O	1:D:189:ILE:HG13	2.09	0.52
1:B:41:LEU:CD2	1:B:69:CYS:HB3	2.40	0.52
1:A:39:ARG:HD3	1:A:72:GLU:O	2.09	0.52
1:A:63:THR:OG1	1:A:186:LYS:HE2	2.10	0.52
1:B:329:CYS:O	1:B:333:PHE:HD1	1.93	0.52
1:C:53:ASN:HB2	1:C:201:ALA:O	2.10	0.52
1:A:24:ASN:HD21	1:B:116:LYS:NZ	2.08	0.52
1:D:41:LEU:HD22	1:D:69:CYS:HB3	1.91	0.52
1:C:130:ASP:HB3	1:C:285:LYS:HD2	1.92	0.52
1:A:59:CYS:O	1:A:60:SER:HB2	2.10	0.52
1:A:287:THR:HG21	1:A:428:TYR:CZ	2.45	0.51
1:A:295:ASN:HD22	1:A:326:PRO:CG	2.17	0.51
1:C:196:THR:HB	3:C:527:HOH:O	2.10	0.51
1:A:35:ASP:HB3	1:A:38:TRP:CE3	2.45	0.51
1:B:223:PHE:O	1:B:264:ASN:HB2	2.10	0.51
1:B:312:PRO:HA	1:B:321:SER:O	2.11	0.51
1:A:11:HIS:CD2	1:A:33:VAL:HB	2.45	0.51
1:A:9:GLU:OE1	1:A:33:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:CB	1:A:285:LYS:HG3	2.39	0.51
1:B:188:ASN:OD1	1:B:205:PRO:HG2	2.10	0.51
1:B:177:ALA:HB3	1:B:208:SER:OG	2.10	0.51
1:A:179:ASP:OD1	1:A:180:LEU:HD23	2.11	0.51
1:A:155:MET:HG3	1:A:164:GLY:CA	2.39	0.51
1:D:276:LYS:HE3	3:D:614:HOH:O	2.10	0.51
1:A:82:GLY:CA	1:A:93:LYS:HD2	2.41	0.51
1:A:252:PHE:CD2	1:A:339:ARG:HD3	2.46	0.51
1:D:182:PHE:CE1	1:D:187:ALA:HB2	2.46	0.51
1:C:65:CYS:O	1:C:69:CYS:HB2	2.10	0.51
1:A:340:ASN:ND2	1:A:342:PHE:HB3	2.25	0.51
1:B:50:TYR:HH	1:B:192:TRP:HZ2	1.57	0.51
1:B:102:THR:HG22	1:B:102:THR:O	2.10	0.51
1:A:340:ASN:HD22	1:A:343:GLU:H	1.55	0.51
1:B:66:ALA:HB2	1:B:182:PHE:HE1	1.75	0.51
1:A:53:ASN:O	1:A:194:SER:OG	2.29	0.51
1:A:332:MET:O	1:A:336:PHE:HB2	2.11	0.51
1:D:325:THR:HG21	3:D:480:HOH:O	2.09	0.51
1:A:299:GLN:O	1:A:310:ILE:HD13	2.11	0.51
1:B:300:TYR:CD1	1:B:307:LYS:HE3	2.45	0.51
1:B:96:THR:CG2	1:B:103:ASN:HB3	2.41	0.51
1:A:366:TRP:HB3	3:A:562:HOH:O	2.11	0.51
1:D:125:ASN:HD22	1:D:423:PRO:CA	2.19	0.51
1:B:2:ARG:HE	1:B:70:MET:HG2	1.76	0.51
1:C:111:MET:HE1	1:C:166:ARG:HA	1.92	0.51
1:D:40:TRP:CE3	1:D:72:GLU:HG3	2.46	0.51
1:D:379:ILE:HD13	1:D:397:THR:HG23	1.93	0.51
1:A:114:PRO:O	1:A:166:ARG:HB3	2.10	0.51
1:B:315:TRP:CH2	1:B:388:PRO:HA	2.46	0.51
1:B:253:ALA:O	1:B:254:GLY:O	2.29	0.51
1:B:55:TRP:O	1:B:56:THR:O	2.29	0.51
1:A:7:THR:OG1	1:D:98:HIS:HA	2.10	0.50
1:A:80:THR:HG21	1:D:99:GLU:HG2	1.93	0.50
1:B:56:THR:HA	3:B:571:HOH:O	2.12	0.50
1:B:313:PRO:HD2	1:B:319:PRO:O	2.10	0.50
1:B:123:MET:HE3	1:B:123:MET:HA	1.93	0.50
1:A:247:TYR:HD1	1:A:370:TYR:HH	1.59	0.50
1:B:137:GLU:HG3	1:B:409:PHE:CD1	2.47	0.50
1:D:243:CYS:O	1:D:253:ALA:HB3	2.12	0.50
1:B:51:ASP:O	1:B:54:GLN:O	2.30	0.50
1:B:54:GLN:OE1	1:B:192:TRP:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:HG	1:B:84:SER:HB3	1.93	0.50
1:A:373:MET:CG	1:A:376:LEU:HD23	2.42	0.50
1:A:367:ASP:OD2	1:A:406:GLU:OE2	2.30	0.50
1:B:315:TRP:CZ2	1:B:388:PRO:HA	2.47	0.50
1:C:230:CYS:HB2	1:C:232:THR:O	2.11	0.50
1:B:292:PHE:HB3	1:B:355:LEU:CD2	2.35	0.50
1:A:324:ILE:HG22	1:A:324:ILE:O	2.10	0.50
1:A:295:ASN:OD1	1:A:352:ASN:OD1	2.30	0.50
1:B:274:TYR:HD1	1:B:280:LEU:HD12	1.76	0.50
1:D:18:ARG:HH12	1:D:26:GLN:NE2	2.10	0.50
1:C:394:ASP:HA	3:C:457:HOH:O	2.10	0.50
1:B:170:GLY:HA2	3:B:672:HOH:O	2.11	0.50
1:A:139:GLY:HA3	1:A:400:GLY:HA2	1.92	0.50
1:D:59:CYS:O	1:D:60:SER:HB3	2.11	0.50
1:A:331:THR:O	1:A:334:ASP:OD1	2.29	0.50
1:A:301:PHE:HB2	1:A:308:ILE:HB	1.94	0.50
1:B:96:THR:CG2	1:B:103:ASN:HD22	2.17	0.50
1:A:147:VAL:HG23	1:A:147:VAL:O	2.11	0.50
1:A:173:ASP:HB2	1:A:212:GLU:OE1	2.11	0.50
1:A:291:ARG:HD2	1:A:298:SER:HB3	1.94	0.50
1:D:104:VAL:HG21	1:D:406:GLU:OE1	2.12	0.50
1:A:288:VAL:O	1:A:288:VAL:HG12	2.12	0.50
1:A:257:ASP:HA	1:A:341:ARG:HG3	1.93	0.50
1:B:8:PRO:HD2	1:C:78:LEU:HD21	1.94	0.50
1:B:376:LEU:O	1:B:376:LEU:HD12	2.10	0.50
1:A:82:GLY:HA2	1:A:93:LYS:HD2	1.93	0.50
1:B:402:PRO:O	1:B:406:GLU:HB2	2.12	0.50
1:B:8:PRO:O	1:B:73:GLY:O	2.30	0.50
1:A:111:MET:O	1:A:118:GLN:HB2	2.11	0.50
1:B:342:PHE:O	1:B:347:GLY:HA2	2.11	0.50
1:D:331:THR:O	1:D:334:ASP:HB2	2.12	0.50
1:C:49:CYS:O	1:C:56:THR:HG23	2.12	0.49
1:C:64:ASP:O	1:C:68:LYS:HB2	2.12	0.49
1:B:144:LEU:CD1	1:B:363:MET:HG2	2.43	0.49
1:B:377:ASP:HB2	1:B:395:CYS:SG	2.52	0.49
1:D:2:ARG:HA	1:D:162:GLN:HB2	1.92	0.49
1:C:45:ASN:OD1	1:C:47:GLN:OE1	2.30	0.49
1:B:58:ALA:O	1:B:68:LYS:HD2	2.12	0.49
1:A:232:THR:O	1:A:232:THR:HG22	2.11	0.49
1:A:1:PCA:OE	1:A:161:ASN:HB2	2.12	0.49
1:C:137:GLU:HG3	1:C:409:PHE:CD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:GLU:OE2	1:D:214:ASP:OD1	2.30	0.49
1:B:46:MET:HG2	1:C:97:LYS:HD3	1.94	0.49
1:A:144:LEU:CD2	1:A:361:LEU:HD11	2.42	0.49
1:A:225:PHE:CE1	1:A:299:GLN:HB2	2.48	0.49
1:B:350:GLN:O	1:B:350:GLN:OE1	2.30	0.49
1:B:133:LEU:HD21	1:B:286:PHE:CZ	2.47	0.49
1:B:278:LYS:O	1:B:281:ASP:OD2	2.30	0.49
1:B:107:ARG:HA	1:B:364:SER:CB	2.41	0.49
1:B:274:TYR:C	1:B:278:LYS:HD2	2.33	0.49
1:A:321:SER:HB2	3:A:498:HOH:O	2.12	0.49
1:B:268:MET:O	1:B:313:PRO:HA	2.12	0.49
1:D:155:MET:HG3	1:D:164:GLY:CA	2.43	0.49
1:D:18:ARG:HH12	1:D:26:GLN:HE22	1.61	0.49
1:B:346:GLY:O	1:B:350:GLN:HB2	2.13	0.49
1:B:95:VAL:HG22	1:B:104:VAL:HA	1.94	0.49
1:B:106:SER:O	1:B:364:SER:HB2	2.12	0.49
1:B:160:SER:OG	1:B:185:GLY:O	2.30	0.49
1:B:214:ASP:OD2	1:B:217:GLU:OE2	2.30	0.49
1:D:367:ASP:OD2	1:D:406:GLU:OE2	2.30	0.49
1:B:266:TYR:OH	1:B:394:ASP:OD2	2.30	0.49
1:C:82:GLY:CA	1:C:96:THR:HG21	2.42	0.49
1:A:4:GLY:C	1:A:70:MET:HE2	2.18	0.49
1:A:134:SER:HB3	1:A:283:SER:O	2.13	0.49
1:A:216:TRP:CZ3	1:A:288:VAL:HG11	2.48	0.49
1:C:136:VAL:HG12	1:C:219:ASN:CB	2.43	0.49
1:A:189:ILE:HG13	3:A:620:HOH:O	2.13	0.49
1:B:53:ASN:HD22	1:B:195:SER:N	1.97	0.49
1:A:150:GLU:HB2	3:A:616:HOH:O	2.12	0.49
1:B:78:LEU:O	1:B:82:GLY:HA2	2.13	0.49
1:B:295:ASN:H	1:B:352:ASN:HD21	1.61	0.49
1:D:227:PRO:HD2	1:D:261:CYS:O	2.13	0.49
1:C:268:MET:O	1:C:313:PRO:HA	2.13	0.49
1:C:250:ASP:HB3	1:C:253:ALA:HB2	1.94	0.49
1:A:41:LEU:CD1	1:A:49:CYS:HB2	2.43	0.48
1:A:110:LEU:HD12	1:A:111:MET:H	1.78	0.48
1:A:273:PHE:O	1:A:278:LYS:HB3	2.13	0.48
1:D:97:LYS:HG2	1:D:102:THR:OG1	2.13	0.48
1:A:287:THR:HG21	1:A:428:TYR:CE1	2.47	0.48
1:B:103:ASN:OD1	1:B:105:GLY:O	2.30	0.48
1:C:415:VAL:HG21	3:C:535:HOH:O	2.12	0.48
1:A:381:PRO:HB2	1:A:383:GLU:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ALA:HB3	1:C:420:ARG:HB2	1.94	0.48
1:C:114:PRO:O	1:C:166:ARG:HG2	2.13	0.48
1:B:65:CYS:O	1:B:69:CYS:HB2	2.14	0.48
1:A:112:ASN:O	1:A:116:LYS:HG2	2.13	0.48
1:A:95:VAL:O	1:A:95:VAL:HG12	2.13	0.48
1:D:198:ASP:HA	1:D:199:PRO:HD3	1.66	0.48
1:D:255:LYS:HE2	3:D:698:HOH:O	2.13	0.48
1:B:213:ILE:O	1:B:215:VAL:HG23	2.13	0.48
1:A:325:THR:OG1	1:A:327:GLU:OE1	2.30	0.48
1:C:132:ASP:CB	1:C:415:VAL:HG22	2.40	0.48
1:A:147:VAL:C	1:A:359:MET:HB3	2.34	0.48
1:A:172:CYS:HA	1:A:208:SER:O	2.13	0.48
1:D:183:VAL:HG12	1:D:183:VAL:O	2.13	0.48
1:C:139:GLY:HA3	1:C:400:GLY:HA2	1.95	0.48
1:A:4:GLY:HA2	1:A:70:MET:CG	2.42	0.48
1:B:146:PHE:HB3	1:B:359:MET:HB3	1.96	0.48
1:B:144:LEU:HD21	1:B:361:LEU:CD1	2.43	0.48
1:B:213:ILE:O	1:B:213:ILE:HG22	2.13	0.48
1:B:307:LYS:HD2	1:B:430:PHE:CD2	2.49	0.48
1:A:104:VAL:HG11	1:A:406:GLU:HG2	1.96	0.48
1:B:98:HIS:CD2	1:B:100:TYR:H	2.31	0.48
1:A:56:THR:HG1	1:A:58:ALA:HB3	1.79	0.48
1:B:144:LEU:CG	1:B:363:MET:HG2	2.42	0.48
1:A:320:ASN:HB2	3:A:565:HOH:O	2.14	0.48
1:A:129:PHE:CD1	1:A:144:LEU:HD13	2.49	0.48
1:C:295:ASN:HA	1:C:348:PHE:CE2	2.48	0.48
1:B:154:GLY:HA2	3:B:616:HOH:O	2.13	0.48
1:B:280:LEU:HD22	1:B:303:GLN:OE1	2.13	0.48
1:B:122:LEU:HD11	1:B:146:PHE:CD1	2.48	0.48
1:A:49:CYS:HA	1:A:56:THR:HG1	1.78	0.48
1:A:368:ASP:HB3	1:A:373:MET:N	2.29	0.48
1:C:7:THR:HB	1:C:72:GLU:OE1	2.14	0.48
1:B:383:GLU:HA	1:B:383:GLU:OE2	2.05	0.48
1:C:117:TYR:OH	1:C:168:GLY:HA2	2.14	0.48
1:C:147:VAL:HG23	1:C:149:MET:HG3	1.95	0.47
1:A:223:PHE:O	1:A:264:ASN:HA	2.14	0.47
1:D:82:GLY:CA	1:D:96:THR:HG21	2.44	0.47
1:A:81:TYR:OH	1:D:99:GLU:OE2	2.32	0.47
1:B:48:ASN:HD22	1:B:50:TYR:H	1.62	0.47
1:D:285:LYS:HG2	1:D:286:PHE:N	2.29	0.47
1:A:295:ASN:HA	1:A:348:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:PHE:HD1	1:B:308:ILE:HG22	1.79	0.47
1:A:217:GLU:O	1:A:218:SER:HB3	2.15	0.47
1:D:47:GLN:CG	1:D:58:ALA:HB2	2.36	0.47
1:A:130:ASP:OD1	1:A:287:THR:OG1	2.30	0.47
1:A:341:ARG:HA	1:A:341:ARG:HD2	1.50	0.47
1:C:126:GLU:HG2	1:C:424:ILE:HA	1.96	0.47
1:A:384:LYS:HG3	1:A:385:GLU:O	2.14	0.47
1:B:371:ALA:HB1	1:B:380:TYR:CE1	2.49	0.47
1:B:6:GLU:HG3	1:B:72:GLU:OE2	2.15	0.47
1:A:122:LEU:HD23	1:A:359:MET:HE3	1.97	0.47
1:A:274:TYR:HD1	1:A:280:LEU:HD12	1.78	0.47
1:B:351:LEU:HG	1:B:355:LEU:HD12	1.96	0.47
1:A:263:TYR:CB	1:A:324:ILE:HD11	2.38	0.47
1:D:7:THR:HG22	1:D:8:PRO:O	2.15	0.47
1:B:144:LEU:HA	1:B:362:VAL:O	2.15	0.47
1:B:136:VAL:HG13	1:B:140:ILE:CG2	2.45	0.47
1:A:17:GLN:HB3	1:A:26:GLN:O	2.15	0.47
1:A:276:LYS:HD3	3:A:510:HOH:O	2.15	0.47
1:A:52:GLY:O	1:A:200:ASN:HA	2.15	0.47
1:B:16:TRP:HB2	1:B:419:ILE:HG22	1.96	0.47
1:C:275:GLY:O	1:C:278:LYS:HB2	2.15	0.47
1:C:101:GLY:O	1:C:102:THR:OG1	2.31	0.47
1:B:122:LEU:HD21	1:B:146:PHE:CD1	2.50	0.46
1:B:228:HIS:CE1	2:B:431:CBI:H2	2.50	0.46
1:A:231:THR:OG1	1:A:255:LYS:HD2	2.15	0.46
1:B:365:ILE:O	1:B:365:ILE:HG23	2.15	0.46
1:D:181:LYS:HD2	3:D:689:HOH:O	2.14	0.46
1:B:130:ASP:O	1:B:131:VAL:HB	2.14	0.46
1:A:155:MET:HA	1:A:161:ASN:O	2.15	0.46
1:B:56:THR:HG22	3:B:571:HOH:O	2.14	0.46
1:D:53:ASN:CG	1:D:194:SER:HB3	2.36	0.46
1:D:356:ARG:HG2	1:D:356:ARG:NH1	2.30	0.46
1:B:140:ILE:HD11	1:B:405:VAL:HG12	1.97	0.46
1:B:383:GLU:HB2	3:B:642:HOH:O	2.16	0.46
1:B:231:THR:OG1	1:B:255:LYS:HB3	2.15	0.46
1:B:127:LEU:HG	1:B:128:ALA:N	2.31	0.46
1:A:387:GLN:HB3	1:A:388:PRO:HD2	1.98	0.46
1:A:263:TYR:CZ	1:A:322:SER:HA	2.50	0.46
1:B:181:LYS:HB2	1:B:181:LYS:HE3	1.47	0.46
1:B:147:VAL:HB	1:B:172:CYS:O	2.15	0.46
1:D:356:ARG:HD2	3:D:644:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:PHE:HA	1:C:388:PRO:O	2.14	0.46
1:B:349:GLU:HA	1:B:352:ASN:HB2	1.97	0.46
1:A:315:TRP:CZ3	1:A:388:PRO:HA	2.50	0.46
1:A:137:GLU:C	1:A:140:ILE:HD12	2.35	0.46
1:A:30:ALA:HB3	1:A:110:LEU:HD11	1.98	0.46
1:A:112:ASN:HB2	1:A:118:GLN:HA	1.98	0.46
1:B:339:ARG:HD3	1:B:339:ARG:HA	1.51	0.46
1:B:190:GLU:HG3	3:B:677:HOH:O	2.16	0.46
1:C:137:GLU:OE2	1:C:221:TYR:OH	2.32	0.46
1:C:80:THR:HG23	1:C:98:HIS:ND1	2.31	0.46
1:D:379:ILE:HD11	3:D:763:HOH:O	2.16	0.46
1:B:298:SER:O	1:B:299:GLN:HB2	2.14	0.46
1:C:17:GLN:OE1	1:C:420:ARG:NE	2.49	0.46
1:A:281:ASP:OD1	1:A:283:SER:OG	2.31	0.46
1:A:296:LYS:CG	1:A:325:THR:HG22	2.37	0.46
1:B:284:ARG:HE	1:B:284:ARG:HB3	1.58	0.46
1:A:47:GLN:HE21	1:A:58:ALA:HB2	1.81	0.46
1:A:137:GLU:H	1:A:140:ILE:CD1	2.29	0.45
1:B:286:PHE:HB3	1:B:303:GLN:HE21	1.80	0.45
1:B:2:ARG:O	1:B:70:MET:HA	2.16	0.45
1:A:179:ASP:HB3	1:A:247:TYR:CZ	2.51	0.45
1:B:353:ASN:HA	1:B:356:ARG:HD2	1.98	0.45
1:A:382:PRO:O	1:A:384:LYS:N	2.49	0.45
1:B:287:THR:O	1:B:301:PHE:HA	2.15	0.45
1:B:59:CYS:CB	1:B:189:ILE:HD13	2.43	0.45
1:B:136:VAL:HG13	1:B:140:ILE:HG22	1.98	0.45
1:B:321:SER:OG	1:B:322:SER:N	2.49	0.45
1:A:117:TYR:HB3	1:A:360:VAL:HG22	1.98	0.45
1:D:383:GLU:HA	1:D:383:GLU:OE2	2.15	0.45
1:A:264:ASN:OD1	1:A:266:TYR:N	2.49	0.45
1:A:380:TYR:O	1:A:392:ARG:NH2	2.50	0.45
1:B:375:TRP:CA	1:B:392:ARG:HH11	2.29	0.45
1:B:251:ARG:HG2	1:B:252:PHE:CD2	2.52	0.45
1:A:257:ASP:OD2	1:A:342:PHE:HA	2.15	0.45
1:D:50:TYR:O	1:D:51:ASP:OD2	2.35	0.45
1:C:251:ARG:NH2	2:C:431:CBI:O3'	2.50	0.45
1:A:107:ARG:O	1:A:107:ARG:HG3	2.16	0.45
1:B:96:THR:HG23	1:B:96:THR:O	2.16	0.45
1:B:409:PHE:HD2	3:B:654:HOH:O	2.00	0.45
1:A:300:TYR:HA	1:A:310:ILE:HD12	1.99	0.45
1:B:53:ASN:HB2	1:B:194:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ARG:HB3	1:B:203:VAL:HG13	1.97	0.45
1:B:251:ARG:HG2	1:B:252:PHE:CE2	2.51	0.45
1:B:139:GLY:N	1:B:377:ASP:OD2	2.49	0.45
1:D:183:VAL:HG11	1:D:207:GLY:H	1.81	0.45
1:C:340:ASN:HB3	3:C:728:HOH:O	2.15	0.45
1:C:385:GLU:OE2	1:C:386:GLY:N	2.50	0.45
1:A:21:ALA:HB3	1:A:24:ASN:CB	2.42	0.45
1:A:21:ALA:O	1:A:23:GLY:N	2.50	0.45
1:B:41:LEU:O	1:B:48:ASN:ND2	2.49	0.45
1:B:185:GLY:O	1:B:186:LYS:HD3	2.17	0.45
1:A:148:ALA:N	1:A:359:MET:HB3	2.32	0.45
1:A:147:VAL:O	1:A:149:MET:N	2.49	0.45
1:B:339:ARG:HB3	3:B:622:HOH:O	2.16	0.45
1:A:377:ASP:O	1:A:395:CYS:HB2	2.15	0.45
1:D:418:ASN:ND2	3:D:487:HOH:O	2.49	0.45
1:C:54:GLN:NE2	1:C:55:TRP:O	2.50	0.45
1:C:57:ASN:ND2	3:C:723:HOH:O	2.50	0.45
1:B:297:LEU:CD2	1:B:351:LEU:HD21	2.45	0.45
1:A:341:ARG:NH1	1:A:344:GLU:OE1	2.49	0.45
1:B:9:GLU:OE2	1:B:39:ARG:NH1	2.50	0.45
1:C:400:GLY:HA2	1:C:405:VAL:HG11	1.97	0.45
1:C:278:LYS:HA	1:C:278:LYS:HD2	1.69	0.45
1:C:309:GLU:OE1	1:D:306:ARG:NE	2.50	0.45
1:D:76:ASP:OD2	1:D:78:LEU:N	2.49	0.45
1:A:99:GLU:HG3	1:D:48:ASN:ND2	2.30	0.45
1:D:287:THR:HB	1:D:302:ILE:HB	1.97	0.45
1:C:4:GLY:N	1:C:71:ILE:O	2.50	0.45
1:C:152:ASP:OD2	1:C:155:MET:N	2.50	0.45
1:A:251:ARG:NH2	2:A:431:CBI:H61	2.31	0.45
1:A:41:LEU:HD13	1:A:69:CYS:HB3	1.99	0.45
1:B:240:THR:OG1	1:B:241:THR:N	2.49	0.45
1:D:276:LYS:HG2	1:D:283:SER:HB3	1.99	0.45
1:B:196:THR:HB	3:B:468:HOH:O	2.16	0.45
1:D:175:GLN:O	1:D:245:GLY:HA3	2.17	0.45
1:A:281:ASP:O	1:A:303:GLN:NE2	2.50	0.45
1:B:101:GLY:O	1:B:102:THR:OG1	2.30	0.45
1:B:56:THR:OG1	1:B:57:ASN:N	2.50	0.45
1:B:318:MET:HG2	1:B:331:THR:OG1	2.17	0.45
1:A:177:ALA:HB3	1:A:208:SER:OG	2.17	0.45
1:B:270:ASN:OD1	1:B:270:ASN:N	2.50	0.45
1:D:2:ARG:NH1	1:D:67:GLU:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ALA:O	1:A:364:SER:N	2.49	0.45
1:D:117:TYR:OH	1:D:168:GLY:HA2	2.16	0.45
1:C:107:ARG:HD3	1:C:107:ARG:HH11	1.64	0.45
1:C:404:GLU:O	1:C:408:GLN:HG2	2.17	0.44
1:C:7:THR:HG21	1:C:73:GLY:O	2.16	0.44
1:B:93:LYS:HG3	3:B:454:HOH:O	2.16	0.44
1:D:315:TRP:HB3	1:D:335:VAL:HG11	1.99	0.44
1:B:366:TRP:HB3	3:B:492:HOH:O	2.17	0.44
1:D:379:ILE:HD12	1:D:379:ILE:N	2.32	0.44
1:A:71:ILE:HG13	1:A:167:TYR:HD1	1.81	0.44
1:B:357:VAL:HG13	1:B:358:PRO:HD2	1.97	0.44
1:D:361:LEU:HD12	1:D:362:VAL:N	2.31	0.44
1:D:35:ASP:HB3	1:D:38:TRP:CE3	2.53	0.44
1:D:35:ASP:OD2	1:D:37:ASN:HB2	2.16	0.44
1:A:109:TYR:CE1	1:A:362:VAL:HG22	2.52	0.44
1:B:307:LYS:HD2	1:B:430:PHE:HB3	1.99	0.44
1:B:380:TYR:HB3	1:B:392:ARG:NH1	2.32	0.44
1:B:99:GLU:HB3	1:B:100:TYR:CD1	2.52	0.44
1:B:122:LEU:HD11	1:B:146:PHE:CE1	2.52	0.44
1:C:387:GLN:HG2	1:C:388:PRO:CD	2.47	0.44
1:C:196:THR:O	1:C:196:THR:HG23	2.17	0.44
1:C:405:VAL:HA	1:C:408:GLN:CG	2.47	0.44
1:C:368:ASP:CG	1:C:371:ALA:H	2.21	0.44
1:A:193:LYS:N	1:A:203:VAL:O	2.50	0.44
1:A:384:LYS:HB3	1:A:387:GLN:HE21	1.82	0.44
1:B:274:TYR:O	1:B:278:LYS:HD2	2.18	0.44
1:B:357:VAL:O	1:B:359:MET:HG2	2.18	0.44
1:B:145:TYR:CE2	1:B:147:VAL:HG13	2.53	0.44
1:A:394:ASP:HA	3:A:505:HOH:O	2.17	0.44
1:A:368:ASP:HB2	1:A:373:MET:CE	2.47	0.44
1:A:2:ARG:NH2	1:A:68:LYS:HA	2.33	0.44
1:A:413:GLN:NE2	3:A:542:HOH:O	2.50	0.44
1:A:94:PHE:O	1:A:104:VAL:HA	2.17	0.44
1:B:141:ASN:N	1:B:366:TRP:O	2.50	0.44
1:D:351:LEU:O	1:D:355:LEU:HG	2.18	0.44
1:B:267:ARG:HG2	1:B:336:PHE:CE2	2.52	0.44
1:B:371:ALA:HB1	1:B:380:TYR:HE1	1.83	0.44
1:A:139:GLY:CA	1:A:400:GLY:HA2	2.48	0.44
1:B:126:GLU:HB2	1:B:290:SER:O	2.18	0.44
1:B:139:GLY:HA2	1:B:373:MET:CB	2.48	0.44
1:B:378:SER:OG	1:B:379:ILE:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASP:OD2	1:A:156:ALA:HB2	2.18	0.44
1:A:84:SER:CB	1:A:91:THR:HB	2.44	0.44
1:A:63:THR:HG22	1:A:64:ASP:N	2.32	0.44
1:B:310:ILE:O	1:B:322:SER:HB3	2.17	0.44
1:B:68:LYS:HB3	1:B:68:LYS:HE3	1.30	0.44
1:A:12:PRO:HA	1:A:13:PRO:HD3	1.91	0.44
1:C:200:ASN:ND2	3:C:548:HOH:O	2.50	0.44
1:A:145:TYR:CE1	1:A:362:VAL:HB	2.53	0.44
1:A:21:ALA:O	1:A:24:ASN:N	2.51	0.44
1:B:11:HIS:ND1	1:B:31:GLU:OE2	2.49	0.44
1:B:38:TRP:CZ2	1:B:106:SER:HA	2.53	0.44
1:B:308:ILE:HG22	1:B:308:ILE:O	2.18	0.44
1:B:218:SER:HA	1:B:376:LEU:HD21	2.00	0.44
1:A:333:PHE:O	1:A:337:ASN:N	2.50	0.44
1:D:232:THR:CG2	1:D:234:GLU:HG2	2.47	0.44
1:B:114:PRO:O	1:B:166:ARG:HB3	2.17	0.44
1:B:94:PHE:N	1:B:412:ALA:O	2.50	0.44
1:A:86:SER:O	1:A:89:ALA:N	2.50	0.44
1:B:53:ASN:HB3	1:B:201:ALA:O	2.18	0.44
1:B:53:ASN:OD1	1:B:53:ASN:N	2.51	0.44
1:A:384:LYS:HE3	1:A:384:LYS:HA	1.99	0.44
1:A:415:VAL:HG23	1:A:415:VAL:O	2.17	0.44
1:D:98:HIS:HE1	1:D:103:ASN:H	1.66	0.44
1:A:37:ASN:OD1	1:A:181:LYS:N	2.50	0.44
1:C:90:LEU:HD21	1:C:92:LEU:HD21	2.00	0.44
1:C:296:LYS:HE3	1:C:296:LYS:HB3	1.60	0.44
1:A:133:LEU:HD12	1:A:133:LEU:H	1.83	0.44
1:B:134:SER:N	3:B:649:HOH:O	2.50	0.44
1:A:144:LEU:HD21	1:A:361:LEU:HD11	2.00	0.43
1:A:176:CYS:O	1:A:178:ARG:N	2.49	0.43
1:A:178:ARG:NH1	1:A:248:SER:OG	2.49	0.43
1:B:175:GLN:O	1:B:176:CYS:HB2	2.18	0.43
1:A:179:ASP:HB3	1:A:247:TYR:CE2	2.52	0.43
1:A:214:ASP:OD2	1:A:228:HIS:NE2	2.50	0.43
1:B:53:ASN:O	1:B:194:SER:OG	2.30	0.43
1:B:96:THR:O	1:B:102:THR:HA	2.18	0.43
2:A:431:CBI:HO6	2:A:431:CBI:HO3'	1.65	0.43
1:A:279:THR:HG22	1:A:280:LEU:N	2.32	0.43
1:A:95:VAL:HB	1:A:410:PRO:O	2.17	0.43
1:A:203:VAL:HG12	3:A:590:HOH:O	2.17	0.43
1:A:246:THR:HB	1:A:251:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:TYR:O	1:B:169:THR:N	2.52	0.43
1:D:122:LEU:HD11	1:D:146:PHE:CE1	2.53	0.43
1:A:378:SER:HB2	1:A:379:ILE:H	1.51	0.43
1:D:250:ASP:CB	1:D:253:ALA:HB2	2.40	0.43
1:B:75:GLY:HA2	1:C:78:LEU:HD22	1.99	0.43
1:B:153:GLY:O	1:B:170:GLY:HA3	2.19	0.43
1:B:341:ARG:HG3	1:B:341:ARG:O	2.17	0.43
1:C:18:ARG:HD3	3:C:651:HOH:O	2.18	0.43
1:C:34:ILE:HD11	1:C:38:TRP:CG	2.53	0.43
1:D:94:PHE:HA	1:D:365:ILE:HD13	2.00	0.43
1:A:34:ILE:HG13	1:A:108:PHE:CE1	2.53	0.43
1:B:112:ASN:HB2	1:B:118:GLN:HA	2.00	0.43
1:A:40:TRP:O	1:A:71:ILE:HA	2.19	0.43
1:B:83:ALA:CB	1:B:92:LEU:HD23	2.48	0.43
1:B:123:MET:HE2	1:B:292:PHE:O	2.19	0.43
1:B:99:GLU:OE1	1:C:81:TYR:OH	2.29	0.43
1:B:281:ASP:HB2	1:B:284:ARG:HD2	2.00	0.43
1:C:147:VAL:HG11	1:C:172:CYS:O	2.19	0.43
1:A:141:ASN:HA	1:A:218:SER:O	2.19	0.43
1:B:262:ASP:N	1:B:262:ASP:OD1	2.50	0.43
1:A:223:PHE:HE1	1:A:299:GLN:OE1	2.01	0.43
1:A:379:ILE:O	1:A:379:ILE:HG22	2.19	0.43
1:B:267:ARG:HG2	1:B:336:PHE:HE2	1.83	0.43
1:B:296:LYS:C	1:B:297:LEU:HD13	2.38	0.43
1:B:239:GLU:HG3	1:B:240:THR:HG23	2.00	0.43
1:B:173:ASP:HB2	1:B:212:GLU:OE1	2.19	0.43
1:A:123:MET:HB2	1:A:355:LEU:O	2.19	0.43
1:A:144:LEU:H	1:A:216:TRP:HB3	1.83	0.43
2:A:431:CBI:O3'	2:A:431:CBI:O5	2.29	0.43
1:D:295:ASN:HA	1:D:348:PHE:CE2	2.54	0.43
1:B:147:VAL:HG22	1:B:362:VAL:CG2	2.49	0.43
1:C:125:ASN:HD22	1:C:423:PRO:HA	1.83	0.43
1:B:65:CYS:HB2	1:B:187:ALA:CB	2.49	0.42
1:B:367:ASP:N	1:B:367:ASP:OD1	2.50	0.42
1:C:250:ASP:HB3	1:C:253:ALA:CB	2.49	0.42
1:B:149:MET:HG2	1:B:170:GLY:O	2.18	0.42
1:B:144:LEU:HD21	1:B:361:LEU:CG	2.49	0.42
1:A:37:ASN:CG	1:A:180:LEU:HA	2.39	0.42
1:A:189:ILE:O	1:A:191:GLY:N	2.52	0.42
1:A:76:ASP:OD2	1:A:78:LEU:N	2.50	0.42
1:D:77:TYR:HB3	1:D:83:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:GLU:O	1:D:223:PHE:HA	2.18	0.42
1:C:95:VAL:HB	1:C:410:PRO:CA	2.50	0.42
1:A:268:MET:HA	1:A:315:TRP:HE1	1.84	0.42
1:A:343:GLU:HG2	1:A:344:GLU:N	2.35	0.42
1:B:408:GLN:HG2	1:B:409:PHE:CE1	2.55	0.42
1:A:115:ASP:OD1	1:A:166:ARG:NE	2.50	0.42
1:A:289:VAL:HB	1:A:300:TYR:CE1	2.55	0.42
1:A:177:ALA:HB1	1:A:180:LEU:CG	2.48	0.42
1:A:158:TYR:HA	3:A:572:HOH:O	2.18	0.42
1:A:155:MET:HG2	1:A:161:ASN:O	2.18	0.42
1:D:95:VAL:HG11	1:D:97:LYS:NZ	2.34	0.42
1:B:126:GLU:HA	1:B:290:SER:O	2.18	0.42
1:B:217:GLU:O	1:B:218:SER:HB3	2.18	0.42
1:A:14:LEU:HD11	1:A:90:LEU:HB2	2.02	0.42
1:D:325:THR:HB	1:D:326:PRO:HD2	2.01	0.42
1:A:267:ARG:HD3	3:A:632:HOH:O	2.20	0.42
1:D:341:ARG:O	1:D:344:GLU:HB2	2.20	0.42
1:B:351:LEU:HG	1:B:355:LEU:CD1	2.50	0.42
1:A:327:GLU:O	1:A:330:SER:OG	2.29	0.42
1:B:95:VAL:HG13	1:B:102:THR:O	2.20	0.42
1:A:275:GLY:N	1:A:282:THR:HG23	2.33	0.42
1:C:126:GLU:HB3	1:C:291:ARG:HG2	2.01	0.42
1:B:233:ASN:HB2	3:B:489:HOH:O	2.19	0.42
1:C:166:ARG:NH1	3:C:584:HOH:O	2.52	0.42
1:C:12:PRO:HA	1:C:13:PRO:HD2	1.59	0.42
1:C:141:ASN:O	1:C:365:ILE:HA	2.19	0.42
1:B:193:LYS:HB2	1:B:193:LYS:NZ	2.35	0.42
1:B:129:PHE:HD2	1:B:130:ASP:O	2.03	0.42
1:C:270:ASN:HA	1:C:271:PRO:HD2	1.90	0.42
1:B:166:ARG:HG3	1:B:166:ARG:H	1.46	0.42
1:C:408:GLN:H	1:C:408:GLN:HG2	1.60	0.42
1:D:141:ASN:O	1:D:365:ILE:HA	2.20	0.42
1:A:18:ARG:HG3	1:A:28:VAL:HG21	2.00	0.42
1:C:263:TYR:CE2	1:C:322:SER:HB2	2.55	0.42
1:B:234:GLU:H	1:B:234:GLU:HG2	1.35	0.42
1:D:68:LYS:HB2	1:D:68:LYS:HE2	1.14	0.42
1:A:379:ILE:HG21	1:A:385:GLU:HB2	2.01	0.42
1:A:295:ASN:HB3	1:A:326:PRO:CD	2.50	0.42
1:B:401:VAL:HA	1:B:402:PRO:HD3	1.92	0.42
1:C:240:THR:OG1	1:C:241:THR:N	2.49	0.42
1:A:116:LYS:NZ	3:A:496:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:PRO:O	1:A:406:GLU:HB2	2.20	0.42
1:A:129:PHE:CE1	1:A:144:LEU:HD13	2.55	0.41
1:B:368:ASP:OD1	1:B:370:TYR:HB2	2.20	0.41
1:B:17:GLN:O	1:B:420:ARG:HA	2.19	0.41
1:B:70:MET:HB2	1:B:70:MET:HE2	1.84	0.41
1:A:291:ARG:N	1:A:298:SER:O	2.50	0.41
1:A:198:ASP:HB2	1:A:369:HIS:CD2	2.55	0.41
1:B:302:ILE:HD13	1:B:430:PHE:HE1	1.85	0.41
1:D:72:GLU:HA	1:D:72:GLU:OE1	2.20	0.41
1:B:369:HIS:ND1	1:B:402:PRO:HG2	2.36	0.41
1:C:45:ASN:O	1:C:47:GLN:HG3	2.20	0.41
1:D:9:GLU:OE2	1:D:9:GLU:HA	2.20	0.41
1:B:297:LEU:N	1:B:297:LEU:HD13	2.36	0.41
1:A:214:ASP:CB	1:A:226:THR:HB	2.49	0.41
1:C:318:MET:CE	1:C:332:MET:HA	2.50	0.41
1:A:363:MET:HB3	1:A:416:TRP:CE2	2.55	0.41
1:D:12:PRO:HD2	1:D:32:VAL:O	2.20	0.41
1:A:144:LEU:O	1:A:145:TYR:HB3	2.20	0.41
1:B:55:TRP:HB2	1:B:189:ILE:HD12	2.02	0.41
1:C:318:MET:HE2	1:C:335:VAL:HB	2.02	0.41
1:A:90:LEU:HD23	1:A:363:MET:SD	2.60	0.41
1:C:401:VAL:HG11	1:C:404:GLU:OE2	2.21	0.41
1:C:262:ASP:N	1:C:262:ASP:OD1	2.50	0.41
1:B:37:ASN:O	1:B:181:LYS:HE2	2.20	0.41
1:A:172:CYS:SG	1:A:235:TYR:HD1	2.42	0.41
1:A:12:PRO:HD2	1:A:32:VAL:O	2.21	0.41
1:A:2:ARG:HG2	1:A:162:GLN:NE2	2.36	0.41
1:B:293:GLU:H	1:B:297:LEU:CD1	2.33	0.41
1:C:40:TRP:NE1	1:C:48:ASN:OD1	2.52	0.41
1:A:76:ASP:CG	1:D:76:ASP:HB3	2.40	0.41
1:B:179:ASP:HB3	1:B:247:TYR:CE1	2.54	0.41
1:B:336:PHE:CD2	1:B:389:GLY:HA3	2.55	0.41
1:B:18:ARG:HH11	1:B:26:GLN:CD	2.24	0.41
1:B:284:ARG:HG3	1:B:303:GLN:NE2	2.36	0.41
1:B:65:CYS:HB2	1:B:187:ALA:HB2	2.02	0.41
1:B:145:TYR:CE1	1:B:362:VAL:HB	2.56	0.41
1:B:377:ASP:O	1:B:378:SER:HB2	2.21	0.41
1:D:74:ALA:HB3	1:D:77:TYR:CZ	2.56	0.41
1:D:127:LEU:HD21	1:D:144:LEU:HD21	2.03	0.41
1:B:117:TYR:CZ	1:B:165:ALA:HA	2.55	0.41
1:B:232:THR:HG22	1:B:236:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:PHE:HZ	1:C:216:TRP:CG	2.38	0.41
1:A:120:PHE:CD1	1:A:146:PHE:HE2	2.38	0.41
1:A:424:ILE:H	1:A:424:ILE:HG12	1.70	0.41
1:A:284:ARG:HB2	1:A:285:LYS:H	1.18	0.41
1:B:150:GLU:OE2	1:B:154:GLY:HA2	2.21	0.41
1:A:176:CYS:HB3	1:A:207:GLY:HA3	2.03	0.41
1:B:9:GLU:HB2	1:B:73:GLY:HA3	2.03	0.41
1:B:4:GLY:CA	1:B:70:MET:HE3	2.47	0.41
1:B:189:ILE:HG23	1:B:190:GLU:N	2.36	0.41
1:A:122:LEU:HD23	1:A:359:MET:CE	2.50	0.41
1:A:373:MET:HG3	1:A:376:LEU:HB3	2.03	0.41
1:A:76:ASP:OD1	1:D:76:ASP:N	2.50	0.41
1:A:288:VAL:HG22	1:A:301:PHE:CD2	2.56	0.41
1:B:252:PHE:CD2	1:B:341:ARG:HD3	2.56	0.41
1:B:144:LEU:HG	1:B:362:VAL:O	2.20	0.41
1:A:377:ASP:O	1:A:393:GLY:HA3	2.21	0.41
1:C:287:THR:HB	1:C:302:ILE:HB	2.03	0.41
1:A:301:PHE:CD1	1:A:310:ILE:HD11	2.57	0.40
1:B:8:PRO:CG	1:C:78:LEU:HD21	2.48	0.40
1:B:311:PRO:HA	1:B:312:PRO:HD3	1.67	0.40
1:D:6:GLU:HB2	1:D:72:GLU:OE2	2.21	0.40
1:A:183:VAL:CG1	1:A:237:VAL:HG22	2.51	0.40
1:A:127:LEU:HD11	1:A:419:ILE:HG23	2.03	0.40
1:B:273:PHE:CD2	1:B:274:TYR:HB2	2.56	0.40
1:C:327:GLU:O	1:C:331:THR:HG23	2.21	0.40
1:B:190:GLU:HB3	3:B:677:HOH:O	2.21	0.40
1:A:35:ASP:HB3	1:A:38:TRP:HE3	1.87	0.40
1:A:123:MET:HE1	1:A:355:LEU:HB2	2.04	0.40
1:C:378:SER:OG	1:C:379:ILE:N	2.51	0.40
1:B:248:SER:HB3	3:B:540:HOH:O	2.21	0.40
1:D:409:PHE:HE1	3:D:597:HOH:O	2.03	0.40
1:D:263:TYR:CE1	1:D:322:SER:HA	2.56	0.40
1:A:300:TYR:HA	1:A:310:ILE:CD1	2.51	0.40
1:A:64:ASP:OD2	1:A:65:CYS:N	2.54	0.40
1:A:30:ALA:CB	1:A:110:LEU:HD11	2.51	0.40
1:A:155:MET:HE3	1:A:155:MET:HB3	1.91	0.40
1:D:7:THR:O	1:D:73:GLY:HA3	2.22	0.40
1:A:31:GLU:OE1	1:A:114:PRO:N	2.54	0.40
1:B:27:THR:O	1:B:27:THR:HG22	2.21	0.40
1:A:421:PHE:HD2	1:A:422:GLY:N	2.15	0.40
1:B:250:ASP:HB3	1:B:253:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:O	1:A:413:GLN:HA	2.21	0.40
1:B:129:PHE:CZ	1:B:288:VAL:HB	2.57	0.40
1:B:147:VAL:HG22	1:B:362:VAL:HG21	2.02	0.40
1:A:218:SER:HB2	1:A:222:ALA:O	2.21	0.40
1:B:416:TRP:O	1:B:417:SER:HB3	2.21	0.40
1:C:16:TRP:CD1	1:C:110:LEU:HD21	2.57	0.40
1:C:369:HIS:HA	1:C:402:PRO:HG2	2.03	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	428/430 (100%)	357 (83%)	55 (13%)	16 (4%)	4 0
1	B	428/430 (100%)	340 (79%)	58 (14%)	30 (7%)	1 0
1	C	428/430 (100%)	403 (94%)	19 (4%)	6 (1%)	14 2
1	D	428/430 (100%)	391 (91%)	27 (6%)	10 (2%)	8 1
All	All	1712/1720 (100%)	1491 (87%)	159 (9%)	62 (4%)	4 0

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	A	240	THR
1	A	383	GLU
1	B	14	LEU
1	B	51	ASP
1	B	56	THR
1	B	74	ALA
1	B	103	ASN

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Mol	Chain	Res	Type
1	B	140	ILE
1	B	149	MET
1	B	180	LEU
1	B	337	ASN
1	B	383	GLU
1	C	383	GLU
1	A	60	SER
1	A	164	GLY
1	A	176	CYS
1	A	177	ALA
1	A	190	GLU
1	A	347	GLY
1	B	62	ALA
1	B	87	GLY
1	B	102	THR
1	B	131	VAL
1	B	168	GLY
1	B	176	CYS
1	B	182	PHE
1	B	194	SER
1	B	197	SER
1	B	246	THR
1	B	254	GLY
1	B	330	SER
1	C	240	THR
1	C	382	PRO
1	D	60	SER
1	D	99	GLU
1	D	176	CYS
1	D	177	ALA
1	D	332	MET
1	A	218	SER
1	B	214	ASP
1	B	220	ALA
1	B	378	SER
1	C	176	CYS
1	C	330	SER
1	D	240	THR
1	D	383	GLU
1	A	76	ASP
1	B	296	LYS
1	B	373	MET

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Mol	Chain	Res	Type
1	D	46	MET
1	A	30	ALA
1	A	385	GLU
1	A	401	VAL
1	D	22	PRO
1	D	206	TYR
1	A	245	GLY
1	B	60	SER
1	B	13	PRO
1	C	75	GLY
1	A	402	PRO
1	B	215	VAL

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	354/354 (100%)	275 (78%)	79 (22%)	1 0
1	B	354/354 (100%)	281 (79%)	73 (21%)	1 0
1	C	354/354 (100%)	314 (89%)	40 (11%)	7 1
1	D	354/354 (100%)	316 (89%)	38 (11%)	8 1
All	All	1416/1416 (100%)	1186 (84%)	230 (16%)	3 0

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	GLU
1	A	14	LEU
1	A	27	THR
1	A	34	ILE
1	A	41	LEU
1	A	46	MET
1	A	51	ASP
1	A	54	GLN

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Mol	Chain	Res	Type
1	A	59	CYS
1	A	68	LYS
1	A	78	LEU
1	A	84	SER
1	A	85	THR
1	A	86	SER
1	A	96	THR
1	A	97	LYS
1	A	107	ARG
1	A	122	LEU
1	A	133	LEU
1	A	145	TYR
1	A	155	MET
1	A	162	GLN
1	A	166	ARG
1	A	179	ASP
1	A	181	LYS
1	A	190	GLU
1	A	193	LYS
1	A	194	SER
1	A	196	THR
1	A	215	VAL
1	A	228	HIS
1	A	230	CYS
1	A	234	GLU
1	A	236	HIS
1	A	241	THR
1	A	246	THR
1	A	248	SER
1	A	256	CYS
1	A	276	LYS
1	A	278	LYS
1	A	279	THR
1	A	283	SER
1	A	284	ARG
1	A	289	VAL
1	A	290	SER
1	A	291	ARG
1	A	293	GLU
1	A	296	LYS
1	A	298	SER
1	A	300	TYR

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Mol	Chain	Res	Type
1	A	303	GLN
1	A	306	ARG
1	A	307	LYS
1	A	309	GLU
1	A	316	GLU
1	A	320	ASN
1	A	321	SER
1	A	322	SER
1	A	328	LEU
1	A	333	PHE
1	A	335	VAL
1	A	337	ASN
1	A	340	ASN
1	A	341	ARG
1	A	343	GLU
1	A	344	GLU
1	A	348	PHE
1	A	363	MET
1	A	376	LEU
1	A	378	SER
1	A	384	LYS
1	A	385	GLU
1	A	394	ASP
1	A	402	PRO
1	A	411	ASP
1	A	416	TRP
1	A	421	PHE
1	A	424	ILE
1	B	2	ARG
1	B	26	GLN
1	B	27	THR
1	B	32	VAL
1	B	41	LEU
1	B	43	ASP
1	B	46	MET
1	B	47	GLN
1	B	48	ASN
1	B	51	ASP
1	B	53	ASN
1	B	54	GLN
1	B	57	ASN
1	B	60	SER

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Mol	Chain	Res	Type
1	B	64	ASP
1	B	68	LYS
1	B	70	MET
1	B	71	ILE
1	B	78	LEU
1	B	80	THR
1	B	92	LEU
1	B	97	LYS
1	B	103	ASN
1	B	106	SER
1	B	116	LYS
1	B	123	MET
1	B	125	ASN
1	B	127	LEU
1	B	130	ASP
1	B	133	LEU
1	B	135	THR
1	B	147	VAL
1	B	149	MET
1	B	151	GLU
1	B	162	GLN
1	B	166	ARG
1	B	181	LYS
1	B	189	ILE
1	B	190	GLU
1	B	208	SER
1	B	234	GLU
1	B	239	GLU
1	B	242	ASN
1	B	246	THR
1	B	247	TYR
1	B	251	ARG
1	B	264	ASN
1	B	270	ASN
1	B	276	LYS
1	B	278	LYS
1	B	281	ASP
1	B	284	ARG
1	B	296	LYS
1	B	297	LEU
1	B	320	ASN
1	B	328	LEU

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Mol	Chain	Res	Type
1	B	337	ASN
1	B	338	ASP
1	B	339	ARG
1	B	340	ASN
1	B	348	PHE
1	B	350	GLN
1	B	365	ILE
1	B	369	HIS
1	B	373	MET
1	B	383	GLU
1	B	385	GLU
1	B	388	PRO
1	B	392	ARG
1	B	394	ASP
1	B	401	VAL
1	B	404	GLU
1	B	413	GLN
1	C	17	GLN
1	C	26	GLN
1	C	37	ASN
1	C	45	ASN
1	C	48	ASN
1	C	54	GLN
1	C	64	ASP
1	C	67	GLU
1	C	71	ILE
1	C	93	LYS
1	C	96	THR
1	C	100	TYR
1	C	115	ASP
1	C	116	LYS
1	C	122	LEU
1	C	133	LEU
1	C	155	MET
1	C	175	GLN
1	C	190	GLU
1	C	193	LYS
1	C	196	THR
1	C	239	GLU
1	C	278	LYS
1	C	284	ARG
1	C	293	GLU

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Mol	Chain	Res	Type
1	C	328	LEU
1	C	334	ASP
1	C	340	ASN
1	C	348	PHE
1	C	361	LEU
1	C	365	ILE
1	C	368	ASP
1	C	383	GLU
1	C	384	LYS
1	C	385	GLU
1	C	387	GLN
1	C	397	THR
1	C	408	GLN
1	C	415	VAL
1	C	429	ASP
1	D	2	ARG
1	D	6	GLU
1	D	18	ARG
1	D	37	ASN
1	D	46	MET
1	D	47	GLN
1	D	54	GLN
1	D	59	CYS
1	D	60	SER
1	D	68	LYS
1	D	71	ILE
1	D	78	LEU
1	D	98	HIS
1	D	115	ASP
1	D	166	ARG
1	D	183	VAL
1	D	189	ILE
1	D	190	GLU
1	D	193	LYS
1	D	196	THR
1	D	278	LYS
1	D	283	SER
1	D	296	LYS
1	D	328	LEU
1	D	332	MET
1	D	333	PHE
1	D	338	ASP

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Mol	Chain	Res	Type
1	D	340	ASN
1	D	343	GLU
1	D	349	GLU
1	D	361	LEU
1	D	384	LYS
1	D	385	GLU
1	D	387	GLN
1	D	405	VAL
1	D	408	GLN
1	D	415	VAL
1	D	429	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	26	GLN
1	A	29	ASN
1	A	47	GLN
1	A	98	HIS
1	A	112	ASN
1	A	125	ASN
1	A	162	GLN
1	A	340	ASN
1	A	352	ASN
1	A	387	GLN
1	A	408	GLN
1	A	413	GLN
1	B	24	ASN
1	B	48	ASN
1	B	53	ASN
1	B	57	ASN
1	B	98	HIS
1	B	103	ASN
1	B	125	ASN
1	B	233	ASN
1	B	242	ASN
1	B	295	ASN
1	B	320	ASN
1	B	340	ASN
1	B	352	ASN
1	B	353	ASN

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Mol	Chain	Res	Type
1	B	369	HIS
1	B	372	ASN
1	B	387	GLN
1	C	5	ASN
1	C	10	ASN
1	C	29	ASN
1	C	47	GLN
1	C	54	GLN
1	C	125	ASN
1	C	200	ASN
1	C	242	ASN
1	C	320	ASN
1	C	340	ASN
1	C	352	ASN
1	C	353	ASN
1	C	369	HIS
1	D	26	GLN
1	D	29	ASN
1	D	45	ASN
1	D	125	ASN
1	D	320	ASN
1	D	340	ASN
1	D	352	ASN
1	D	353	ASN
1	D	372	ASN
1	D	408	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	PCA	A	1	1	7,8,9	1.73	1 (14%)	9,10,12	1.52	1 (11%)
1	PCA	B	1	1	7,8,9	1.72	1 (14%)	9,10,12	1.93	1 (11%)
1	PCA	C	1	1	7,8,9	1.77	1 (14%)	9,10,12	1.75	4 (44%)
1	PCA	D	1	1	7,8,9	1.76	1 (14%)	9,10,12	1.54	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	PCA	CD-N	4.13	1.47	1.33
1	A	1	PCA	CD-N	4.29	1.48	1.33
1	D	1	PCA	CD-N	4.42	1.48	1.33
1	B	1	PCA	CD-N	4.44	1.48	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1	PCA	CB-CA-C	-4.81	106.18	112.76
1	D	1	PCA	CB-CA-C	-3.81	107.55	112.76
1	A	1	PCA	CB-CA-C	-3.23	108.35	112.76
1	C	1	PCA	OE-CD-CG	-2.88	120.37	126.81
1	C	1	PCA	O-C-CA	-2.76	118.14	125.44
1	C	1	PCA	CB-CA-C	-2.28	109.65	112.76
1	C	1	PCA	CB-CG-CD	2.15	108.60	104.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	2	0
1	B	1	PCA	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	CBI	A	431	-	24,24,24	0.44	0	35,35,35	1.44	5 (14%)
2	CBI	B	431	-	24,24,24	0.51	0	35,35,35	1.57	5 (14%)
2	CBI	C	431	-	24,24,24	0.47	0	35,35,35	1.23	3 (8%)
2	CBI	D	431	-	24,24,24	0.56	0	35,35,35	0.80	0

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	CBI	A	431	-	-	0/8/48/48	0/2/2/2
2	CBI	B	431	-	-	0/8/48/48	0/2/2/2
2	CBI	C	431	-	-	0/8/48/48	0/2/2/2
2	CBI	D	431	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	431	CBI	C1-O4'-C4'	-3.36	109.23	118.01
2	B	431	CBI	C4-C3-C2	-3.14	104.92	110.79
2	C	431	CBI	C1'-O5'-C5'	-3.09	107.75	113.47
2	C	431	CBI	C1-O4'-C4'	-3.08	109.97	118.01
2	A	431	CBI	C1-O5-C5	-3.05	107.83	113.75
2	A	431	CBI	C1'-O5'-C5'	-2.78	108.34	113.47
2	B	431	CBI	C1-O4'-C4'	-2.75	110.82	118.01
2	C	431	CBI	O5-C5-C4	-2.30	105.36	109.68
2	A	431	CBI	C2'-C3'-C4'	2.51	115.11	109.60
2	B	431	CBI	O5-C5-C6	3.05	114.07	106.36
2	A	431	CBI	C3'-C4'-C5'	3.63	119.04	110.84
2	B	431	CBI	C2'-C3'-C4'	3.95	118.28	109.60
2	B	431	CBI	C1'-C2'-C3'	4.05	116.45	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	431	CBI	4	0
2	B	431	CBI	5	0
2	C	431	CBI	1	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^{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	429/430 (99%)	0.32	15 (3%) 48 52	7, 26, 39, 52	0
1	B	429/430 (99%)	0.37	15 (3%) 48 52	12, 26, 46, 62	0
1	C	429/430 (99%)	-0.36	0 100 100	4, 14, 30, 58	0
1	D	429/430 (99%)	-0.40	3 (0%) 89 91	3, 12, 26, 57	0
All	All	1716/1720 (99%)	-0.02	33 (1%) 70 74	3, 21, 39, 62	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	PRO	5.4
1	B	210	CYS	3.5
1	D	100	TYR	3.1
1	B	273	PHE	3.1
1	A	330	SER	2.9
1	A	405	VAL	2.8
1	A	24	ASN	2.7
1	B	55	TRP	2.7
1	B	428	TYR	2.7
1	D	98	HIS	2.7
1	A	286	PHE	2.6
1	A	333	PHE	2.6
1	A	380	TYR	2.6
1	B	244	GLY	2.6
1	B	75	GLY	2.5
1	A	127	LEU	2.5
1	A	366	TRP	2.5
1	A	289	VAL	2.4
1	A	163	ALA	2.4
1	B	139	GLY	2.4
1	B	407	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	46	MET	2.3
1	A	124	GLY	2.3
1	B	207	GLY	2.1
1	B	76	ASP	2.1
1	B	189	ILE	2.1
1	B	104	VAL	2.1
1	B	100	TYR	2.1
1	A	400	GLY	2.1
1	A	389	GLY	2.0
1	A	27	THR	2.0
1	B	232	THR	2.0
1	A	300	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PCA	A	1	8/9	0.95	0.10	-	8,24,34,47	0
1	PCA	B	1	8/9	0.94	0.07	-	16,20,23,29	0
1	PCA	C	1	8/9	0.96	0.08	-	7,14,21,32	0
1	PCA	D	1	8/9	0.95	0.08	-	6,13,18,20	0

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
2	CBI	C	431	23/23	0.97	0.08	1.06	3,15,33,57	0
2	CBI	D	431	23/23	0.96	0.08	0.83	4,12,20,32	0
2	CBI	A	431	23/23	0.92	0.11	0.29	4,32,42,71	0
2	CBI	B	431	23/23	0.94	0.11	0.17	9,22,37,67	0

6.5 Other polymers (i)

There are no such residues in this entry.