Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:00 AM GMT

PDB ID	:	2VK4
Title	:	CRYSTAL STRUCTURE OF PYRUVATE DECARBOXYLASE FROM KLUYVEROMYCES LACTIS
Authors	:	Kutter, S.; Relle, S.; Wille, G.; Weiss, M.S.; Konig, S.
Deposited on	:	2007-12-17
Resolution	:	1.95 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:

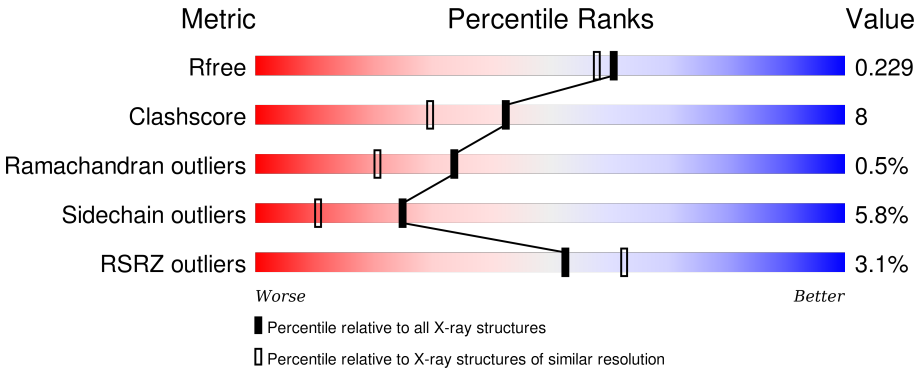
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	563	3% 82% 14%
1	B	563	4% 81% 14%
1	C	563	3% 82% 15%
1	D	563	2% 80% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	601	-	-	-	X

2 Entry composition

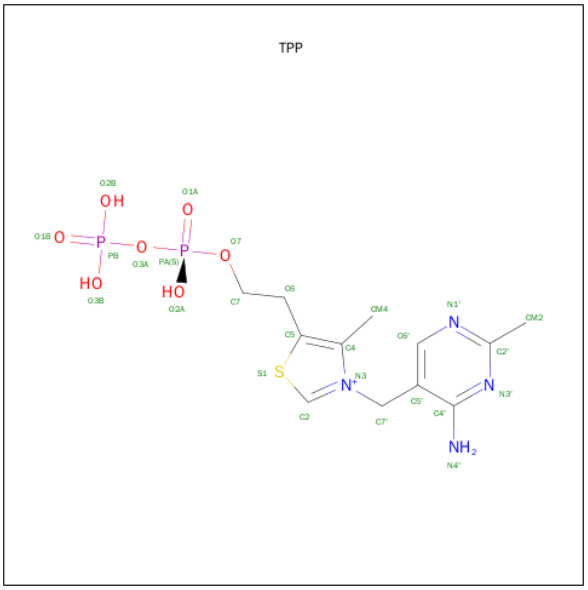
There are 4 unique types of molecules in this entry. The entry contains 18654 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRUVATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			4324	2754	723	833	14			
1	B	557	Total	C	N	O	S	0	0	0
			4293	2733	716	830	14			
1	C	555	Total	C	N	O	S	0	0	0
			4286	2731	715	826	14			
1	D	560	Total	C	N	O	S	0	0	0
			4324	2754	723	833	14			

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

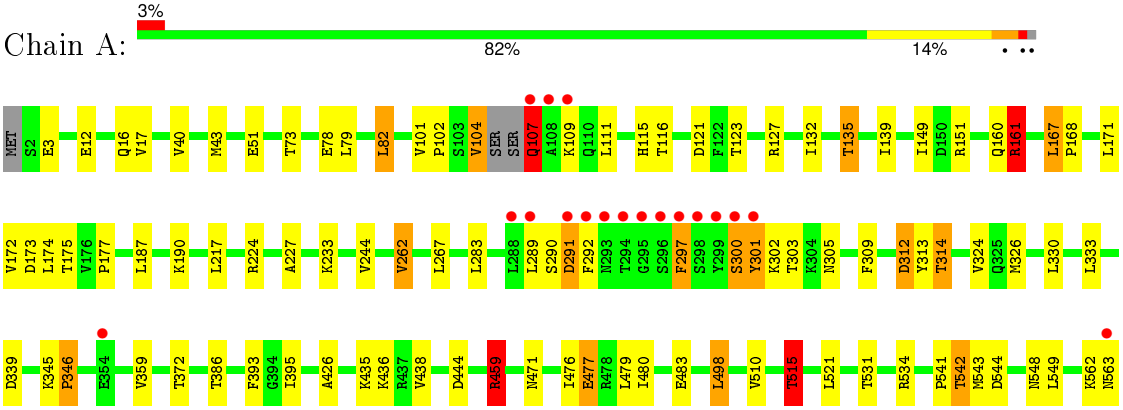
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O	0	0
			310	310		
4	B	326	Total	O	0	0
			326	326		
4	C	376	Total	O	0	0
			376	376		
4	D	307	Total	O	0	0
			307	307		

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.

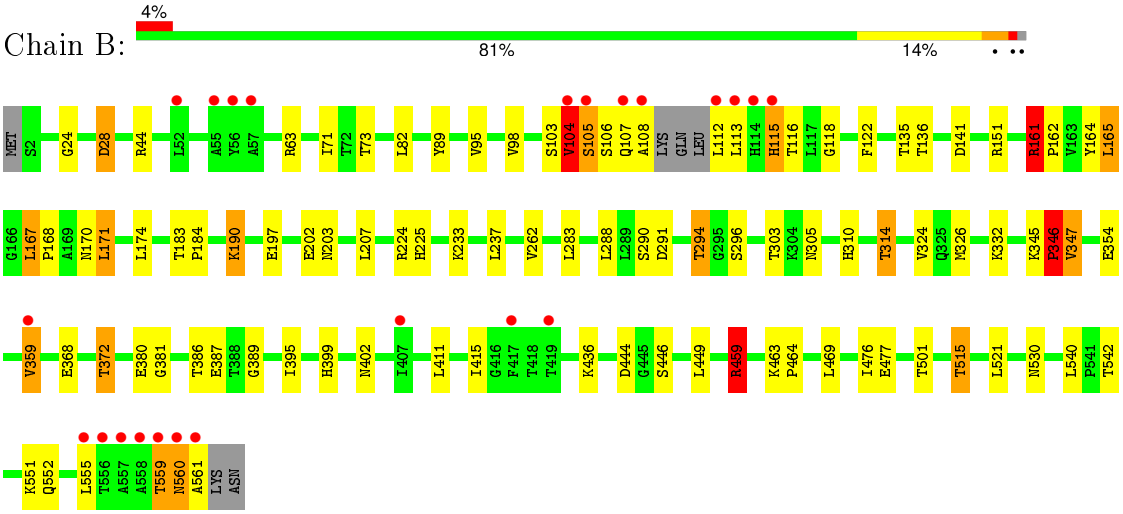
- Molecule 1: PYRUVATE DECARBOXYLASE

Chain A:



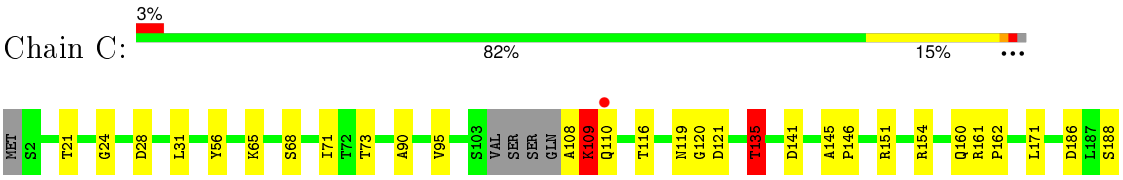
- Molecule 1: PYRUVATE DECARBOXYLASE

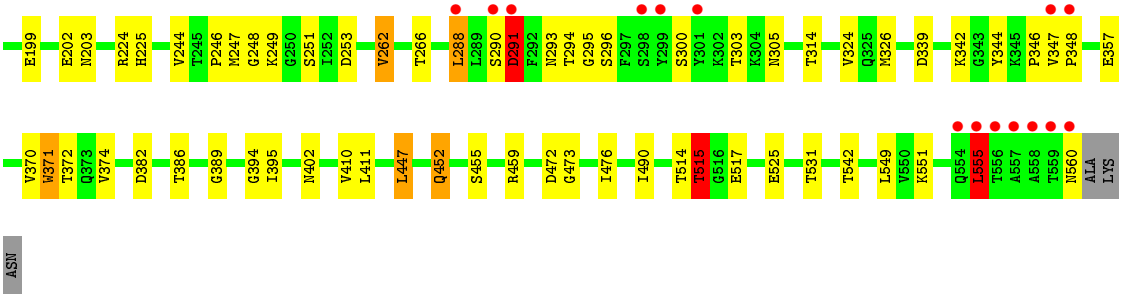
Chain B:



- Molecule 1: PYRUVATE DECARBOXYLASE

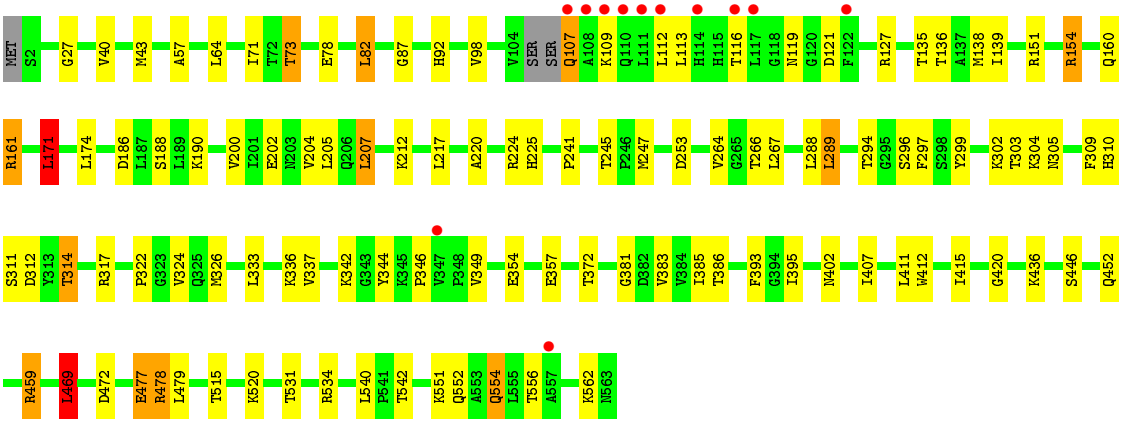
Chain C:





- Molecule 1: PYRUVATE DECARBOXYLASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.71Å 203.18Å 79.81Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	48.45 – 1.95 48.47 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.45-1.95) 85.4 (48.47-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.230 0.177 , 0.229	Depositor DCC
R_{free} test set	7819 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.4	EDS
Estimated twinning fraction	0.006 for l,k,-h 0.033 for h,-k,-l 0.025 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 156058 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18654	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: MG, TPP

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	0.89	2/4415 (0.0%)	0.85	8/6009 (0.1%)
1	B	0.87	1/4384 (0.0%)	0.96	12/5969 (0.2%)
1	C	0.91	2/4377 (0.0%)	0.86	7/5958 (0.1%)
1	D	0.88	3/4415 (0.1%)	0.86	8/6009 (0.1%)
All	All	0.89	8/17591 (0.0%)	0.88	35/23945 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	1
1	B	4	2
1	C	6	1
1	D	7	0
All	All	21	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	HIS	CA-CB	-13.55	1.24	1.53
1	D	107	GLN	CA-CB	-8.75	1.34	1.53
1	C	371	TRP	CB-CG	6.47	1.61	1.50
1	B	561	ALA	CA-C	6.20	1.69	1.52
1	D	73	THR	C-O	-6.16	1.11	1.23
1	D	202	GLU	CG-CD	6.02	1.60	1.51
1	C	56	TYR	CD1-CE1	5.36	1.47	1.39
1	A	115	HIS	N-CA	5.35	1.57	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	561	ALA	N-CA-C	-26.55	39.32	111.00
1	B	161	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	B	161	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	D	107	GLN	N-CA-CB	9.12	127.01	110.60
1	D	478	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	D	459	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	115	HIS	N-CA-CB	7.14	123.45	110.60
1	D	459	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	555	LEU	CA-CB-CG	6.86	131.08	115.30
1	C	247	MET	CG-SD-CE	-6.69	89.49	100.20
1	B	44	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	C	447	LEU	CB-CG-CD2	6.48	122.02	111.00
1	D	161	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	63	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	161	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	C	515	THR	N-CA-CB	-6.27	98.39	110.30
1	B	444	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	561	ALA	N-CA-CB	-6.07	101.60	110.10
1	B	105	SER	N-CA-CB	-5.96	101.56	110.50
1	A	312	ASP	N-CA-CB	-5.82	100.12	110.60
1	B	108	ALA	N-CA-C	5.82	126.72	111.00
1	A	444	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	82	LEU	CB-CG-CD1	-5.65	101.40	111.00
1	C	28	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	135	THR	CB-CA-C	-5.52	96.71	111.60
1	A	515	THR	N-CA-CB	-5.50	99.85	110.30
1	A	115	HIS	CB-CA-C	5.39	121.17	110.40
1	C	382	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	115	HIS	N-CA-C	5.33	125.39	111.00
1	A	301	TYR	N-CA-C	5.26	125.21	111.00
1	D	171	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	459	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	459	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	469	LEU	CA-CB-CG	5.04	126.89	115.30
1	D	154	ARG	NE-CZ-NH2	-5.04	117.78	120.30

All (21) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	73	THR	CB
1	A	116	THR	CB
1	A	303	THR	CB
1	A	372	THR	CB

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Mol	Chain	Res	Type	Atom
1	B	73	THR	CB
1	B	135	THR	CB
1	B	303	THR	CB
1	B	542	THR	CB
1	C	73	THR	CB
1	C	116	THR	CB
1	C	303	THR	CB
1	C	314	THR	CB
1	C	372	THR	CB
1	C	542	THR	CB
1	D	73	THR	CB
1	D	116	THR	CB
1	D	135	THR	CB
1	D	303	THR	CB
1	D	372	THR	CB
1	D	531	THR	CB
1	D	542	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	GLN	Peptide
1	B	104	VAL	Mainchain
1	B	107	GLN	Peptide
1	C	108	ALA	Peptide

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	4324	0	4300	85	0
1	B	4293	0	4259	76	0
1	C	4286	0	4259	65	0
1	D	4324	0	4300	78	0
2	A	26	0	16	0	0
2	B	26	0	16	1	0
2	C	26	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	26	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	310	0	0	15	0
4	B	326	0	0	9	0
4	C	376	0	0	18	0
4	D	307	0	0	11	0
All	All	18654	0	17182	285	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 8.

All (285) 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:D:303:THR:HG22	1:D:305:ASN:N	1.67	1.09
1:B:303:THR:HG22	1:B:305:ASN:H	1.15	1.08
1:D:303:THR:HG22	1:D:305:ASN:H	0.91	1.06
1:B:294:THR:HG22	1:B:296:SER:H	1.15	1.06
1:D:303:THR:CG2	1:D:305:ASN:H	1.70	1.05
1:A:372:THR:HG22	4:A:2205:HOH:O	1.56	1.02
1:A:107:GLN:O	1:A:107:GLN:HG3	1.60	0.99
1:A:303:THR:HG22	1:A:305:ASN:H	1.25	0.99
1:D:477:GLU:HG2	4:D:2252:HOH:O	1.60	0.97
1:C:303:THR:HG22	1:C:305:ASN:H	1.33	0.94
1:D:372:THR:HG22	4:D:2203:HOH:O	1.67	0.94
1:A:393:PHE:HE2	1:A:476:ILE:HD11	1.34	0.91
1:C:542:THR:HG21	4:C:2300:HOH:O	1.71	0.88
1:C:203:ASN:HB3	4:C:2130:HOH:O	1.72	0.88
1:B:141:ASP:OD2	1:D:135:THR:HG23	1.74	0.86
1:C:21:THR:O	4:C:2018:HOH:O	1.92	0.86
1:B:112:LEU:HD11	1:B:122:PHE:HE2	1.41	0.86
1:B:113:LEU:O	1:B:116:THR:HG22	1.76	0.85
1:C:288:LEU:HD13	1:C:411:LEU:HD13	1.58	0.84
1:C:135:THR:HG21	1:C:151:ARG:HH12	1.42	0.84
1:A:135:THR:HG21	1:A:151:ARG:HH12	1.42	0.83
1:B:372:THR:HG21	4:B:2188:HOH:O	1.79	0.82
1:A:393:PHE:CE2	1:A:476:ILE:HD11	2.16	0.80
1:B:542:THR:HG21	4:B:2260:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:O	1:B:104:VAL:HG22	1.82	0.79
1:D:542:THR:HG21	4:D:2241:HOH:O	1.82	0.79
1:B:303:THR:HG22	1:B:305:ASN:N	1.96	0.79
1:B:135:THR:HG21	1:B:151:ARG:HH12	1.48	0.79
1:A:302:LYS:H	1:D:304:LYS:HZ2	1.31	0.78
1:A:515:THR:CG2	4:A:2179:HOH:O	2.31	0.77
1:D:294:THR:HG22	1:D:296:SER:H	1.49	0.77
1:C:515:THR:HG23	4:C:2224:HOH:O	1.85	0.76
1:B:346:PRO:O	1:B:347:VAL:HB	1.86	0.76
1:A:121:ASP:OD1	1:A:127:ARG:NH1	2.19	0.76
1:A:302:LYS:H	1:D:304:LYS:NZ	1.84	0.75
1:A:515:THR:HG23	4:A:2179:HOH:O	1.84	0.74
1:A:300:SER:O	1:A:302:LYS:HG3	1.87	0.74
1:B:294:THR:HG22	1:B:296:SER:N	1.97	0.74
1:B:112:LEU:HD12	1:B:112:LEU:O	1.88	0.73
1:C:303:THR:HG22	1:C:305:ASN:N	2.04	0.72
1:B:112:LEU:HD12	1:B:112:LEU:C	2.12	0.71
1:B:190:LYS:HG3	4:B:2104:HOH:O	1.92	0.70
1:A:267:LEU:HD11	1:A:297:PHE:HB3	1.73	0.70
1:C:372:THR:HG21	4:C:2216:HOH:O	1.92	0.69
1:C:357:GLU:HG2	4:C:2219:HOH:O	1.93	0.69
1:C:135:THR:HG21	1:C:151:ARG:NH1	2.07	0.69
1:A:173:ASP:OD1	4:A:2091:HOH:O	2.11	0.69
1:D:267:LEU:HD12	1:D:297:PHE:HB3	1.76	0.68
1:B:559:THR:HG22	1:B:560:ASN:OD1	1.93	0.67
1:A:116:THR:HB	1:B:411:LEU:HD21	1.75	0.67
1:C:160:GLN:OE1	4:C:2096:HOH:O	2.12	0.67
1:A:303:THR:HG22	1:A:305:ASN:N	2.03	0.67
1:D:303:THR:HG21	1:D:305:ASN:HB3	1.76	0.66
1:A:292:PHE:HB3	1:B:113:LEU:HD13	1.77	0.66
1:D:135:THR:HG21	1:D:151:ARG:HH12	1.60	0.66
1:A:459:ARG:NH2	4:A:2234:HOH:O	2.28	0.66
1:B:303:THR:CG2	1:B:305:ASN:HB2	2.27	0.65
1:A:386:THR:HG21	1:A:395:ILE:HB	1.77	0.65
1:C:314:THR:HG22	4:C:2188:HOH:O	1.98	0.64
1:C:288:LEU:CD1	1:C:411:LEU:HD13	2.28	0.64
1:C:411:LEU:O	1:D:116:THR:HG21	1.98	0.64
1:A:477:GLU:HG2	4:A:2243:HOH:O	1.98	0.64
1:A:127:ARG:NH2	4:A:2068:HOH:O	2.25	0.63
1:B:104:VAL:O	1:B:104:VAL:CG2	2.47	0.63
1:A:123:THR:OG1	1:A:127:ARG:NH1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:THR:HG22	4:C:2263:HOH:O	2.00	0.62
1:C:116:THR:HG21	1:D:411:LEU:O	2.00	0.62
1:B:165:LEU:HD22	1:B:167:LEU:HD13	1.82	0.62
1:C:348:PRO:HB3	4:C:2203:HOH:O	1.99	0.61
1:C:339:ASP:O	1:C:342:LYS:HB2	2.00	0.60
1:D:309:PHE:HB3	1:D:326:MET:HG3	1.83	0.60
1:C:290:SER:O	1:C:291:ASP:HB3	2.02	0.60
1:A:116:THR:HB	1:B:411:LEU:CD2	2.32	0.60
1:A:116:THR:HG21	1:B:411:LEU:O	2.02	0.59
1:A:127:ARG:NE	4:A:2068:HOH:O	2.29	0.59
1:C:95:VAL:O	1:C:162:PRO:HA	2.03	0.59
1:B:346:PRO:O	1:B:347:VAL:CB	2.51	0.59
1:D:469:LEU:HD13	1:D:540:LEU:HD11	1.85	0.58
1:B:203:ASN:HB3	4:B:2112:HOH:O	2.02	0.58
1:D:121:ASP:OD1	1:D:127:ARG:NH1	2.36	0.58
1:C:154:ARG:NE	1:C:186:ASP:O	2.32	0.58
1:C:386:THR:HG21	1:C:395:ILE:HB	1.86	0.58
1:D:73:THR:HG22	4:D:2045:HOH:O	2.03	0.58
1:C:344:TYR:CE2	1:C:346:PRO:HA	2.39	0.58
1:C:199:GLU:OE1	4:C:2129:HOH:O	2.17	0.58
1:A:289:LEU:HD23	1:A:292:PHE:HE2	1.68	0.57
1:B:354:GLU:HG3	1:B:399:HIS:CE1	2.39	0.57
1:A:135:THR:HG22	1:C:141:ASP:OD2	2.03	0.57
1:D:78:GLU:O	1:D:82:LEU:HD13	2.05	0.57
1:A:82:LEU:HG	1:A:132:ILE:HD11	1.86	0.56
1:D:220:ALA:HB2	1:D:247:MET:HB3	1.87	0.56
1:A:548:ASN:HB3	4:A:2148:HOH:O	2.06	0.56
1:D:317:ARG:HD3	4:D:2152:HOH:O	2.06	0.56
1:D:241:PRO:HB3	1:D:349:VAL:HG12	1.87	0.55
1:B:112:LEU:CD1	1:B:122:PHE:HE2	2.17	0.55
1:C:372:THR:HG22	4:C:2212:HOH:O	2.06	0.55
1:A:227:ALA:CB	1:A:326:MET:HE3	2.36	0.55
1:A:302:LYS:N	1:D:304:LYS:HZ2	2.03	0.55
1:A:139:ILE:HG22	1:A:171:LEU:HD12	1.89	0.54
1:D:478:ARG:NH2	4:D:2243:HOH:O	2.38	0.54
1:A:135:THR:HG21	1:A:151:ARG:NH1	2.17	0.54
1:A:542:THR:HG21	4:A:2239:HOH:O	2.06	0.54
1:A:531:THR:HG21	4:A:2287:HOH:O	2.08	0.54
1:C:225:HIS:HB2	1:C:326:MET:HE3	1.90	0.54
1:A:73:THR:HG22	4:A:2044:HOH:O	2.07	0.54
1:A:542:THR:HG22	4:A:2295:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:THR:HG22	1:C:296:SER:H	1.73	0.53
1:C:248:GLY:O	1:C:251:SER:HB2	2.08	0.53
1:D:225:HIS:CD2	1:D:311:SER:HB3	2.44	0.53
1:B:459:ARG:NH2	4:B:2250:HOH:O	2.33	0.53
1:D:478:ARG:NE	4:D:2243:HOH:O	1.96	0.53
1:D:207:LEU:HD11	1:D:317:ARG:HH21	1.74	0.53
1:A:562:LYS:HB3	1:D:322:PRO:HG2	1.91	0.53
1:D:217:LEU:HD11	1:D:245:THR:HG23	1.91	0.52
1:B:559:THR:C	1:B:560:ASN:OD1	2.48	0.52
1:A:477:GLU:CG	4:A:2243:HOH:O	2.57	0.52
1:A:78:GLU:O	1:A:82:LEU:HD13	2.09	0.52
1:B:135:THR:CG2	1:B:151:ARG:HH12	2.21	0.52
1:B:112:LEU:HD11	1:B:122:PHE:CE2	2.32	0.52
1:D:303:THR:HG21	1:D:305:ASN:CB	2.40	0.52
1:D:303:THR:CG2	1:D:305:ASN:CB	2.88	0.51
1:A:393:PHE:CE2	1:A:476:ILE:CD1	2.92	0.51
1:C:459:ARG:NH2	4:C:2290:HOH:O	2.32	0.51
1:A:562:LYS:HE3	4:A:2307:HOH:O	2.10	0.51
1:A:51:GLU:OE2	2:B:600:TPP:N1'	2.44	0.51
1:C:452:GLN:O	1:C:455:SER:HB3	2.11	0.51
1:B:303:THR:HG22	1:B:305:ASN:HB2	1.93	0.50
1:D:135:THR:CG2	1:D:151:ARG:HH12	2.24	0.50
1:C:160:GLN:O	1:C:161:ARG:HG2	2.11	0.50
1:A:531:THR:HG22	1:A:534:ARG:HH22	1.75	0.50
1:D:245:THR:HG22	1:D:299:TYR:OH	2.12	0.50
1:C:288:LEU:HD13	1:C:411:LEU:CD1	2.37	0.50
1:B:135:THR:HG22	1:B:136:THR:N	2.27	0.50
1:D:225:HIS:HB2	1:D:326:MET:HE1	1.93	0.50
1:A:104:VAL:HG22	1:A:168:PRO:CB	2.42	0.50
1:A:483:GLU:HG3	1:A:543:MET:CE	2.41	0.50
1:D:531:THR:HG22	1:D:534:ARG:HH22	1.77	0.50
1:C:370:VAL:O	1:C:374:VAL:HG23	2.12	0.50
1:C:68:SER:HA	4:C:2050:HOH:O	2.11	0.49
1:B:314:THR:HG23	1:B:324:VAL:HB	1.94	0.49
1:A:359:VAL:HG23	1:A:515:THR:HG21	1.94	0.49
1:A:510:VAL:HG21	1:A:521:LEU:CD2	2.43	0.49
1:C:119:ASN:ND2	1:C:121:ASP:HB3	2.28	0.49
1:A:302:LYS:N	1:D:304:LYS:NZ	2.59	0.49
1:D:381:GLY:O	1:D:436:LYS:HG3	2.12	0.49
1:D:200:VAL:O	1:D:204:VAL:HG23	2.13	0.49
1:A:393:PHE:HE2	1:A:476:ILE:CD1	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:GLY:HA3	1:C:71:ILE:O	2.12	0.49
1:C:73:THR:HG22	4:C:2051:HOH:O	2.12	0.49
1:A:562:LYS:HG2	1:A:563:ASN:H	1.78	0.49
1:B:359:VAL:HG23	1:B:515:THR:HG21	1.95	0.48
1:C:246:PRO:HB2	1:C:410:VAL:HG21	1.93	0.48
1:C:31:LEU:HD11	1:D:477:GLU:HG3	1.95	0.48
1:A:121:ASP:CG	1:A:127:ARG:HH12	2.16	0.48
1:D:552:GLN:O	1:D:556:THR:HG23	2.12	0.48
1:C:514:THR:OG1	1:C:517:GLU:HG3	2.13	0.48
1:B:135:THR:HG22	1:B:136:THR:H	1.78	0.48
1:A:314:THR:HG22	1:A:324:VAL:O	2.14	0.47
1:C:202:GLU:HG2	4:C:2198:HOH:O	2.15	0.47
1:D:386:THR:HG21	1:D:395:ILE:HB	1.96	0.47
1:D:92:HIS:CD2	1:D:288:LEU:CD1	2.97	0.47
1:A:17:VAL:HG12	1:A:187:LEU:HD11	1.97	0.47
1:B:314:THR:HG22	1:B:324:VAL:O	2.14	0.47
1:C:389:GLY:HA2	1:C:476:ILE:HG21	1.97	0.47
1:D:205:LEU:HD11	1:D:336:LYS:HB2	1.96	0.47
1:C:473:GLY:HA2	1:C:490:ILE:HG12	1.96	0.47
1:B:560:ASN:N	1:B:560:ASN:OD1	2.48	0.47
1:B:411:LEU:O	1:B:411:LEU:HD23	2.14	0.47
2:C:600:TPP:H7'1	1:D:27:GLY:HA2	1.97	0.47
1:D:135:THR:HG22	1:D:136:THR:H	1.80	0.47
1:B:112:LEU:CD1	1:B:112:LEU:C	2.83	0.47
1:B:28:ASP:CG	4:B:2012:HOH:O	2.52	0.47
1:A:101:VAL:HB	1:A:102:PRO:CD	2.45	0.46
1:B:135:THR:HG21	1:B:151:ARG:NH1	2.24	0.46
1:C:244:VAL:HG21	1:C:249:LYS:HA	1.98	0.46
1:A:471:ASN:O	1:A:542:THR:HB	2.16	0.46
1:D:154:ARG:NH2	1:D:188:SER:O	2.49	0.46
1:C:293:ASN:HB2	1:D:113:LEU:HB3	1.96	0.46
1:A:510:VAL:HG21	1:A:521:LEU:HD22	1.97	0.46
1:D:385:ILE:HG12	1:D:407:ILE:HB	1.98	0.46
1:B:411:LEU:HD23	1:B:411:LEU:C	2.36	0.46
1:A:498:LEU:HD12	1:B:501:THR:CG2	2.46	0.46
1:B:310:HIS:O	1:B:326:MET:HB2	2.16	0.46
1:D:344:TYR:CE2	1:D:346:PRO:HA	2.51	0.46
1:B:73:THR:HG22	4:B:2037:HOH:O	2.16	0.45
1:A:562:LYS:CG	1:A:563:ASN:H	2.29	0.45
1:A:436:LYS:HB2	1:A:436:LYS:HE2	1.74	0.45
1:B:387:GLU:HG2	1:B:446:SER:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ILE:HG22	1:D:171:LEU:HD12	1.98	0.45
1:D:310:HIS:O	1:D:326:MET:HB2	2.16	0.45
1:D:154:ARG:NE	1:D:186:ASP:O	2.43	0.45
1:D:87:GLY:HA2	1:D:412:TRP:CG	2.52	0.45
1:C:90:ALA:HB1	1:C:411:LEU:CD2	2.47	0.45
1:C:135:THR:CG2	1:C:151:ARG:HH12	2.22	0.45
1:A:3:GLU:HG2	1:A:177:PRO:HA	1.98	0.45
1:D:64:LEU:HD21	1:D:383:VAL:HG21	1.97	0.45
1:B:303:THR:HG21	1:B:305:ASN:HB2	1.99	0.45
1:D:459:ARG:NH2	4:D:2233:HOH:O	2.48	0.45
1:C:145:ALA:HB3	1:C:146:PRO:HD3	1.99	0.45
1:C:225:HIS:HB2	1:C:326:MET:CE	2.46	0.45
1:B:168:PRO:HB2	1:B:171:LEU:HD23	1.99	0.45
1:C:109:LYS:HB3	1:C:109:LYS:HE3	1.63	0.44
1:C:314:THR:HG23	1:C:324:VAL:O	2.17	0.44
1:C:154:ARG:NH2	1:C:188:SER:O	2.50	0.44
1:B:103:SER:CB	1:B:170:ASN:OD1	2.66	0.44
1:D:314:THR:HG22	1:D:324:VAL:O	2.17	0.44
1:A:40:VAL:HB	1:A:43:MET:HG3	2.00	0.44
1:A:435:LYS:HA	1:A:435:LYS:HD2	1.78	0.44
1:A:3:GLU:HB3	1:A:175:THR:HB	2.00	0.44
1:B:463:LYS:N	1:B:464:PRO:CD	2.81	0.44
1:A:314:THR:HG23	1:A:324:VAL:HB	2.00	0.44
1:D:554:GLN:HG3	4:D:2304:HOH:O	2.17	0.44
1:D:469:LEU:HD13	1:D:540:LEU:CD1	2.47	0.43
1:B:141:ASP:CG	1:D:135:THR:HG23	2.38	0.43
1:B:71:ILE:HA	1:B:98:VAL:O	2.18	0.43
1:C:288:LEU:CD1	1:C:411:LEU:CD1	2.96	0.43
1:C:551:LYS:O	1:C:555:LEU:HB3	2.18	0.43
1:B:89:TYR:O	1:B:161:ARG:HD3	2.17	0.43
1:B:290:SER:HB2	4:B:2157:HOH:O	2.18	0.43
1:D:312:ASP:OD2	1:D:312:ASP:N	2.50	0.43
1:D:40:VAL:HB	1:D:43:MET:HG3	1.99	0.43
1:C:244:VAL:HG23	1:C:262:VAL:HB	2.00	0.43
1:B:225:HIS:HB2	1:B:326:MET:HE1	2.01	0.43
1:A:312:ASP:HB3	1:A:313:TYR:HD1	1.84	0.43
1:C:472:ASP:HB3	1:C:542:THR:HG22	2.00	0.43
1:B:372:THR:HB	4:B:2220:HOH:O	2.19	0.43
1:D:267:LEU:HD13	1:D:393:PHE:CE1	2.54	0.43
1:B:98:VAL:CG1	1:B:167:LEU:HD22	2.49	0.43
1:B:381:GLY:O	1:B:436:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:THR:HG21	1:D:151:ARG:NH1	2.31	0.43
1:A:227:ALA:HB3	1:A:326:MET:HE3	2.01	0.43
1:A:101:VAL:HB	1:A:102:PRO:HD2	2.00	0.42
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.78	0.42
1:D:107:GLN:N	1:D:107:GLN:OE1	2.52	0.42
1:A:12:GLU:O	1:A:16:GLN:HG3	2.19	0.42
1:A:135:THR:CG2	1:C:141:ASP:OD2	2.67	0.42
1:A:426:ALA:HA	1:A:438:VAL:HG21	1.99	0.42
1:C:120:GLY:HA2	4:C:2072:HOH:O	2.19	0.42
1:C:347:VAL:HA	1:C:348:PRO:HD2	1.90	0.42
1:A:82:LEU:HA	1:A:82:LEU:HD12	1.95	0.42
1:C:459:ARG:NH1	4:C:2291:HOH:O	2.53	0.42
1:A:160:GLN:O	1:A:161:ARG:HG2	2.19	0.42
1:A:289:LEU:O	1:A:289:LEU:HD23	2.20	0.42
1:A:309:PHE:HB3	1:A:326:MET:HG3	2.02	0.42
1:C:294:THR:HG22	1:C:295:GLY:N	2.35	0.41
1:D:372:THR:HG21	4:D:2165:HOH:O	2.20	0.41
1:A:386:THR:HG21	1:A:395:ILE:CB	2.46	0.41
1:C:253:ASP:HB3	1:C:402:ASN:OD1	2.20	0.41
1:A:541:PRO:HB2	1:A:544:ASP:HB2	2.02	0.41
1:D:135:THR:HG22	1:D:136:THR:N	2.35	0.41
1:B:71:ILE:HG12	1:B:98:VAL:HB	2.03	0.41
1:C:371:TRP:CD1	1:C:394:GLY:HA3	2.55	0.41
1:A:483:GLU:HG3	1:A:543:MET:HE2	2.01	0.41
1:D:289:LEU:HD22	1:D:411:LEU:HD21	2.02	0.41
1:A:563:ASN:OD1	1:B:106:SER:HB2	2.20	0.41
1:B:380:GLU:HG2	1:B:402:ASN:O	2.21	0.41
1:A:345:LYS:HA	1:A:346:PRO:HD3	1.72	0.41
1:A:244:VAL:HG23	1:A:262:VAL:HB	2.03	0.41
1:D:415:ILE:HB	1:D:446:SER:OG	2.20	0.41
1:B:345:LYS:O	1:B:346:PRO:O	2.39	0.41
1:B:24:GLY:HA3	1:B:71:ILE:O	2.20	0.41
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.93	0.41
1:B:294:THR:CG2	1:B:296:SER:H	2.06	0.41
1:A:267:LEU:CD1	1:A:297:PHE:HB3	2.47	0.41
1:B:233:LYS:HE3	1:B:237:LEU:HD21	2.03	0.41
1:B:116:THR:HG23	1:B:118:GLY:H	1.86	0.41
1:D:472:ASP:HB3	1:D:542:THR:HG22	2.03	0.41
1:D:314:THR:HG23	1:D:324:VAL:HB	2.02	0.41
1:B:469:LEU:HB3	1:B:540:LEU:HD12	2.03	0.41
1:D:57:ALA:HA	1:D:420:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:THR:HA	1:B:184:PRO:HD3	1.97	0.40
1:B:197:GLU:OE2	1:B:332:LYS:HD3	2.21	0.40
1:B:136:THR:HA	1:B:164:TYR:O	2.21	0.40
1:D:71:ILE:HA	1:D:98:VAL:O	2.21	0.40
1:B:386:THR:HG21	1:B:395:ILE:HB	2.03	0.40
1:D:160:GLN:O	1:D:161:ARG:HG2	2.21	0.40
1:B:389:GLY:HA2	1:B:476:ILE:HG21	2.03	0.40
1:B:95:VAL:O	1:B:162:PRO:HA	2.22	0.40
1:D:119:ASN:ND2	4:D:2061:HOH:O	2.29	0.40
1:D:303:THR:HG22	1:D:305:ASN:CA	2.48	0.40
1:D:303:THR:CG2	1:D:304:LYS:N	2.84	0.40
1:A:345:LYS:HA	1:A:345:LYS:HD3	1.91	0.40
1:B:463:LYS:HD2	1:B:530:ASN:O	2.22	0.40
1:B:415:ILE:HG13	1:B:449:LEU:HD22	2.03	0.40
1:D:253:ASP:HB3	1:D:402:ASN:OD1	2.22	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	556/563 (99%)	527 (95%)	24 (4%)	5 (1%)	21 9
1	B	553/563 (98%)	538 (97%)	11 (2%)	4 (1%)	26 14
1	C	551/563 (98%)	535 (97%)	14 (2%)	2 (0%)	39 27
1	D	556/563 (99%)	539 (97%)	17 (3%)	0	100 100
All	All	2216/2252 (98%)	2139 (96%)	66 (3%)	11 (0%)	34 21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	TYR
1	B	346	PRO
1	B	347	VAL
1	B	559	THR
1	C	109	LYS
1	A	291	ASP
1	A	300	SER
1	A	290	SER
1	B	104	VAL
1	C	291	ASP
1	A	346	PRO

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	471/474 (99%)	440 (93%)	31 (7%)	21 7
1	B	468/474 (99%)	438 (94%)	30 (6%)	22 8
1	C	467/474 (98%)	448 (96%)	19 (4%)	37 22
1	D	471/474 (99%)	442 (94%)	29 (6%)	23 8
All	All	1877/1896 (99%)	1768 (94%)	109 (6%)	25 10

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	104	VAL
1	A	107	GLN
1	A	109	LYS
1	A	111	LEU
1	A	135	THR
1	A	149	ILE
1	A	161	ARG
1	A	167	LEU
1	A	172	VAL
1	A	174	LEU

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Mol	Chain	Res	Type
1	A	190	LYS
1	A	217	LEU
1	A	224	ARG
1	A	233	LYS
1	A	262	VAL
1	A	283	LEU
1	A	291	ASP
1	A	297	PHE
1	A	314	THR
1	A	330	LEU
1	A	333	LEU
1	A	339	ASP
1	A	459	ARG
1	A	477	GLU
1	A	479	LEU
1	A	480	ILE
1	A	498	LEU
1	A	515	THR
1	A	542	THR
1	A	549	LEU
1	B	28	ASP
1	B	105	SER
1	B	115	HIS
1	B	161	ARG
1	B	165	LEU
1	B	167	LEU
1	B	171	LEU
1	B	174	LEU
1	B	190	LYS
1	B	202	GLU
1	B	207	LEU
1	B	224	ARG
1	B	262	VAL
1	B	283	LEU
1	B	288	LEU
1	B	291	ASP
1	B	294	THR
1	B	314	THR
1	B	346	PRO
1	B	359	VAL
1	B	368	GLU
1	B	372	THR

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Mol	Chain	Res	Type
1	B	459	ARG
1	B	477	GLU
1	B	515	THR
1	B	521	LEU
1	B	551	LYS
1	B	552	GLN
1	B	555	LEU
1	B	560	ASN
1	C	65	LYS
1	C	109	LYS
1	C	110	GLN
1	C	135	THR
1	C	171	LEU
1	C	224	ARG
1	C	262	VAL
1	C	266	THR
1	C	288	LEU
1	C	291	ASP
1	C	300	SER
1	C	447	LEU
1	C	452	GLN
1	C	515	THR
1	C	525	GLU
1	C	531	THR
1	C	549	LEU
1	C	555	LEU
1	C	560	ASN
1	D	82	LEU
1	D	109	LYS
1	D	112	LEU
1	D	138	MET
1	D	171	LEU
1	D	174	LEU
1	D	190	LYS
1	D	207	LEU
1	D	212	LYS
1	D	224	ARG
1	D	264	VAL
1	D	266	THR
1	D	289	LEU
1	D	302	LYS
1	D	314	THR

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Mol	Chain	Res	Type
1	D	333	LEU
1	D	337	VAL
1	D	342	LYS
1	D	354	GLU
1	D	357	GLU
1	D	452	GLN
1	D	469	LEU
1	D	477	GLU
1	D	479	LEU
1	D	515	THR
1	D	520	LYS
1	D	551	LYS
1	D	554	GLN
1	D	562	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	114	HIS
1	D	107	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TPP	A	600	3	20,27,27	1.39	4 (20%)	31,40,40	1.87	8 (25%)
2	TPP	B	600	3	20,27,27	1.67	5 (25%)	31,40,40	1.66	7 (22%)
2	TPP	C	600	3	20,27,27	1.42	2 (10%)	31,40,40	1.71	9 (29%)
2	TPP	D	600	3	20,27,27	1.40	4 (20%)	31,40,40	1.75	5 (16%)

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	TPP	A	600	3	-	0/16/17/17	0/2/2/2
2	TPP	B	600	3	-	0/16/17/17	0/2/2/2
2	TPP	C	600	3	-	0/16/17/17	0/2/2/2
2	TPP	D	600	3	-	0/16/17/17	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	TPP	C4-N3	-2.66	1.37	1.39
2	A	600	TPP	PB-O2B	-2.29	1.46	1.54
2	A	600	TPP	C4-N3	-2.22	1.37	1.39
2	B	600	TPP	C6'-C5'	2.05	1.42	1.37
2	B	600	TPP	C4'-N3'	2.32	1.38	1.35
2	A	600	TPP	C2'-N3'	2.52	1.38	1.34
2	C	600	TPP	C2'-N3'	2.53	1.38	1.34
2	D	600	TPP	C2'-N1'	2.62	1.38	1.34
2	D	600	TPP	C6'-N1'	2.63	1.40	1.34
2	B	600	TPP	C2'-N3'	2.67	1.39	1.34
2	D	600	TPP	C4'-N3'	2.67	1.39	1.35
2	A	600	TPP	C6'-N1'	2.82	1.40	1.34
2	B	600	TPP	C2'-N1'	3.20	1.39	1.34
2	C	600	TPP	C4'-N3'	3.22	1.40	1.35
2	B	600	TPP	C6'-N1'	4.39	1.43	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	TPP	C6-C5-S1	-3.69	115.07	120.24
2	A	600	TPP	N1'-C2'-N3'	-3.66	118.82	125.60
2	A	600	TPP	C6-C5-S1	-3.56	115.25	120.24
2	A	600	TPP	C5'-C6'-N1'	-3.45	117.87	123.86
2	D	600	TPP	N1'-C2'-N3'	-3.35	119.41	125.60
2	D	600	TPP	C6-C5-S1	-3.34	115.57	120.24
2	C	600	TPP	N1'-C2'-N3'	-3.12	119.84	125.60
2	B	600	TPP	C5'-C6'-N1'	-3.06	118.55	123.86
2	C	600	TPP	CM4-C4-C5	-2.92	122.33	128.90
2	C	600	TPP	C6-C5-S1	-2.56	116.65	120.24
2	C	600	TPP	C5'-C6'-N1'	-2.43	119.64	123.86
2	B	600	TPP	N1'-C2'-N3'	-2.21	121.51	125.60
2	C	600	TPP	O3A-PA-O7	-2.11	97.33	102.94
2	D	600	TPP	C6'-C5'-C4'	2.03	118.64	115.72
2	A	600	TPP	CM2-C2'-N3'	2.18	120.91	117.20
2	B	600	TPP	C6'-N1'-C2'	2.25	119.70	115.77
2	B	600	TPP	C6-C5-C4	2.36	129.68	127.56
2	C	600	TPP	CM2-C2'-N1'	2.40	119.91	117.03
2	D	600	TPP	C6'-N1'-C2'	2.43	120.01	115.77
2	B	600	TPP	C6'-C5'-C4'	2.44	119.22	115.72
2	C	600	TPP	C6'-C5'-C4'	2.65	119.52	115.72
2	A	600	TPP	CM2-C2'-N1'	2.70	120.27	117.03
2	C	600	TPP	CM4-C4-N3	2.98	126.56	122.59
2	A	600	TPP	C6'-C5'-C4'	3.02	120.06	115.72
2	C	600	TPP	C6'-N1'-C2'	3.04	121.09	115.77
2	A	600	TPP	C6-C5-C4	3.60	130.79	127.56
2	A	600	TPP	C6'-N1'-C2'	3.75	122.33	115.77
2	B	600	TPP	CM2-C2'-N1'	4.86	122.86	117.03
2	D	600	TPP	CM2-C2'-N1'	5.43	123.55	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	TPP	1	0
2	C	600	TPP	1	0

5.7 Other polymers (i)

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	560/563 (99%)	-0.04	18 (3%)	51	61	9, 21, 44, 74	0
1	B	557/563 (98%)	0.18	23 (4%)	41	52	9, 20, 37, 79	0
1	C	555/563 (98%)	-0.07	16 (2%)	55	65	8, 17, 41, 81	0
1	D	560/563 (99%)	-0.09	12 (2%)	67	75	8, 20, 42, 68	0
All	All	2232/2252 (99%)	-0.01	69 (3%)	52	62	8, 19, 42, 81	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	558	ALA	10.1
1	C	559	THR	9.6
1	C	560	ASN	8.6
1	D	107	GLN	7.5
1	B	561	ALA	7.5
1	B	560	ASN	6.6
1	C	290	SER	6.5
1	B	113	LEU	6.2
1	B	559	THR	5.8
1	A	292	PHE	5.7
1	D	108	ALA	5.6
1	A	107	GLN	5.5
1	C	558	ALA	5.2
1	A	301	TYR	4.7
1	B	557	ALA	4.7
1	A	563	ASN	4.7
1	D	111	LEU	4.7
1	C	555	LEU	4.5
1	B	555	LEU	4.4
1	B	556	THR	4.4
1	C	347	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	289	LEU	4.1
1	A	299	TYR	4.1
1	B	112	LEU	3.9
1	C	299	TYR	3.8
1	A	297	PHE	3.8
1	A	294	THR	3.5
1	A	109	LYS	3.4
1	A	108	ALA	3.3
1	D	112	LEU	3.2
1	C	348	PRO	3.2
1	A	296	SER	3.1
1	B	105	SER	3.1
1	D	109	LYS	2.9
1	D	347	VAL	2.8
1	C	110	GLN	2.8
1	C	554	GLN	2.8
1	B	55	ALA	2.7
1	B	359	VAL	2.6
1	B	108	ALA	2.6
1	A	354	GLU	2.6
1	B	417	PHE	2.6
1	A	300	SER	2.6
1	D	117	LEU	2.6
1	A	291	ASP	2.6
1	A	293	ASN	2.5
1	B	52	LEU	2.5
1	D	122	PHE	2.5
1	C	298	SER	2.5
1	B	107	GLN	2.4
1	C	557	ALA	2.4
1	C	291	ASP	2.4
1	A	288	LEU	2.4
1	C	288	LEU	2.4
1	D	557	ALA	2.3
1	A	295	GLY	2.2
1	A	298	SER	2.2
1	B	114	HIS	2.2
1	B	115	HIS	2.2
1	B	57	ALA	2.2
1	D	110	GLN	2.2
1	B	56	TYR	2.1
1	D	116	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	301	TYR	2.1
1	B	104	VAL	2.1
1	C	556	THR	2.1
1	D	114	HIS	2.1
1	B	419	THR	2.0
1	B	407	ILE	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
3	MG	D	601	1/1	0.98	0.14	5.12	20,20,20,20	0
3	MG	B	601	1/1	0.97	0.09	0.22	17,17,17,17	0
2	TPP	D	600	26/26	0.99	0.10	-0.25	8,14,17,18	0
2	TPP	B	600	26/26	0.99	0.11	-0.25	9,12,15,15	0
2	TPP	C	600	26/26	0.99	0.11	-0.31	7,10,12,14	0
2	TPP	A	600	26/26	0.98	0.10	-0.61	10,13,15,16	0
3	MG	C	601	1/1	0.99	0.09	-0.67	12,12,12,12	0
3	MG	A	601	1/1	0.98	0.06	-1.27	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.