Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:58 PM GMT

PDB ID	:	1DIK
Title	:	PYRUVATE PHOSPHATE DIKINASE
Authors	:	Herzberg, O.; Chen, C.C.H.
Deposited on	:	1995-12-06
Resolution	:	2.30 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 (i)) were used in the production of this report:

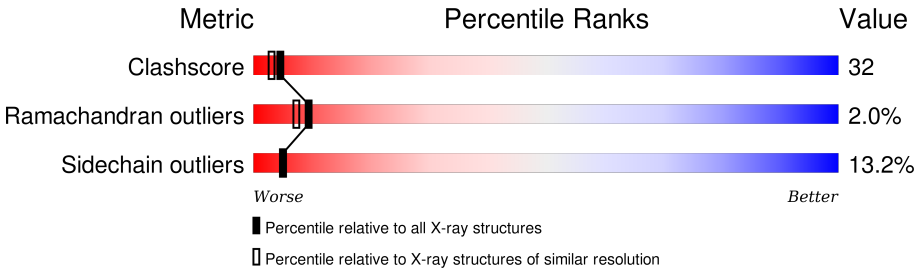
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	874	44% 46% 8% ••

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
2	SO4	A	875	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7161 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.

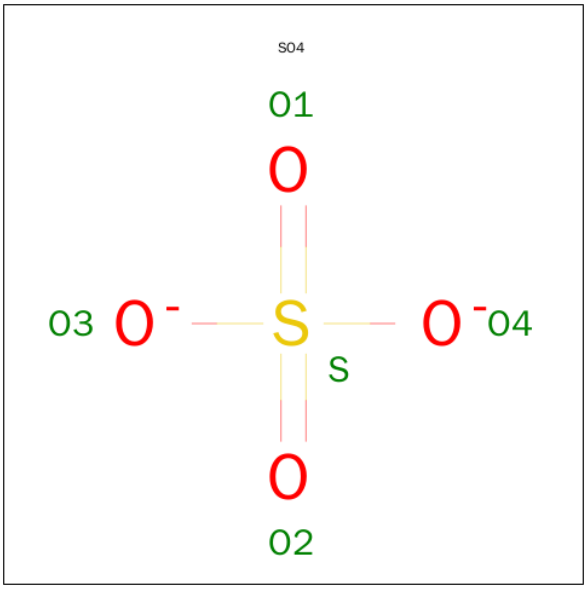
- Molecule 1 is a protein called PYRUVATE PHOSPHATE DIKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	869	Total	C	N	O	S	0	0	0
			6730	4236	1140	1303	51			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	GLY	CONFLICT	UNP P22983

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	416	Total	O	0	0
			416	416		

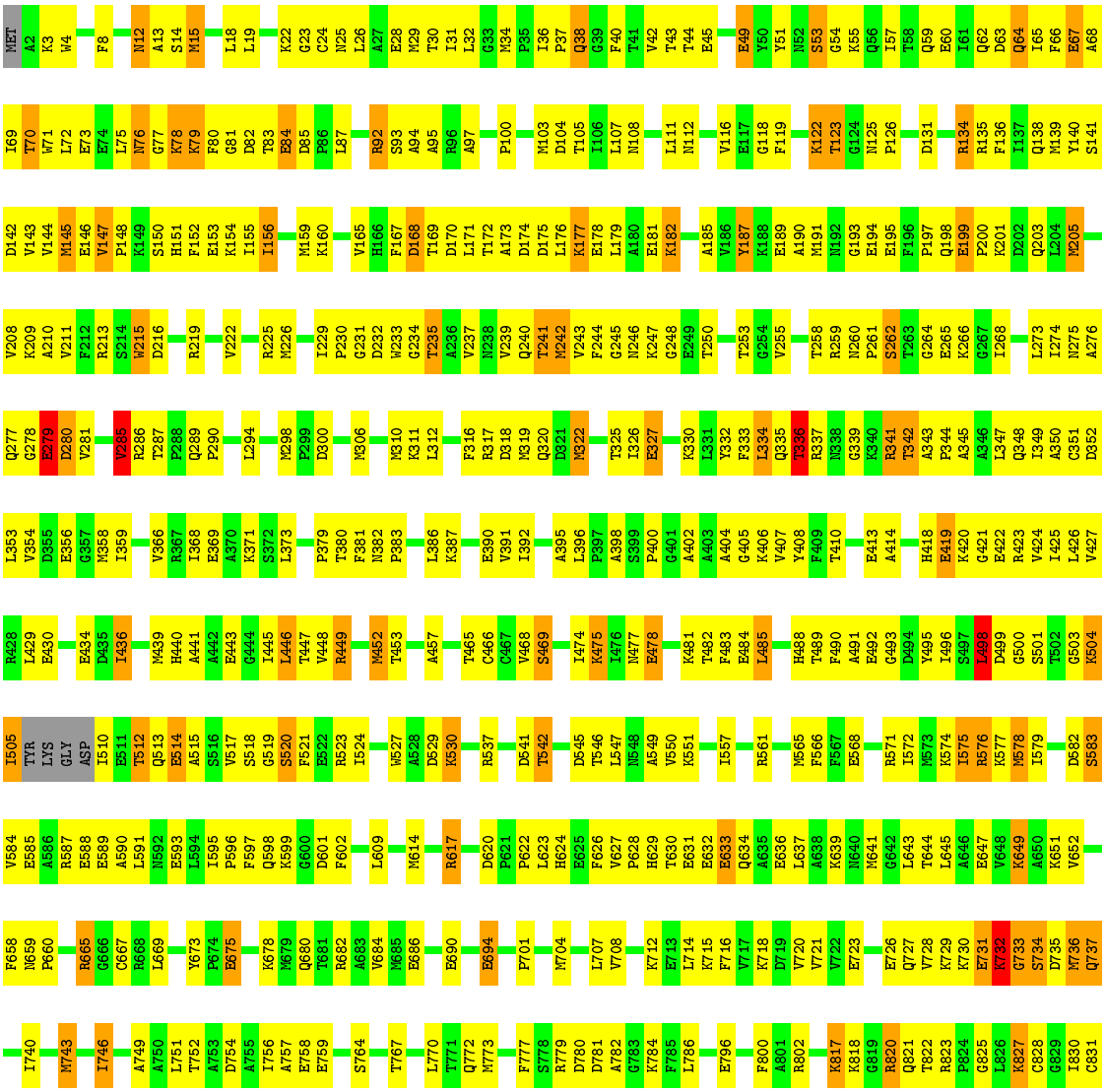
3 Residue-property plots (i)

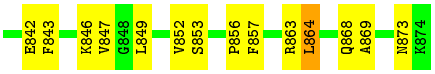
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: PYRUVATE PHOSPHATE DIKINASE

Chain A:




E842
F843
K846
V847
G848
L849
V852
S853
P856
F857
R863
L864
Q868
A869
N873
K874

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	89.80Å 58.80Å 102.00Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	80.0 (8.00-2.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7161	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.87	2/6852 (0.0%)	0.99	12/9234 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	GLU	CG-CD	5.72	1.60	1.51
1	A	667	CYS	CB-SG	-5.14	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	449	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	A	561	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	A	731	GLU	O-C-N	6.69	133.40	122.70
1	A	617	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	736	MET	CG-SD-CE	6.09	109.94	100.20
1	A	242	MET	CG-SD-CE	6.04	109.86	100.20
1	A	498	LEU	CA-CB-CG	6.00	129.09	115.30
1	A	743	MET	CG-SD-CE	5.67	109.27	100.20
1	A	336	THR	N-CA-CB	5.41	120.57	110.30
1	A	820	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	731	GLU	CA-C-N	-5.24	105.67	117.20
1	A	92	ARG	NE-CZ-NH2	-5.15	117.73	120.30

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	6730	0	6653	432	0
2	A	15	0	0	1	0
3	A	416	0	0	24	0
All	All	7161	0	6653	432	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 32.

All (432) 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:373:LEU:HD11	1:A:864:LEU:HD12	1.33	1.11
1:A:76:ASN:O	1:A:78:LYS:HG2	1.55	1.06
1:A:107:LEU:HB3	1:A:242:MET:HE2	1.27	1.06
1:A:342:THR:HG23	1:A:344:PRO:HD2	1.37	1.05
1:A:253:THR:HG21	1:A:278:GLY:N	1.78	0.98
1:A:400:PRO:HA	1:A:499:ASP:HB3	1.45	0.97
1:A:276:ALA:HB1	1:A:281:VAL:CG2	1.94	0.97
1:A:107:LEU:HB3	1:A:242:MET:CE	1.97	0.94
1:A:732:LYS:C	1:A:734:SER:H	1.68	0.94
1:A:419:GLU:HA	1:A:441:ALA:HB1	1.57	0.87
1:A:483:PHE:HE2	1:A:485:LEU:HD12	1.40	0.86
1:A:277:GLN:O	1:A:281:VAL:HG22	1.73	0.86
1:A:493:GLY:HA3	3:A:1070:HOH:O	1.73	0.86
1:A:3:LYS:HG2	3:A:986:HOH:O	1.76	0.86
1:A:107:LEU:HD11	1:A:279:GLU:HB2	1.58	0.85
1:A:153:GLU:HA	1:A:156:ILE:HG22	1.59	0.85
1:A:519:GLY:O	1:A:523:ARG:HG3	1.78	0.83
1:A:737:GLN:HE21	1:A:737:GLN:H	1.28	0.82
1:A:732:LYS:O	1:A:734:SER:N	2.13	0.81
1:A:447:THR:OG1	1:A:469:SER:HA	1.80	0.81
1:A:146:GLU:HG3	1:A:187:TYR:CE2	2.17	0.80
1:A:276:ALA:HB1	1:A:281:VAL:HG23	1.61	0.80
1:A:276:ALA:HB1	1:A:281:VAL:HG21	1.61	0.80
1:A:165:VAL:HG13	1:A:170:ASP:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ALA:HA	1:A:24:CYS:HB2	1.64	0.80
1:A:122:LYS:HD2	1:A:122:LYS:O	1.81	0.79
1:A:347:LEU:HD22	1:A:524:ILE:HG13	1.64	0.78
1:A:408:TYR:HB3	1:A:413:GLU:HG3	1.66	0.78
1:A:392:ILE:HD13	1:A:485:LEU:HD13	1.66	0.77
1:A:576:ARG:HD3	1:A:626:PHE:O	1.83	0.77
1:A:392:ILE:HD11	1:A:495:TYR:CE1	2.20	0.76
1:A:447:THR:HG1	1:A:469:SER:HA	1.48	0.76
1:A:29:MET:HA	1:A:32:LEU:HD12	1.67	0.76
1:A:434:GLU:HB2	3:A:961:HOH:O	1.85	0.76
1:A:381:PHE:CZ	1:A:496:ILE:HG23	2.20	0.76
1:A:732:LYS:C	1:A:734:SER:N	2.38	0.75
1:A:392:ILE:CD1	1:A:485:LEU:HD13	2.18	0.73
1:A:145:MET:C	1:A:145:MET:SD	2.67	0.73
1:A:727:GLN:HG3	3:A:1006:HOH:O	1.89	0.73
1:A:395:ALA:HB3	1:A:468:VAL:HG12	1.70	0.73
1:A:704:MET:SD	1:A:743:MET:HG2	2.29	0.72
1:A:342:THR:HG22	1:A:345:ALA:H	1.54	0.72
1:A:147:VAL:HG12	1:A:148:PRO:HD2	1.69	0.72
1:A:395:ALA:HB3	1:A:468:VAL:CG1	2.20	0.72
1:A:637:LEU:O	1:A:641:MET:HG3	1.90	0.71
1:A:80:PHE:HA	1:A:87:LEU:HB3	1.71	0.71
1:A:57:ILE:CD1	1:A:209:LYS:HG3	2.20	0.71
1:A:146:GLU:HB3	1:A:191:MET:SD	2.30	0.71
1:A:57:ILE:HD11	1:A:209:LYS:HG3	1.73	0.71
1:A:407:VAL:O	1:A:492:GLU:HA	1.91	0.71
1:A:515:ALA:HB3	3:A:1142:HOH:O	1.90	0.70
1:A:825:GLY:HA3	3:A:899:HOH:O	1.91	0.70
1:A:352:ASP:O	1:A:356:GLU:HG3	1.91	0.70
1:A:644:THR:OG1	1:A:647:GLU:HG2	1.92	0.69
1:A:268:ILE:HG13	1:A:306:MET:SD	2.32	0.69
1:A:732:LYS:HD3	1:A:734:SER:HA	1.75	0.69
1:A:42:VAL:HB	1:A:237:VAL:HG12	1.73	0.69
1:A:404:ALA:HB1	1:A:496:ILE:HG13	1.75	0.69
1:A:398:ALA:HB2	1:A:469:SER:OG	1.93	0.69
1:A:146:GLU:HG3	1:A:187:TYR:HE2	1.58	0.68
1:A:141:SER:HG	1:A:187:TYR:HD2	1.42	0.68
1:A:285:VAL:HG22	1:A:286:ARG:H	1.58	0.68
1:A:30:THR:OG1	1:A:36:ILE:HD11	1.93	0.67
1:A:278:GLY:O	1:A:280:ASP:N	2.27	0.67
1:A:737:GLN:NE2	1:A:737:GLN:H	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TYR:CD1	1:A:424:VAL:HG13	2.30	0.67
1:A:312:LEU:HD13	1:A:336:THR:HG21	1.77	0.67
1:A:584:VAL:HG22	1:A:587:ARG:NH1	2.10	0.67
1:A:225:ARG:HG3	1:A:796:GLU:O	1.94	0.67
1:A:38:GLN:NE2	1:A:38:GLN:HA	2.10	0.66
1:A:262:SER:O	1:A:342:THR:HG21	1.96	0.66
1:A:259:ARG:HG2	1:A:266:LYS:HA	1.77	0.66
1:A:276:ALA:HB2	1:A:286:ARG:NH2	2.11	0.66
1:A:474:ILE:HG23	1:A:483:PHE:CD2	2.30	0.66
1:A:609:LEU:HD11	1:A:614:MET:HB2	1.76	0.66
1:A:546:THR:O	1:A:550:VAL:HG23	1.97	0.66
1:A:222:VAL:O	1:A:226:MET:HG2	1.97	0.65
1:A:380:THR:CG2	1:A:515:ALA:HB2	2.27	0.65
1:A:156:ILE:HD12	1:A:179:LEU:HD21	1.78	0.64
1:A:381:PHE:CD2	1:A:402:ALA:HB1	2.32	0.64
1:A:327:GLU:HB2	1:A:332:TYR:HE2	1.63	0.64
1:A:167:PHE:CB	1:A:169:THR:HG22	2.28	0.63
1:A:405:GLY:HA3	1:A:423:ARG:O	1.98	0.63
1:A:400:PRO:HA	1:A:499:ASP:CB	2.26	0.63
1:A:312:LEU:HD13	1:A:336:THR:CG2	2.28	0.63
1:A:379:PRO:HB2	1:A:512:THR:HB	1.80	0.63
1:A:754:ASP:O	1:A:822:THR:HG21	1.98	0.63
1:A:530:LYS:NZ	1:A:530:LYS:HB2	2.13	0.63
1:A:802:ARG:HD2	3:A:1011:HOH:O	1.99	0.63
1:A:498:LEU:HD22	1:A:500:GLY:H	1.64	0.63
1:A:629:HIS:HA	1:A:634:GLN:HE21	1.64	0.62
1:A:43:THR:HG21	1:A:45:GLU:HG3	1.79	0.62
1:A:392:ILE:HD11	1:A:495:TYR:HE1	1.63	0.62
1:A:123:THR:HG23	1:A:125:ASN:H	1.65	0.62
1:A:135:ARG:HH12	1:A:281:VAL:CG1	2.13	0.62
1:A:565:MET:HG2	1:A:601:ASP:OD2	2.00	0.62
1:A:43:THR:CG2	1:A:45:GLU:HG3	2.29	0.62
1:A:182:LYS:O	1:A:185:ALA:HB3	2.00	0.62
1:A:38:GLN:O	1:A:241:THR:HG22	2.00	0.62
1:A:827:LYS:N	1:A:827:LYS:HD2	2.13	0.62
1:A:334:LEU:O	1:A:335:GLN:HB2	2.00	0.61
1:A:395:ALA:O	1:A:501:SER:HB3	2.00	0.61
1:A:153:GLU:HA	1:A:156:ILE:CG2	2.29	0.61
1:A:76:ASN:HD21	1:A:87:LEU:CD1	2.14	0.61
1:A:273:LEU:HD12	1:A:281:VAL:O	2.00	0.61
1:A:651:LYS:HB2	3:A:1122:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:THR:HG22	1:A:545:ASP:H	1.64	0.61
1:A:122:LYS:HD2	1:A:122:LYS:C	2.21	0.61
1:A:85:ASP:OD1	1:A:122:LYS:HG3	2.00	0.61
1:A:18:LEU:HD22	1:A:43:THR:HG21	1.83	0.61
1:A:513:GLN:O	1:A:514:GLU:HB2	2.01	0.60
1:A:258:THR:HG23	1:A:322:MET:CE	2.32	0.60
1:A:215:TRP:CH2	1:A:231:GLY:HA2	2.36	0.60
1:A:491:ALA:O	1:A:492:GLU:HB2	2.01	0.60
1:A:167:PHE:HB3	1:A:169:THR:HG22	1.83	0.60
1:A:578:MET:HG3	1:A:587:ARG:HB3	1.82	0.59
1:A:134:ARG:HG3	1:A:179:LEU:HD23	1.85	0.59
1:A:73:GLU:HG2	1:A:79:LYS:HA	1.85	0.59
1:A:317:ARG:HG2	1:A:358:MET:HG2	1.83	0.59
1:A:751:LEU:O	1:A:818:LYS:NZ	2.34	0.59
1:A:448:VAL:HG22	1:A:474:ILE:HB	1.85	0.58
1:A:587:ARG:NH1	3:A:946:HOH:O	2.31	0.58
1:A:278:GLY:C	1:A:280:ASP:H	2.06	0.58
1:A:60:GLU:O	1:A:64:GLN:HB2	2.02	0.58
1:A:680:GLN:O	1:A:684:VAL:HG23	2.03	0.58
1:A:264:GLY:HA3	1:A:348:GLN:HB3	1.85	0.58
1:A:135:ARG:HH12	1:A:281:VAL:HG11	1.67	0.58
1:A:37:PRO:HB3	1:A:241:THR:HG23	1.86	0.58
1:A:255:VAL:HB	1:A:453:THR:HG21	1.85	0.58
1:A:549:ALA:HB2	1:A:856:PRO:HB3	1.85	0.58
1:A:743:MET:HA	1:A:764:SER:O	2.03	0.58
1:A:630:THR:OG1	1:A:633:GLU:HB2	2.03	0.57
1:A:366:VAL:HA	1:A:868:GLN:HG2	1.86	0.57
1:A:404:ALA:HA	1:A:496:ILE:HA	1.85	0.57
1:A:396:LEU:HD23	1:A:452:MET:SD	2.45	0.57
1:A:43:THR:HG22	1:A:44:THR:N	2.19	0.57
1:A:49:GLU:O	1:A:53:SER:HB2	2.05	0.57
1:A:253:THR:HG21	1:A:278:GLY:CA	2.34	0.57
1:A:630:THR:O	1:A:634:GLN:HG3	2.05	0.57
1:A:259:ARG:CZ	1:A:266:LYS:HD3	2.34	0.57
1:A:589:GLU:HG3	3:A:1223:HOH:O	2.04	0.56
1:A:104:ASP:HB3	1:A:143:VAL:HG13	1.87	0.56
1:A:131:ASP:HB2	1:A:176:LEU:HD13	1.87	0.56
1:A:520:SER:O	1:A:524:ILE:HG12	2.06	0.56
1:A:504:LYS:HG3	1:A:510:ILE:CD1	2.36	0.56
1:A:171:LEU:HD12	1:A:176:LEU:HD23	1.87	0.56
1:A:828:CYS:HB3	1:A:849:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:LYS:HE3	1:A:593:GLU:OE2	2.06	0.56
1:A:12:ASN:OD1	1:A:14:SER:HB2	2.04	0.56
1:A:729:LYS:NZ	1:A:736:MET:O	2.35	0.56
1:A:93:SER:HB2	1:A:235:THR:HG21	1.87	0.56
1:A:410:THR:OG1	1:A:413:GLU:HG2	2.06	0.55
1:A:628:PRO:HG2	1:A:634:GLN:HG2	1.86	0.55
1:A:414:ALA:HB2	1:A:426:LEU:HD13	1.88	0.55
1:A:392:ILE:HG22	1:A:488:HIS:CE1	2.41	0.55
1:A:537:ARG:O	1:A:853:SER:HA	2.06	0.55
1:A:343:ALA:HB3	1:A:344:PRO:HD3	1.88	0.55
1:A:92:ARG:NE	3:A:952:HOH:O	2.39	0.55
1:A:341:ARG:HB3	1:A:345:ALA:HB3	1.88	0.55
1:A:495:TYR:OH	1:A:503:GLY:HA3	2.07	0.54
1:A:382:ASN:OD1	1:A:383:PRO:HD2	2.06	0.54
1:A:496:ILE:HG12	1:A:510:ILE:N	2.21	0.54
1:A:95:ALA:HB3	1:A:97:ALA:O	2.06	0.54
1:A:767:THR:HG21	1:A:830:ILE:HD11	1.89	0.54
1:A:22:LYS:HB2	1:A:94:ALA:CB	2.38	0.54
1:A:624:HIS:HB2	3:A:957:HOH:O	2.05	0.54
1:A:273:LEU:HD11	1:A:286:ARG:O	2.07	0.54
1:A:391:VAL:O	1:A:391:VAL:HG12	2.07	0.54
1:A:199:GLU:OE2	1:A:201:LYS:HB2	2.08	0.54
1:A:258:THR:HG23	1:A:322:MET:HE1	1.89	0.54
1:A:174:ASP:O	1:A:177:LYS:HG3	2.08	0.54
1:A:200:PRO:HA	1:A:203:GLN:OE1	2.08	0.54
1:A:408:TYR:HD1	1:A:424:VAL:HG13	1.70	0.53
1:A:475:LYS:HB2	1:A:484:GLU:HB2	1.88	0.53
1:A:752:THR:O	1:A:756:ILE:HG12	2.08	0.53
1:A:260:ASN:HB2	3:A:954:HOH:O	2.08	0.53
1:A:12:ASN:OD1	1:A:15:MET:HG2	2.09	0.53
1:A:37:PRO:HD2	1:A:240:GLN:NE2	2.23	0.53
1:A:575:ILE:O	1:A:579:ILE:HG13	2.08	0.53
1:A:178:GLU:HA	1:A:178:GLU:OE1	2.09	0.53
1:A:350:ALA:O	1:A:354:VAL:HG23	2.07	0.53
1:A:707:LEU:HG	1:A:746:ILE:CD1	2.39	0.53
1:A:37:PRO:HD2	1:A:240:GLN:HE22	1.74	0.53
1:A:112:ASN:HB2	1:A:198:GLN:OE1	2.08	0.53
1:A:156:ILE:HD12	1:A:179:LEU:CD2	2.38	0.53
1:A:34:MET:SD	1:A:312:LEU:HD21	2.49	0.53
1:A:436:ILE:HD13	1:A:439:MET:HE3	1.90	0.53
1:A:380:THR:HG23	1:A:515:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD13	1:A:242:MET:HE1	1.91	0.53
1:A:419:GLU:O	1:A:421:GLY:N	2.39	0.53
1:A:430:GLU:OE2	1:A:449:ARG:HD2	2.09	0.53
1:A:427:VAL:HG22	1:A:446:LEU:HD12	1.90	0.53
1:A:22:LYS:HB2	1:A:94:ALA:HB2	1.90	0.52
1:A:19:LEU:HD13	3:A:987:HOH:O	2.08	0.52
1:A:139:MET:HG2	3:A:1158:HOH:O	2.10	0.52
1:A:483:PHE:CE2	1:A:485:LEU:HD12	2.32	0.52
1:A:103:MET:HE1	1:A:235:THR:CG2	2.39	0.52
1:A:76:ASN:O	1:A:78:LYS:N	2.43	0.52
1:A:81:GLY:HA3	1:A:200:PRO:HG3	1.91	0.52
1:A:419:GLU:C	1:A:421:GLY:H	2.13	0.52
1:A:171:LEU:HB3	1:A:175:ASP:HB2	1.90	0.52
1:A:391:VAL:HG22	1:A:504:LYS:HE3	1.91	0.52
1:A:104:ASP:HB3	1:A:143:VAL:CG1	2.39	0.52
1:A:244:PHE:N	1:A:244:PHE:CD1	2.78	0.52
1:A:802:ARG:HG2	1:A:802:ARG:HH11	1.75	0.52
1:A:571:ARG:NH1	1:A:601:ASP:OD2	2.43	0.52
1:A:19:LEU:O	1:A:23:GLY:HA3	2.10	0.52
1:A:726:GLU:HA	1:A:726:GLU:OE1	2.10	0.52
1:A:537:ARG:HD2	3:A:941:HOH:O	2.10	0.51
1:A:830:ILE:HG22	1:A:852:VAL:HG22	1.92	0.51
1:A:43:THR:HG22	1:A:45:GLU:H	1.75	0.51
1:A:66:PHE:O	1:A:69:ILE:HB	2.10	0.51
1:A:354:VAL:HG21	1:A:527:TRP:CH2	2.45	0.51
1:A:76:ASN:ND2	1:A:87:LEU:HD13	2.26	0.51
1:A:347:LEU:CD2	1:A:524:ILE:HG13	2.39	0.51
1:A:583:SER:OG	1:A:585:GLU:HG3	2.11	0.51
1:A:843:PHE:HA	1:A:846:LYS:HZ2	1.76	0.51
1:A:474:ILE:HG23	1:A:483:PHE:HD2	1.75	0.51
1:A:320:GLN:HB3	1:A:336:THR:HG22	1.91	0.51
1:A:728:VAL:O	1:A:730:LYS:N	2.41	0.51
1:A:199:GLU:O	1:A:200:PRO:C	2.49	0.51
1:A:79:LYS:HB3	1:A:82:ASP:HB2	1.92	0.51
1:A:229:ILE:HG23	1:A:233:TRP:CZ3	2.45	0.51
1:A:144:VAL:O	1:A:144:VAL:HG12	2.11	0.51
1:A:327:GLU:HB2	1:A:332:TYR:CE2	2.44	0.50
1:A:599:LYS:HD2	1:A:686:GLU:HB3	1.93	0.50
1:A:584:VAL:HG22	1:A:587:ARG:HH12	1.76	0.50
1:A:587:ARG:HD2	1:A:675:GLU:OE1	2.12	0.50
1:A:436:ILE:HA	1:A:439:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PHE:HB2	1:A:169:THR:HG22	1.93	0.50
1:A:51:TYR:OH	1:A:216:ASP:HB2	2.11	0.50
1:A:627:VAL:HB	1:A:652:VAL:HG22	1.94	0.50
1:A:482:THR:HG22	1:A:491:ALA:HB2	1.93	0.50
1:A:716:PHE:C	1:A:716:PHE:CD1	2.85	0.50
1:A:707:LEU:HG	1:A:746:ILE:HD11	1.94	0.50
1:A:390:GLU:OE2	1:A:505:ILE:HD12	2.11	0.50
1:A:733:GLY:O	1:A:734:SER:O	2.28	0.49
1:A:386:LEU:HD12	1:A:510:ILE:HD13	1.95	0.49
1:A:557:ILE:HG13	1:A:609:LEU:HD21	1.95	0.49
1:A:729:LYS:O	1:A:733:GLY:HA2	2.12	0.49
1:A:140:TYR:CZ	1:A:197:PRO:HG3	2.48	0.49
1:A:406:LYS:O	1:A:425:ILE:N	2.43	0.49
1:A:63:ASP:O	1:A:67:GLU:HB2	2.12	0.49
1:A:68:ALA:O	1:A:71:TRP:HB3	2.12	0.49
1:A:714:LEU:HD23	1:A:759:GLU:HB2	1.95	0.49
1:A:398:ALA:HB1	1:A:457:ALA:HA	1.94	0.49
1:A:448:VAL:O	1:A:448:VAL:HG12	2.13	0.49
1:A:380:THR:HG21	1:A:515:ALA:HB2	1.95	0.49
1:A:76:ASN:HD21	1:A:87:LEU:HD13	1.77	0.49
1:A:76:ASN:HD21	1:A:87:LEU:HD11	1.77	0.49
1:A:565:MET:HB3	1:A:598:GLN:HG2	1.95	0.49
1:A:504:LYS:HG3	1:A:510:ILE:HD11	1.95	0.49
1:A:156:ILE:HD11	1:A:168:ASP:HB3	1.94	0.49
1:A:141:SER:OG	1:A:187:TYR:HD2	1.95	0.48
1:A:842:GLU:O	1:A:846:LYS:HG3	2.13	0.48
1:A:582:ASP:O	1:A:583:SER:HB2	2.13	0.48
1:A:585:GLU:O	1:A:589:GLU:HG2	2.13	0.48
1:A:40:PHE:CZ	1:A:239:VAL:HB	2.47	0.48
1:A:575:ILE:HD12	1:A:575:ILE:O	2.13	0.48
1:A:708:VAL:O	1:A:749:ALA:HB2	2.13	0.48
1:A:146:GLU:CG	1:A:187:TYR:CE2	2.92	0.48
1:A:103:MET:HE1	1:A:235:THR:HG23	1.96	0.48
1:A:779:ARG:NH1	1:A:800:PHE:HB3	2.28	0.48
1:A:387:LYS:HB2	1:A:387:LYS:HE3	1.52	0.48
1:A:439:MET:HB3	1:A:445:ILE:HD11	1.96	0.48
1:A:274:ILE:HD12	1:A:298:MET:HE1	1.95	0.48
1:A:80:PHE:CE2	1:A:200:PRO:HB2	2.48	0.48
1:A:100:PRO:HA	2:A:876:SO4:O1	2.13	0.48
1:A:347:LEU:HD13	1:A:521:PHE:HA	1.95	0.47
1:A:406:LYS:HA	1:A:493:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PRO:O	1:A:240:GLN:NE2	2.46	0.47
1:A:244:PHE:HB2	1:A:247:LYS:HG2	1.95	0.47
1:A:211:VAL:HG11	1:A:237:VAL:HG23	1.95	0.47
1:A:244:PHE:HB3	1:A:246:ASN:OD1	2.13	0.47
1:A:54:GLY:O	1:A:55:LYS:HB2	2.15	0.47
1:A:772:GLN:HG2	1:A:777:PHE:O	2.14	0.47
1:A:406:LYS:HB2	1:A:408:TYR:CE1	2.50	0.47
1:A:396:LEU:O	1:A:468:VAL:HA	2.15	0.47
1:A:274:ILE:HD12	1:A:298:MET:CE	2.45	0.47
1:A:574:LYS:HA	1:A:577:LYS:HE2	1.97	0.47
1:A:248:GLY:O	1:A:275:ASN:HB2	2.15	0.47
1:A:66:PHE:O	1:A:70:THR:HG23	2.15	0.47
1:A:155:ILE:HG22	1:A:179:LEU:CD1	2.45	0.46
1:A:259:ARG:HB2	1:A:319:MET:HG3	1.97	0.46
1:A:609:LEU:CD1	1:A:614:MET:HB2	2.44	0.46
1:A:8:PHE:CZ	1:A:26:LEU:HD13	2.50	0.46
1:A:392:ILE:HD11	1:A:495:TYR:CZ	2.49	0.46
1:A:818:LYS:HA	1:A:821:GLN:HG3	1.96	0.46
1:A:678:LYS:HG3	1:A:720:VAL:CG1	2.46	0.46
1:A:572:ILE:O	1:A:576:ARG:HG3	2.16	0.46
1:A:658:PHE:HD1	3:A:1018:HOH:O	1.98	0.46
1:A:782:ALA:O	1:A:786:LEU:HB2	2.16	0.46
1:A:396:LEU:CD2	1:A:452:MET:SD	3.04	0.46
1:A:842:GLU:HG2	1:A:842:GLU:O	2.15	0.46
1:A:200:PRO:O	1:A:203:GLN:HB2	2.15	0.46
1:A:429:LEU:HA	1:A:448:VAL:HB	1.98	0.46
1:A:404:ALA:CB	1:A:496:ILE:HG13	2.43	0.46
1:A:566:PHE:O	1:A:572:ILE:HA	2.15	0.46
1:A:557:ILE:HB	1:A:614:MET:HA	1.98	0.46
1:A:215:TRP:HH2	1:A:231:GLY:C	2.19	0.46
1:A:429:LEU:O	1:A:449:ARG:HG2	2.16	0.46
1:A:153:GLU:HG2	3:A:1134:HOH:O	2.15	0.46
1:A:368:ILE:O	1:A:868:GLN:NE2	2.49	0.46
1:A:645:LEU:O	1:A:649:LYS:HB3	2.16	0.46
1:A:620:ASP:O	1:A:665:ARG:HB2	2.17	0.46
1:A:658:PHE:C	1:A:660:PRO:HD3	2.36	0.45
1:A:622:PRO:HG3	3:A:925:HOH:O	2.16	0.45
1:A:146:GLU:C	1:A:147:VAL:HG22	2.36	0.45
1:A:59:GLN:HG2	1:A:60:GLU:H	1.79	0.45
1:A:353:LEU:CB	1:A:359:ILE:HG12	2.46	0.45
1:A:146:GLU:CB	1:A:187:TYR:CE2	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:HG23	1:A:233:TRP:CE3	2.52	0.45
1:A:665:ARG:HA	1:A:669:LEU:HG	1.99	0.45
1:A:617:ARG:HD2	3:A:879:HOH:O	2.14	0.45
1:A:402:ALA:HA	1:A:498:LEU:HB3	1.99	0.45
1:A:643:LEU:HB3	1:A:647:GLU:HG3	1.97	0.45
1:A:701:PRO:HD2	1:A:737:GLN:O	2.17	0.45
1:A:145:MET:HE1	1:A:148:PRO:HD3	1.99	0.45
1:A:83:THR:O	1:A:118:GLY:HA3	2.16	0.45
1:A:318:ASP:CG	1:A:341:ARG:HH22	2.20	0.45
1:A:150:SER:O	1:A:154:LYS:HG3	2.16	0.45
1:A:73:GLU:HG2	1:A:80:PHE:H	1.81	0.45
1:A:465:THR:HG22	1:A:466:CYS:N	2.32	0.45
1:A:325:THR:HB	1:A:334:LEU:HD21	1.98	0.45
1:A:715:LYS:HB3	1:A:715:LYS:HE2	1.66	0.45
1:A:843:PHE:CZ	1:A:847:VAL:HG21	2.52	0.45
1:A:369:GLU:OE2	1:A:371:LYS:HB2	2.16	0.44
1:A:76:ASN:ND2	1:A:87:LEU:CD1	2.81	0.44
1:A:59:GLN:HG2	1:A:60:GLU:N	2.32	0.44
1:A:43:THR:HG22	1:A:44:THR:H	1.82	0.44
1:A:495:TYR:CE1	1:A:504:LYS:O	2.70	0.44
1:A:285:VAL:HG13	1:A:286:ARG:N	2.32	0.44
1:A:159:MET:SD	1:A:171:LEU:HD13	2.58	0.44
1:A:632:GLU:HA	3:A:1039:HOH:O	2.18	0.44
1:A:715:LYS:HB2	1:A:759:GLU:HG3	2.00	0.44
1:A:258:THR:HA	1:A:268:ILE:HD13	2.00	0.44
1:A:57:ILE:HD13	1:A:208:VAL:CG1	2.48	0.44
1:A:718:LYS:HG3	1:A:740:ILE:HG21	2.00	0.44
1:A:478:GLU:O	1:A:481:LYS:N	2.50	0.44
1:A:155:ILE:HG22	1:A:179:LEU:HD12	1.99	0.43
1:A:551:LYS:HE3	1:A:551:LYS:HB2	1.62	0.43
1:A:504:LYS:HG3	1:A:510:ILE:HD12	2.00	0.43
1:A:215:TRP:CH2	1:A:234:GLY:N	2.83	0.43
1:A:817:LYS:O	1:A:821:GLN:HG3	2.19	0.43
1:A:483:PHE:O	1:A:489:THR:HA	2.18	0.43
1:A:147:VAL:CG1	1:A:151:HIS:HD2	2.31	0.43
1:A:352:ASP:O	1:A:356:GLU:CG	2.63	0.43
1:A:265:GLU:HG3	3:A:943:HOH:O	2.17	0.43
1:A:144:VAL:HA	1:A:210:ALA:CB	2.48	0.43
1:A:258:THR:CG2	1:A:322:MET:HE1	2.47	0.43
1:A:587:ARG:O	1:A:591:LEU:HG	2.19	0.43
1:A:97:ALA:HB2	1:A:233:TRP:HZ3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:ARG:HA	1:A:728:VAL:HG21	2.01	0.43
1:A:353:LEU:HB2	1:A:359:ILE:HG12	2.01	0.43
1:A:259:ARG:NH1	1:A:266:LYS:HD3	2.34	0.43
1:A:639:LYS:HD2	1:A:639:LYS:HA	1.73	0.43
1:A:28:GLU:HG2	1:A:316:PHE:CE1	2.54	0.43
1:A:386:LEU:HA	1:A:386:LEU:HD12	1.71	0.43
1:A:131:ASP:HB2	1:A:176:LEU:CD1	2.48	0.43
1:A:869:ALA:O	1:A:873:ASN:HB2	2.18	0.43
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.80	0.42
1:A:781:ASP:O	1:A:784:LYS:HG2	2.19	0.42
1:A:197:PRO:HB2	1:A:203:GLN:HG3	2.01	0.42
1:A:482:THR:HG22	1:A:491:ALA:CB	2.49	0.42
1:A:673:TYR:HA	1:A:675:GLU:OE2	2.18	0.42
1:A:351:CYS:HB3	3:A:1009:HOH:O	2.18	0.42
1:A:651:LYS:HA	1:A:651:LYS:HD2	1.78	0.42
1:A:12:ASN:ND2	1:A:14:SER:H	2.17	0.42
1:A:392:ILE:HD12	1:A:392:ILE:C	2.40	0.42
1:A:107:LEU:HD22	1:A:242:MET:HE1	2.00	0.42
1:A:177:LYS:HB2	1:A:177:LYS:HE3	1.60	0.42
1:A:547:LEU:HA	1:A:547:LEU:HD23	1.85	0.42
1:A:381:PHE:HZ	1:A:496:ILE:HG23	1.78	0.42
1:A:165:VAL:HG11	1:A:171:LEU:HD23	2.01	0.42
1:A:37:PRO:CB	1:A:241:THR:HG23	2.49	0.42
1:A:423:ARG:HA	1:A:443:GLU:CG	2.50	0.42
1:A:4:TRP:CH2	1:A:49:GLU:HG3	2.55	0.42
1:A:712:LYS:HA	1:A:715:LYS:HE2	2.01	0.42
1:A:721:VAL:CG1	1:A:740:ILE:HD12	2.49	0.42
1:A:108:ASN:HB2	1:A:136:PHE:HB2	2.02	0.42
1:A:690:GLU:HB3	1:A:694:GLU:OE2	2.19	0.42
1:A:529:ASP:CG	1:A:863:ARG:HH21	2.22	0.42
1:A:211:VAL:HG11	1:A:237:VAL:CG2	2.49	0.42
1:A:602:PHE:CE2	1:A:684:VAL:HG22	2.54	0.42
1:A:477:ASN:O	1:A:481:LYS:N	2.53	0.42
1:A:36:ILE:HG22	1:A:333:PHE:O	2.19	0.42
1:A:326:ILE:HA	1:A:330:LYS:O	2.20	0.42
1:A:381:PHE:CZ	1:A:496:ILE:CG2	2.98	0.41
1:A:574:LYS:O	1:A:590:ALA:HB1	2.19	0.41
1:A:103:MET:CE	1:A:235:THR:HG21	2.50	0.41
1:A:140:TYR:O	1:A:144:VAL:HB	2.19	0.41
1:A:729:LYS:HG2	1:A:734:SER:HB3	2.02	0.41
1:A:349:ILE:O	1:A:353:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:HA	1:A:210:ALA:HB1	2.02	0.41
1:A:155:ILE:HG21	1:A:182:LYS:HB3	2.01	0.41
1:A:319:MET:SD	1:A:339:GLY:HA3	2.60	0.41
1:A:757:ALA:HB3	1:A:822:THR:OG1	2.19	0.41
1:A:268:ILE:HG23	1:A:268:ILE:HD12	1.77	0.41
1:A:758:GLU:O	1:A:823:ARG:NH2	2.53	0.41
1:A:820:ARG:HD2	1:A:820:ARG:HH11	1.70	0.41
1:A:529:ASP:OD2	1:A:863:ARG:NH2	2.50	0.41
1:A:406:LYS:HB2	1:A:408:TYR:HE1	1.86	0.41
1:A:312:LEU:HD13	1:A:336:THR:HG23	2.03	0.41
1:A:405:GLY:CA	1:A:423:ARG:O	2.66	0.41
1:A:767:THR:HA	1:A:770:LEU:HB3	2.03	0.41
1:A:72:LEU:O	1:A:75:LEU:HB3	2.21	0.41
1:A:524:ILE:HG23	1:A:524:ILE:HD12	1.75	0.41
1:A:347:LEU:HA	1:A:347:LEU:HD23	1.79	0.41
1:A:57:ILE:CD1	1:A:208:VAL:HG12	2.51	0.41
1:A:631:GLU:HA	1:A:634:GLN:HB2	2.02	0.41
1:A:659:ASN:N	1:A:660:PRO:HD3	2.36	0.41
1:A:111:LEU:HD22	1:A:116:VAL:HA	2.02	0.41
1:A:623:LEU:HD23	1:A:623:LEU:HA	1.88	0.41
1:A:857:PHE:HD1	1:A:857:PHE:HA	1.71	0.41
1:A:138:GLN:HG3	1:A:152:PHE:CG	2.56	0.41
1:A:147:VAL:HG11	1:A:190:ALA:CB	2.51	0.41
1:A:830:ILE:CG2	1:A:852:VAL:HG22	2.51	0.41
1:A:25:ASN:ND2	1:A:337:ARG:HA	2.35	0.41
1:A:160:LYS:HD3	1:A:168:ASP:N	2.36	0.40
1:A:230:PRO:HG2	1:A:233:TRP:CE2	2.56	0.40
1:A:69:ILE:HD13	1:A:69:ILE:HA	1.73	0.40
1:A:126:PRO:HB2	1:A:173:ALA:HB1	2.02	0.40
1:A:289:GLN:HA	1:A:290:PRO:HD3	1.96	0.40
1:A:593:GLU:O	1:A:597:PHE:CE1	2.75	0.40
1:A:624:HIS:O	1:A:627:VAL:HG22	2.21	0.40
1:A:595:ILE:N	1:A:596:PRO:HD2	2.36	0.40
1:A:65:ILE:HD12	1:A:205:MET:HE1	2.04	0.40
1:A:482:THR:HA	1:A:490:PHE:O	2.21	0.40
1:A:119:PHE:O	1:A:123:THR:HB	2.22	0.40
1:A:245:GLY:O	1:A:275:ASN:HA	2.22	0.40
1:A:147:VAL:CG1	1:A:151:HIS:CD2	3.05	0.40
1:A:371:LYS:HB3	3:A:1165:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	865/874 (99%)	783 (90%)	65 (8%)	17 (2%)	9 7

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	77	GLY
1	A	279	GLU
1	A	285	VAL
1	A	419	GLU
1	A	420	LYS
1	A	518	SER
1	A	732	LYS
1	A	734	SER
1	A	280	ASP
1	A	514	GLU
1	A	583	SER
1	A	733	GLY
1	A	187	TYR
1	A	193	GLY
1	A	418	HIS
1	A	287	THR

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	711/715 (99%)	617 (87%)	94 (13%)	5 5

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	15	MET
1	A	31	ILE
1	A	38	GLN
1	A	49	GLU
1	A	62	GLN
1	A	64	GLN
1	A	67	GLU
1	A	70	THR
1	A	76	ASN
1	A	78	LYS
1	A	79	LYS
1	A	84	GLU
1	A	105	THR
1	A	122	LYS
1	A	123	THR
1	A	134	ARG
1	A	142	ASP
1	A	145	MET
1	A	147	VAL
1	A	156	ILE
1	A	168	ASP
1	A	172	THR
1	A	177	LYS
1	A	181	GLU
1	A	182	LYS
1	A	189	GLU
1	A	194	GLU
1	A	195	GLU
1	A	199	GLU
1	A	205	MET
1	A	213	ARG
1	A	215	TRP
1	A	219	ARG
1	A	232	ASP
1	A	235	THR
1	A	241	THR
1	A	243	VAL

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Mol	Chain	Res	Type
1	A	250	THR
1	A	261	PRO
1	A	262	SER
1	A	279	GLU
1	A	285	VAL
1	A	294	LEU
1	A	300	ASP
1	A	310	MET
1	A	311	LYS
1	A	322	MET
1	A	327	GLU
1	A	334	LEU
1	A	336	THR
1	A	341	ARG
1	A	342	THR
1	A	422	GLU
1	A	436	ILE
1	A	440	HIS
1	A	446	LEU
1	A	452	MET
1	A	469	SER
1	A	475	LYS
1	A	478	GLU
1	A	485	LEU
1	A	498	LEU
1	A	504	LYS
1	A	505	ILE
1	A	512	THR
1	A	517	VAL
1	A	520	SER
1	A	530	LYS
1	A	541	ASP
1	A	542	THR
1	A	568	GLU
1	A	575	ILE
1	A	576	ARG
1	A	578	MET
1	A	588	GLU
1	A	633	GLU
1	A	636	GLU
1	A	649	LYS
1	A	665	ARG

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Mol	Chain	Res	Type
1	A	675	GLU
1	A	694	GLU
1	A	723	GLU
1	A	731	GLU
1	A	732	LYS
1	A	735	ASP
1	A	737	GLN
1	A	746	ILE
1	A	773	MET
1	A	780	ASP
1	A	817	LYS
1	A	827	LYS
1	A	831	CYS
1	A	864	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	52	ASN
1	A	64	GLN
1	A	76	ASN
1	A	151	HIS
1	A	166	HIS
1	A	564	HIS
1	A	592	ASN
1	A	640	ASN
1	A	656	HIS
1	A	737	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	SO4	A	875	-	4,4,4	1.89	2 (50%)	6,6,6	1.82	2 (33%)
2	SO4	A	876	-	4,4,4	1.79	1 (25%)	6,6,6	0.95	0
2	SO4	A	877	-	4,4,4	1.29	1 (25%)	6,6,6	0.90	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	SO4	A	875	-	-	0/0/0/0	0/0/0/0
2	SO4	A	876	-	-	0/0/0/0	0/0/0/0
2	SO4	A	877	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	875	SO4	O4-S	-2.53	1.38	1.47
2	A	876	SO4	O2-S	-2.28	1.39	1.47
2	A	875	SO4	O2-S	-2.23	1.39	1.47
2	A	877	SO4	O4-S	2.06	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	875	SO4	O2-S-O1	-2.30	102.22	109.50
2	A	875	SO4	O4-S-O3	3.67	123.90	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	876	SO4	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.