



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:38 PM UTC

PDB ID : 1DIK / pdb_00001dik
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

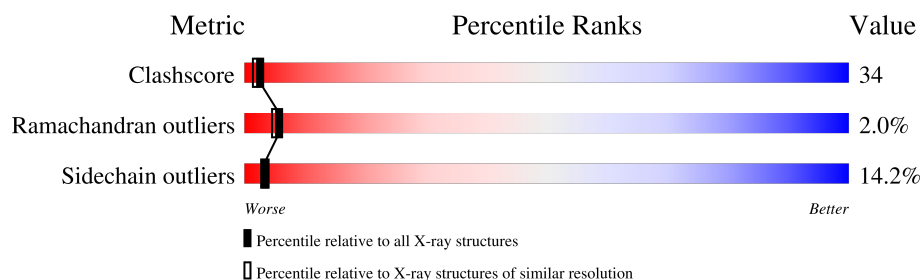
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	874	

2 Entry composition [i](#)

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.

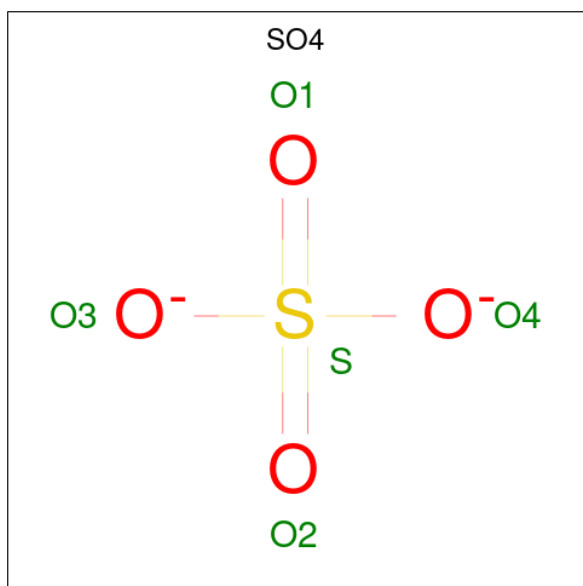
- Molecule 1 is a protein called PYRUVATE PHOSPHATE DIKINASE.

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

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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

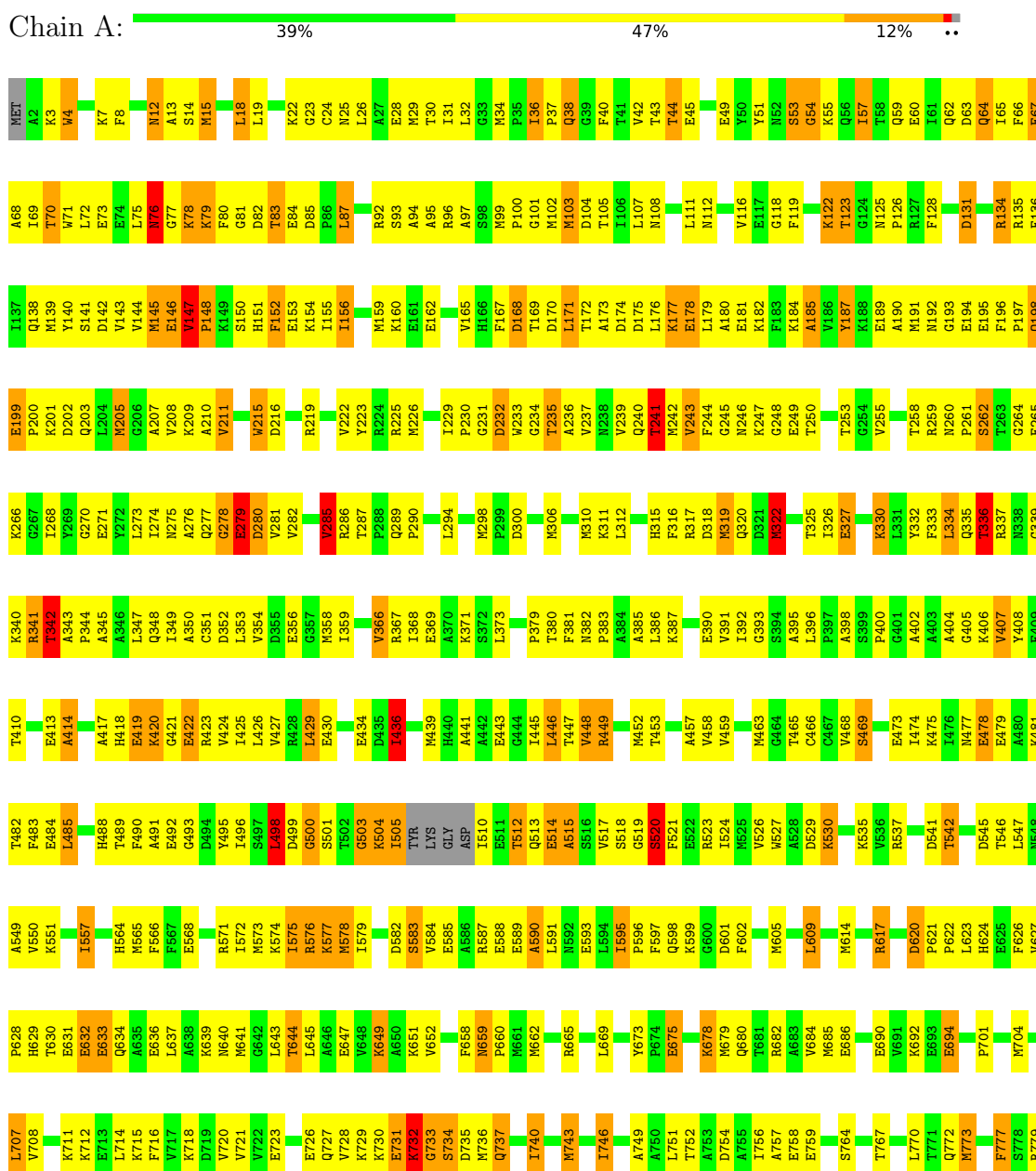
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	416	Total 416	O 416	0	0

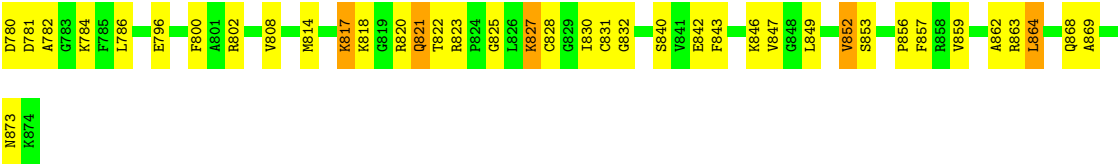
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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	1.10	11/6852 (0.2%)	1.38	74/9234 (0.8%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	685	MET	SD-CE	-7.80	1.60	1.79
1	A	322	MET	SD-CE	-7.67	1.60	1.79
1	A	605	MET	SD-CE	7.04	1.97	1.79
1	A	595	ILE	CA-CB	6.18	1.57	1.54
1	A	814	MET	SD-CE	6.16	1.95	1.79
1	A	103	MET	SD-CE	-5.49	1.65	1.79
1	A	319	MET	SD-CE	-5.48	1.65	1.79
1	A	862	ALA	CA-CB	-5.27	1.44	1.53
1	A	557	ILE	CA-CB	-5.22	1.47	1.54
1	A	590	ALA	CA-CB	-5.13	1.45	1.53
1	A	57	ILE	CA-CB	5.08	1.59	1.53

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	659	ASN	CA-C-N	10.93	133.50	119.84
1	A	659	ASN	C-N-CA	10.93	133.50	119.84
1	A	577	LYS	N-CA-C	-9.86	100.22	110.97
1	A	621	PRO	N-CA-C	9.26	120.49	110.58
1	A	632	GLU	N-CA-C	-9.24	100.78	111.03
1	A	731	GLU	O-C-N	9.06	133.40	122.26
1	A	500	GLY	N-CA-C	-8.48	101.19	115.34
1	A	131	ASP	N-CA-C	-8.43	102.04	111.14
1	A	232	ASP	N-CA-C	-8.25	103.00	113.23
1	A	282	VAL	N-CA-C	-7.84	104.22	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	SER	N-CA-C	-7.68	102.55	112.23
1	A	342	THR	N-CA-C	-7.67	100.20	110.55
1	A	429	LEU	N-CA-C	-7.48	101.27	112.04
1	A	417	ALA	N-CA-C	-7.30	104.11	113.16
1	A	96	ARG	N-CA-C	-7.09	103.55	111.28
1	A	692	LYS	N-CA-C	-7.01	103.71	111.36
1	A	162	GLU	N-CA-C	-6.97	104.65	113.43
1	A	707	LEU	N-CA-C	6.91	121.07	111.74
1	A	498	LEU	N-CA-C	6.88	117.67	108.38
1	A	832	GLY	N-CA-C	6.79	120.51	110.60
1	A	458	VAL	N-CA-C	6.77	116.92	110.42
1	A	148	PRO	N-CA-C	6.70	122.87	111.68
1	A	859	VAL	CA-C-N	-6.70	112.09	119.19
1	A	859	VAL	C-N-CA	-6.70	112.09	119.19
1	A	731	GLU	N-CA-C	-6.68	104.44	112.59
1	A	236	ALA	N-CA-C	-6.49	101.18	110.59
1	A	609	LEU	N-CA-C	6.47	119.32	111.82
1	A	192	ASN	O-C-N	6.41	128.96	122.03
1	A	620	ASP	CA-C-N	6.41	124.28	119.66
1	A	620	ASP	C-N-CA	6.41	124.28	119.66
1	A	7	LYS	N-CA-C	-6.37	102.57	110.41
1	A	4	TRP	N-CA-C	-6.29	105.64	113.38
1	A	146	GLU	N-CA-C	-6.29	105.74	113.41
1	A	147	VAL	CA-C-N	6.26	126.77	120.14
1	A	147	VAL	C-N-CA	6.26	126.77	120.14
1	A	184	LYS	N-CA-C	-6.25	105.51	113.01
1	A	180	ALA	N-CA-C	-6.25	104.47	111.28
1	A	171	LEU	N-CA-C	-6.23	102.30	110.53
1	A	414	ALA	N-CA-C	-6.19	104.08	111.69
1	A	385	ALA	N-CA-C	-6.18	104.44	112.23
1	A	315	HIS	N-CA-C	6.16	118.07	111.36
1	A	535	LYS	N-CA-C	-6.03	101.07	110.42
1	A	436	ILE	N-CA-C	6.02	121.86	109.34
1	A	185	ALA	N-CA-C	-5.95	103.56	111.24
1	A	241	THR	N-CA-C	-5.83	101.22	109.96
1	A	152	PHE	N-CA-C	5.78	117.26	111.07
1	A	821	GLN	N-CA-C	-5.77	104.59	111.69
1	A	336	THR	N-CA-CB	5.75	120.57	111.43
1	A	44	THR	N-CA-C	-5.73	105.17	111.82
1	A	202	ASP	N-CA-C	-5.69	105.45	112.90
1	A	198	GLN	N-CA-C	-5.59	106.14	113.12
1	A	278	GLY	O-C-N	5.50	127.46	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	ARG	N-CA-C	5.47	120.07	112.90
1	A	340	LYS	N-CA-C	-5.45	100.41	109.46
1	A	515	ALA	N-CA-C	5.43	117.05	108.96
1	A	83	THR	N-CA-C	5.40	117.25	111.36
1	A	840	SER	N-CA-C	-5.40	105.48	111.36
1	A	207	ALA	N-CA-C	-5.37	105.07	111.03
1	A	449	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	178	GLU	N-CA-C	-5.29	105.43	111.14
1	A	54	GLY	N-CA-C	5.29	122.40	115.47
1	A	243	VAL	N-CA-C	-5.28	100.59	108.46
1	A	515	ALA	O-C-N	5.22	129.11	123.10
1	A	18	LEU	N-CA-C	-5.19	104.54	111.24
1	A	678	LYS	N-CA-C	-5.15	105.58	111.14
1	A	777	PHE	N-CA-C	5.10	117.14	109.23
1	A	808	VAL	CB-CA-C	-5.09	105.38	112.04
1	A	448	VAL	O-C-N	-5.08	116.22	122.12
1	A	76	ASN	O-C-N	5.08	129.49	122.83
1	A	503	GLY	N-CA-C	-5.07	102.58	111.46
1	A	620	ASP	N-CA-C	5.06	120.99	109.81
1	A	644	THR	N-CA-C	-5.05	102.29	110.32
1	A	393	GLY	N-CA-C	5.04	117.94	110.42
1	A	87	LEU	N-CA-C	-5.02	100.55	108.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6730	0	6653	458	0
2	A	15	0	0	1	0
3	A	416	0	0	24	0
All	All	7161	0	6653	458	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 34.

All (458) 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:342:THR:HG23	1:A:344:PRO:HD2	1.37	1.05
1:A:107:LEU:HB3	1:A:242:MET:HE1	1.41	1.01
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:732:LYS:C	1:A:734:SER:H	1.68	0.97
1:A:107:LEU:HB3	1:A:242:MET:CE	1.97	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:H	1:A:737:GLN:HE21	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:258:THR:HG23	1:A:322:MET:HE1	1.63	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:13:ALA:HA	1:A:24:CYS:HB2	1.64	0.80
1:A:165:VAL:HG13	1:A:170:ASP:HB2	1.62	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:145:MET:SD	1:A:145:MET:C	2.67	0.77
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:732:LYS:C	1:A:734:SER:N	2.38	0.77
1:A:392:ILE:HD11	1:A:495:TYR:CE1	2.20	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:447:THR:HG1	1:A:469:SER:HA	1.51	0.75
1:A:392:ILE:CD1	1:A:485:LEU:HD13	2.18	0.73
1:A:395:ALA:HB3	1:A:468:VAL:HG12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:GLN:HG3	3:A:1006:HOH:O	1.89	0.73
1:A:704:MET:SD	1:A:743:MET:HG2	2.29	0.72
1:A:107:LEU:CB	1:A:242:MET:HE1	2.19	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:57:ILE:CD1	1:A:209:LYS:HG3	2.20	0.71
1:A:80:PHE:HA	1:A:87:LEU:HB3	1.71	0.71
1:A:57:ILE:HD11	1:A:209:LYS:HG3	1.73	0.71
1:A:146:GLU:HB3	1:A:191:MET:SD	2.30	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:268:ILE:HG13	1:A:306:MET:SD	2.32	0.69
1:A:644:THR:OG1	1:A:647:GLU:HG2	1.92	0.69
1:A:101:GLY:O	1:A:102:MET:HE2	1.93	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:398:ALA:HB2	1:A:469:SER:OG	1.93	0.69
1:A:404:ALA:HB1	1:A:496:ILE:HG13	1.75	0.69
1:A:146:GLU:HG3	1:A:187:TYR:HE2	1.58	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:H	1:A:737:GLN:NE2	1.92	0.67
1:A:312:LEU:HD13	1:A:336:THR:HG21	1.77	0.67
1:A:408:TYR:CD1	1:A:424:VAL:HG13	2.30	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:259:ARG:HG2	1:A:266:LYS:HA	1.77	0.66
1:A:262:SER:O	1:A:342:THR:HG21	1.96	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:122:LYS:HD2	1:A:122:LYS:C	2.21	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:65:ILE:HD12	1:A:205:MET:HE1	1.80	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:278:GLY:C	1:A:280:ASP:H	2.06	0.63
1:A:754:ASP:O	1:A:822:THR:HG21	1.98	0.63
1:A:530:LYS:HB2	1:A:530:LYS:NZ	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:123:THR:HG23	1:A:125:ASN:H	1.65	0.62
1:A:392:ILE:HD11	1:A:495:TYR:HE1	1.63	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:38:GLN:O	1:A:241:THR:HG22	2.00	0.62
1:A:182:LYS:O	1:A:185:ALA:HB3	2.00	0.62
1:A:827:LYS:HD2	1:A:827:LYS:N	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:542:THR:HG22	1:A:545:ASP:H	1.64	0.61
1:A:651:LYS:HB2	3:A:1122:HOH:O	1.99	0.61
1:A:258:THR:CG2	1:A:322:MET:HE1	2.31	0.61
1:A:18:LEU:HD22	1:A:43:THR:HG21	1.83	0.61
1:A:85:ASP:OD1	1:A:122:LYS:HG3	2.00	0.61
1:A:513:GLN:O	1:A:514:GLU:HB2	2.01	0.60
1:A:215:TRP:CH2	1:A:231:GLY:HA2	2.36	0.60
1:A:436:ILE:HD13	1:A:439:MET:HE3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:258:THR:HG23	1:A:322:MET:CE	2.32	0.58
1:A:60:GLU:O	1:A:64:GLN:HB2	2.02	0.58
1:A:264:GLY:HA3	1:A:348:GLN:HB3	1.85	0.58
1:A:680:GLN:O	1:A:684:VAL:HG23	2.03	0.58
1:A:135:ARG:HH12	1:A:281:VAL:HG11	1.67	0.58
1:A:274:ILE:CD1	1:A:298:MET:HE3	2.34	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:43:THR:HG22	1:A:44:THR:N	2.19	0.57
1:A:396:LEU:HD23	1:A:452:MET:SD	2.45	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:419:GLU:C	1:A:421:GLY:H	2.13	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:573:MET:HE3	1:A:640:ASN:HD22	1.70	0.56
1:A:504:LYS:HG3	1:A:510:ILE:CD1	2.36	0.56
1:A:12:ASN:OD1	1:A:14:SER:HB2	2.04	0.56
1:A:171:LEU:HD12	1:A:176:LEU:HD23	1.87	0.56
1:A:577:LYS:HE3	1:A:593:GLU:OE2	2.06	0.56
1:A:828:CYS:HB3	1:A:849:LEU:HD22	1.88	0.56
1:A:93:SER:HB2	1:A:235:THR:HG21	1.87	0.56
1:A:729:LYS:NZ	1:A:736:MET:O	2.35	0.56
1:A:199:GLU:O	1:A:200:PRO:C	2.49	0.55
1:A:410:THR:OG1	1:A:413:GLU:HG2	2.06	0.55
1:A:414:ALA:HB2	1:A:426:LEU:HD13	1.88	0.55
1:A:628:PRO:HG2	1:A:634:GLN:HG2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:MET:HE3	1:A:223:TYR:CD1	2.41	0.55
1:A:716:PHE:CD1	1:A:716:PHE:C	2.85	0.55
1:A:341:ARG:HB3	1:A:345:ALA:HB3	1.88	0.55
1:A:382:ASN:OD1	1:A:383:PRO:HD2	2.06	0.54
1:A:495:TYR:OH	1:A:503:GLY:HA3	2.07	0.54
1:A:95:ALA:HB3	1:A:97:ALA:O	2.06	0.54
1:A:496:ILE:HG12	1:A:510:ILE:N	2.21	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:HG12	1:A:391:VAL:O	2.07	0.54
1:A:174:ASP:O	1:A:177:LYS:HG3	2.08	0.54
1:A:199:GLU:OE2	1:A:201:LYS:HB2	2.08	0.54
1:A:200:PRO:HA	1:A:203:GLN:OE1	2.08	0.54
1:A:260:ASN:HB2	3:A:954:HOH:O	2.08	0.53
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: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: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:575:ILE:O	1:A:579:ILE:HG13	2.08	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:159:MET:HE1	1:A:179:LEU:HB2	1.91	0.53
1:A:34:MET:SD	1:A:312:LEU:HD21	2.49	0.53
1:A:380:THR:HG23	1:A:515:ALA:HB2	1.90	0.53
1:A:419:GLU:O	1:A:421:GLY:N	2.39	0.53
1:A:427:VAL:HG22	1:A:446:LEU:HD12	1.90	0.53
1:A:430:GLU:OE2	1:A:449:ARG:HD2	2.09	0.53
1:A:19:LEU:HD13	3:A:987:HOH:O	2.08	0.52
1:A:22:LYS:HB2	1:A:94:ALA:HB2	1.90	0.52
1:A:139:MET:HG2	3:A:1158:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:MET:SD	1:A:773:MET:HE1	2.49	0.52
1:A:483:PHE:CE2	1:A:485:LEU:HD12	2.32	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:274:ILE:HD12	1:A:298:MET:HE3	1.91	0.52
1:A:171:LEU:HB3	1:A:175:ASP:HB2	1.90	0.52
1:A:104:ASP:HB3	1:A:143:VAL:CG1	2.39	0.52
1:A:244:PHE:CD1	1:A:244:PHE:N	2.78	0.52
1:A:391:VAL:HG22	1:A:504:LYS:HE3	1.91	0.52
1:A:571:ARG:NH1	1:A:601:ASP:OD2	2.43	0.52
1:A:802:ARG:HG2	1:A:802:ARG:HH11	1.75	0.52
1:A:19:LEU:O	1:A:23:GLY:HA3	2.10	0.52
1:A:726:GLU:OE1	1:A:726:GLU:HA	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:107:LEU:HD22	1:A:242:MET:HE1	1.91	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:320:GLN:HB3	1:A:336:THR:HG22	1.91	0.51
1:A:474:ILE:HG23	1:A:483:PHE:HD2	1.75	0.51
1:A:728:VAL:O	1:A:730:LYS:N	2.41	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:HG12	1:A:144:VAL:O	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:215:TRP:HH2	1:A:231:GLY:C	2.19	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:51:TYR:OH	1:A:216:ASP:HB2	2.11	0.50
1:A:167:PHE:HB2	1:A:169:THR:HG22	1.93	0.50
1:A:658:PHE:C	1:A:660:PRO:HD3	2.36	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:146:GLU:C	1:A:147:VAL:HG22	2.36	0.50
1:A:707:LEU:HG	1:A:746:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ASP:CG	1:A:341:ARG:HH22	2.20	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:107:LEU:HD13	1:A:242:MET:HE1	1.93	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: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:714:LEU:HD23	1:A:759:GLU:HB2	1.95	0.49
1:A:107:LEU:HB3	1:A:242:MET:HE2	1.87	0.49
1:A:398:ALA:HB1	1:A:457:ALA:HA	1.94	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:156:ILE:HD11	1:A:168:ASP:HB3	1.94	0.49
1:A:504:LYS:HG3	1:A:510:ILE:HD11	1.95	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:O	1:A:575:ILE:HD12	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:387:LYS:HB2	1:A:387:LYS:HE3	1.52	0.48
1:A:779:ARG:NH1	1:A:800:PHE:HB3	2.28	0.48
1:A:439:MET:HB3	1:A:445:ILE:HD11	1.96	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:448:VAL:HG12	1:A:448:VAL:O	2.13	0.48
1:A:347:LEU:HD13	1:A:521:PHE:HA	1.95	0.47
1:A:37:PRO:O	1:A:240:GLN:NE2	2.46	0.47
1:A:406:LYS:HA	1:A:493:GLY:O	2.14	0.47
1:A:244:PHE:HB2	1:A:247:LYS:HG2	1.95	0.47
1:A:54:GLY:O	1:A:55:LYS:HB2	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:GLN:HG2	1:A:777:PHE:O	2.14	0.47
1:A:274:ILE:HD12	1:A:298:MET:CE	2.45	0.47
1:A:396:LEU:O	1:A:468:VAL:HA	2.15	0.47
1:A:406:LYS:HB2	1:A:408:TYR:CE1	2.50	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:529:ASP:CG	1:A:863:ARG:HH21	2.22	0.47
1:A:66:PHE:O	1:A:70:THR:HG23	2.15	0.47
1:A:392:ILE:C	1:A:392:ILE:HD12	2.40	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:8:PHE:CZ	1:A:26:LEU:HD13	2.50	0.46
1:A:609:LEU:CD1	1:A:614:MET:HB2	2.44	0.46
1:A:392:ILE:HD11	1:A:495:TYR:CZ	2.49	0.46
1:A:678:LYS:HG3	1:A:720:VAL:CG1	2.46	0.46
1:A:818:LYS:HA	1:A:821:GLN:HG3	1.96	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:O	1:A:842:GLU:HG2	2.15	0.46
1:A:200:PRO:O	1:A:203:GLN:HB2	2.15	0.46
1:A:404:ALA:CB	1:A:496:ILE:HG13	2.43	0.46
1:A:429:LEU:HA	1:A:448:VAL:HB	1.98	0.46
1:A:557:ILE:HB	1:A:614:MET:HA	1.98	0.46
1:A:566:PHE:O	1:A:572:ILE:HA	2.15	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:620:ASP:O	1:A:665:ARG:HB2	2.17	0.46
1:A:645:LEU:O	1:A:649:LYS:HB3	2.16	0.46
1:A:622:PRO:HG3	3:A:925:HOH:O	2.16	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:101:GLY:C	1:A:102:MET:HE2	2.40	0.45
1:A:146:GLU:CB	1:A:187:TYR:CE2	2.99	0.45
1:A:229:ILE:HG23	1:A:233:TRP:CE3	2.52	0.45
1:A:617:ARG:HD2	3:A:879:HOH:O	2.14	0.45
1:A:665:ARG:HA	1:A:669:LEU:HG	1.99	0.45
1:A:145:MET:HE1	1:A:147:VAL:C	2.41	0.45
1:A:402:ALA:HA	1:A:498:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:LEU:HB3	1:A:647:GLU:HG3	1.97	0.45
1:A:83:THR:O	1:A:118:GLY:HA3	2.16	0.45
1:A:701:PRO:HD2	1:A:737:GLN:O	2.17	0.45
1:A:150:SER:O	1:A:154:LYS:HG3	2.16	0.45
1:A:253:THR:HG21	1:A:277:GLN:C	2.39	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:495:TYR:C	1:A:496:ILE:HD12	2.42	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:564:HIS:NE2	1:A:565:MET:HE3	2.33	0.44
1:A:159:MET:SD	1:A:171:LEU:HD13	2.58	0.44
1:A:215:TRP:CH2	1:A:231:GLY:C	2.95	0.44
1:A:285:VAL:HG13	1:A:286:ARG:N	2.32	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:478:GLU:O	1:A:481:LYS:N	2.50	0.44
1:A:718:LYS:HG3	1:A:740:ILE:HG21	2.00	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:215:TRP:CH2	1:A:234:GLY:N	2.83	0.43
1:A:504:LYS:HG3	1:A:510:ILE:HD12	2.00	0.43
1:A:817:LYS:O	1:A:821:GLN:HG3	2.19	0.43
1:A:147:VAL:CG1	1:A:151:HIS:HD2	2.31	0.43
1:A:265:GLU:HG3	3:A:943:HOH:O	2.17	0.43
1:A:352:ASP:O	1:A:356:GLU:CG	2.63	0.43
1:A:478:GLU:O	1:A:479:GLU:C	2.62	0.43
1:A:483:PHE:O	1:A:489:THR:HA	2.18	0.43
1:A:566:PHE:CE2	1:A:679:MET:HE1	2.53	0.43
1:A:144:VAL:HA	1:A:210:ALA:CB	2.48	0.43
1:A:97:ALA:HB2	1:A:233:TRP:HZ3	1.84	0.43
1:A:353:LEU:HB2	1:A:359:ILE:HG12	2.01	0.43
1:A:587:ARG:O	1:A:591:LEU:HG	2.19	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: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:131:ASP:HB2	1:A:176:LEU:CD1	2.48	0.43
1:A:386:LEU:HD12	1:A:386:LEU:HA	1.71	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:278:GLY:C	1:A:280:ASP:N	2.73	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:351:CYS:HB3	3:A:1009:HOH:O	2.18	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:12:ASN:ND2	1:A:14:SER:H	2.17	0.42
1:A:270:GLY:C	1:A:271:GLU:HG3	2.43	0.42
1:A:651:LYS:HA	1:A:651:LYS:HD2	1.78	0.42
1:A:422:GLU:O	1:A:423:ARG:C	2.61	0.42
1:A:177:LYS:HE3	1:A:177:LYS:HB2	1.60	0.42
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.85	0.42
1:A:381:PHE:HZ	1:A:496:ILE:HG23	1.78	0.42
1:A:4:TRP:CH2	1:A:49:GLU:HG3	2.55	0.42
1:A:37:PRO:CB	1:A:241:THR:HG23	2.49	0.42
1:A:165:VAL:HG11	1:A:171:LEU:HD23	2.01	0.42
1:A:423:ARG:HA	1:A:443:GLU:CG	2.50	0.42
1:A:712:LYS:HA	1:A:715:LYS:HE2	2.01	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:721:VAL:CG1	1:A:740:ILE:HD12	2.49	0.42
1:A:211:VAL:HG11	1:A:237:VAL:CG2	2.49	0.42
1:A:477:ASN:O	1:A:481:LYS:N	2.53	0.42
1:A:602:PHE:CE2	1:A:684:VAL:HG22	2.54	0.42
1:A:662:MET:HE3	1:A:662:MET:HB2	1.79	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:103:MET:CE	1:A:235:THR:HG21	2.50	0.41
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:140:TYR:O	1:A:144:VAL:HB	2.19	0.41
1:A:274:ILE:HD11	1:A:298:MET:HE3	2.01	0.41
1:A:729:LYS:HG2	1:A:734:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ILE:O	1:A:353:LEU:HG	2.19	0.41
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:HD12	1:A:268:ILE:HG23	1.77	0.41
1:A:758:GLU:O	1:A:823:ARG:NH2	2.53	0.41
1:A:820:ARG:HH11	1:A:820:ARG:HD2	1.70	0.41
1:A:59:GLN:CD	1:A:59:GLN:H	2.28	0.41
1:A:529:ASP:OD2	1:A:863:ARG:NH2	2.50	0.41
1:A:72:LEU:O	1:A:75:LEU:HB3	2.21	0.41
1:A:167:PHE:C	1:A:169:THR:N	2.77	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:406:LYS:HB2	1:A:408:TYR:HE1	1.86	0.41
1:A:767:THR:HA	1:A:770:LEU:HB3	2.03	0.41
1:A:57:ILE:CD1	1:A:208:VAL:HG12	2.51	0.41
1:A:111:LEU:HD22	1:A:116:VAL:HA	2.02	0.41
1:A:138:GLN:HG3	1:A:152:PHE:CG	2.56	0.41
1:A:347:LEU:HA	1:A:347:LEU:HD23	1.79	0.41
1:A:419:GLU:C	1:A:421:GLY:N	2.78	0.41
1:A:524:ILE:HG23	1:A:524:ILE:HD12	1.75	0.41
1:A:623:LEU:HA	1:A:623:LEU:HD23	1.88	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:857:PHE:HD1	1:A:857:PHE:HA	1.71	0.41
1:A:25:ASN:ND2	1:A:337:ARG:HA	2.35	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: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: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:566:PHE:CZ	1:A:679:MET:HE1	2.56	0.40
1:A:289:GLN:HA	1:A:290:PRO:HD3	1.96	0.40
1:A:107:LEU:CG	1:A:242:MET:HE1	2.51	0.40
1:A:196:PHE:O	1:A:197:PRO:C	2.62	0.40
1:A:215:TRP:CD1	1:A:235:THR:HG1	2.40	0.40
1:A:459:VAL:CG1	1:A:463:MET:HE3	2.51	0.40
1:A:593:GLU:O	1:A:597:PHE:CE1	2.75	0.40
1:A:595:ILE:N	1:A:596:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:HIS:O	1:A:627:VAL:HG22	2.21	0.40
1:A:85:ASP:CG	1:A:122:LYS:HG3	2.46	0.40
1:A:119:PHE:O	1:A:123:THR:HB	2.22	0.40
1:A:128:PHE:CD1	1:A:128:PHE:C	2.98	0.40
1:A:245:GLY:O	1:A:275:ASN:HA	2.22	0.40
1:A:482:THR:HA	1:A:490:PHE:O	2.21	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%)	6 5

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

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Mol	Chain	Res	Type
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%)	610 (86%)	101 (14%)	3 3

All (101) 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	36	ILE
1	A	38	GLN
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

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Mol	Chain	Res	Type
1	A	172	THR
1	A	177	LYS
1	A	181	GLU
1	A	189	GLU
1	A	194	GLU
1	A	195	GLU
1	A	199	GLU
1	A	205	MET
1	A	211	VAL
1	A	215	TRP
1	A	219	ARG
1	A	232	ASP
1	A	235	THR
1	A	241	THR
1	A	243	VAL
1	A	249	GLU
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	330	LYS
1	A	334	LEU
1	A	336	THR
1	A	341	ARG
1	A	342	THR
1	A	366	VAL
1	A	407	VAL
1	A	420	LYS
1	A	422	GLU
1	A	436	ILE
1	A	446	LEU
1	A	469	SER
1	A	473	GLU
1	A	478	GLU
1	A	485	LEU

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Mol	Chain	Res	Type
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	526	VAL
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	617	ARG
1	A	633	GLU
1	A	636	GLU
1	A	649	LYS
1	A	675	GLU
1	A	694	GLU
1	A	711	LYS
1	A	723	GLU
1	A	731	GLU
1	A	732	LYS
1	A	735	ASP
1	A	737	GLN
1	A	740	ILE
1	A	743	MET
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	852	VAL
1	A	864	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN

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Mol	Chain	Res	Type
1	A	52	ASN
1	A	59	GLN
1	A	64	GLN
1	A	76	ASN
1	A	151	HIS
1	A	166	HIS
1	A	238	ASN
1	A	564	HIS
1	A	624	HIS
1	A	634	GLN
1	A	640	ASN
1	A	737	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 oligosaccharides 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	0.83	0	6,6,6	1.40	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	877	-	4,4,4	0.63	0	6,6,6	1.29	1 (16%)
2	SO4	A	876	-	4,4,4	0.78	0	6,6,6	1.28	1 (16%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	875	SO4	O4-S-O3	2.79	123.90	108.54
2	A	877	SO4	O3-S-O2	-2.43	96.86	109.56
2	A	876	SO4	O4-S-O1	-2.05	98.86	109.56

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.