



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:34 AM UTC

PDB ID : 1MZO / pdb_00001mzo
Title : Crystal structure of pyruvate formate-lyase with pyruvate
Authors : Lehtio, L.; Leppanen, V.-M.; Kozarich, J.W.; Goldman, A.
Deposited on : 2002-10-09
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

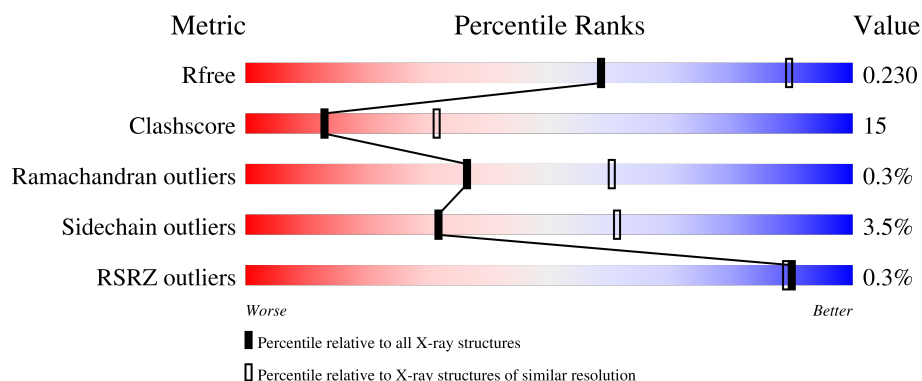
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	759	 69% 28% .
1	B	759	 68% 28% .

2 Entry composition [i](#)

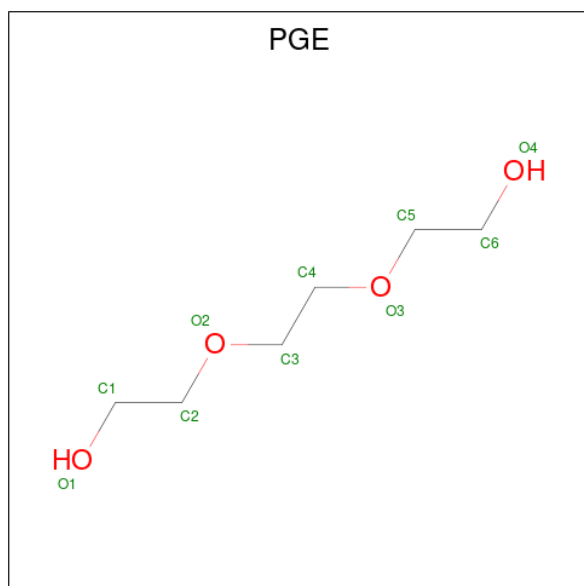
There are 4 unique types of molecules in this entry. The entry contains 12467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 formate-lyase.

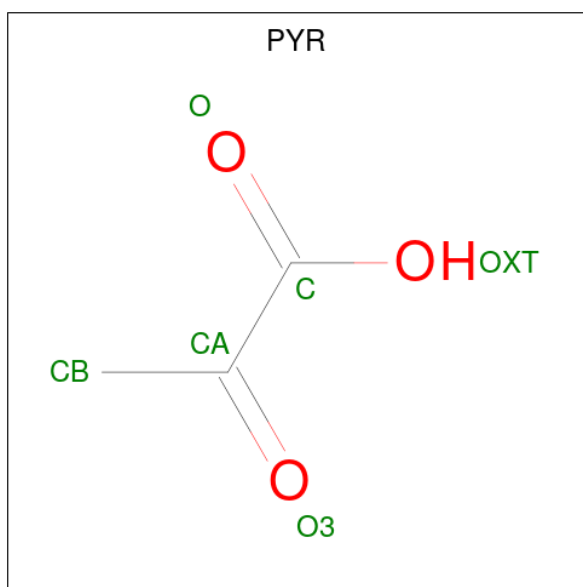
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	756	Total	C	N	O	S	0	0	0
			5965	3770	1020	1139	36			
1	B	756	Total	C	N	O	S	0	0	0
			5965	3770	1020	1139	36			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

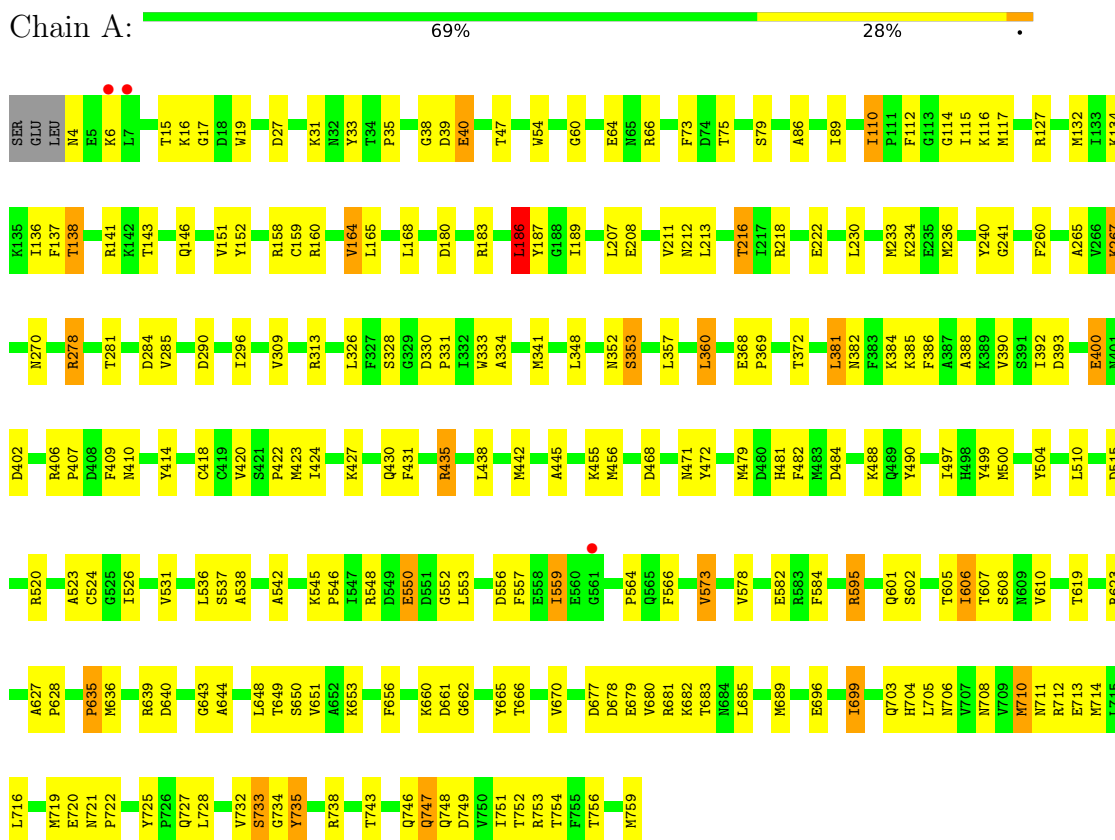
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	276	Total	O	0	0
			276	276		
4	B	239	Total	O	0	0
			239	239		

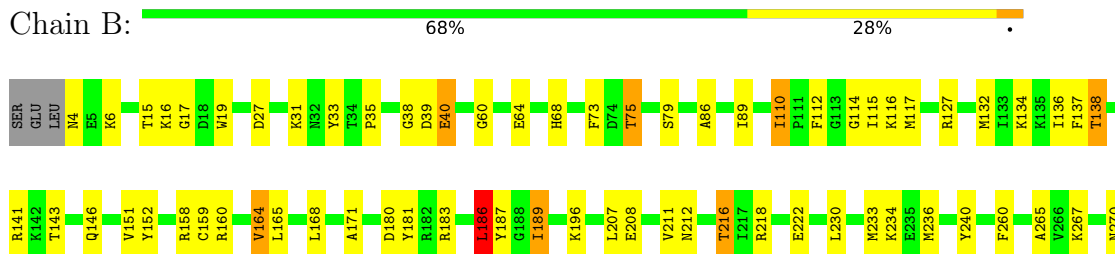
3 Residue-property plots [i](#)

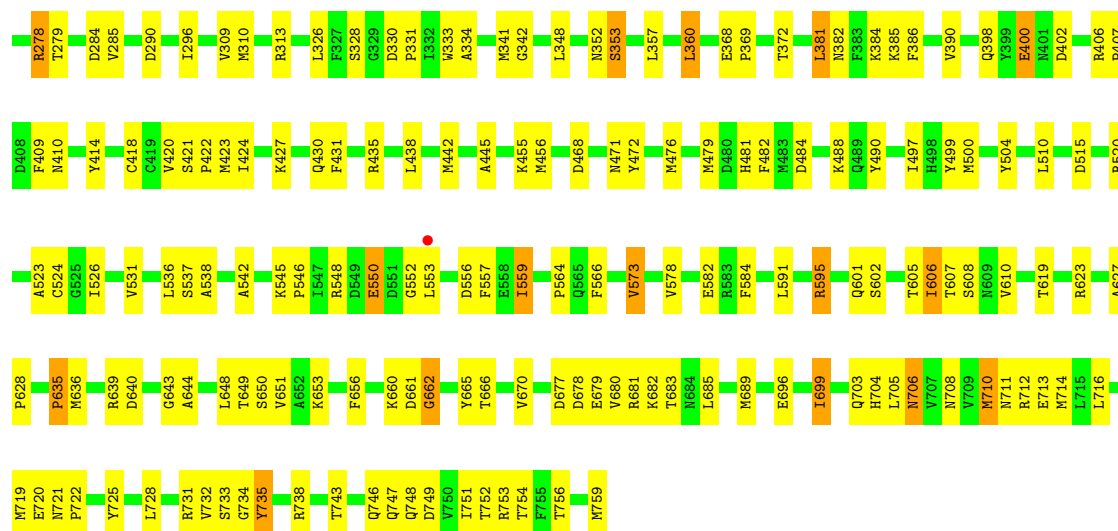
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Pyruvate formate-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	158.35Å 158.35Å 159.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.70) 95.2 (20.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.67Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.235 0.191 , 0.230	Depositor DCC
R_{free} test set	2795 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k 0.004 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12467	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: PGE, PYR

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	0.44	0/6086	0.92	20/8222 (0.2%)
1	B	0.43	0/6086	0.92	24/8222 (0.3%)
All	All	0.43	0/12172	0.92	44/16444 (0.3%)

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	B	0	1

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	89	ILE	N-CA-C	-9.04	102.00	111.58
1	B	89	ILE	N-CA-C	-9.01	102.03	111.58
1	A	499	TYR	N-CA-C	-6.92	103.67	111.14
1	B	499	TYR	N-CA-C	-6.84	103.75	111.14
1	B	662	GLY	N-CA-C	6.61	118.23	111.95
1	A	267	LYS	N-CA-C	-6.33	105.87	113.97
1	B	267	LYS	N-CA-C	-6.24	105.98	113.97
1	A	138	THR	N-CA-C	-6.05	105.14	113.18
1	B	138	THR	N-CA-C	-6.04	105.14	113.18
1	B	410	ASN	N-CA-C	-5.99	103.14	111.52
1	A	410	ASN	N-CA-C	-5.88	103.28	111.52
1	B	137	PHE	N-CA-C	5.80	119.12	112.97
1	A	619	THR	CA-C-N	5.75	126.14	119.47
1	A	619	THR	C-N-CA	5.75	126.14	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	VAL	N-CA-C	-5.71	107.25	112.96
1	B	619	THR	CA-C-N	5.70	126.09	119.47
1	B	619	THR	C-N-CA	5.70	126.09	119.47
1	A	164	VAL	N-CA-C	-5.67	107.29	112.96
1	B	353	SER	N-CA-C	-5.67	105.00	111.07
1	A	334	ALA	N-CA-C	-5.62	100.45	109.39
1	B	334	ALA	N-CA-C	-5.45	100.72	109.39
1	B	635	PRO	N-CA-C	-5.40	103.31	111.41
1	A	137	PHE	N-CA-C	5.35	118.64	112.97
1	A	635	PRO	N-CA-C	-5.34	103.40	111.41
1	A	353	SER	N-CA-C	-5.33	105.36	111.07
1	B	504	TYR	N-CA-C	5.33	119.89	113.17
1	A	504	TYR	N-CA-C	5.29	119.84	113.17
1	B	738	ARG	N-CA-C	-5.29	101.35	109.76
1	B	497	ILE	N-CA-C	5.26	115.89	110.36
1	A	497	ILE	N-CA-C	5.26	115.88	110.36
1	B	523	ALA	N-CA-C	5.24	116.69	109.15
1	B	591	LEU	N-CA-C	5.17	117.93	110.28
1	A	738	ARG	N-CA-C	-5.16	101.55	109.76
1	A	523	ALA	N-CA-C	5.13	116.54	109.15
1	B	279	THR	N-CA-C	5.13	120.40	114.04
1	A	110	ILE	CA-C-N	5.12	124.91	119.28
1	A	110	ILE	C-N-CA	5.12	124.91	119.28
1	B	706	ASN	N-CA-C	-5.08	102.96	110.48
1	A	186	LEU	N-CA-C	5.08	116.50	111.07
1	B	186	LEU	N-CA-C	5.07	116.49	111.07
1	B	110	ILE	CA-C-N	5.05	124.83	119.28
1	B	110	ILE	C-N-CA	5.05	124.83	119.28
1	B	189	ILE	N-CA-C	5.04	115.25	110.42
1	A	747	GLN	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	181	TYR	Sidechain

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	5965	0	5889	181	0
1	B	5965	0	5889	178	0
2	A	10	0	14	1	1
3	A	6	0	0	1	0
3	B	6	0	0	0	0
4	A	276	0	0	13	0
4	B	239	0	0	7	0
All	All	12467	0	11792	357	1

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 15.

All (357) 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:602:SER:HB3	1:A:661:ASP:HB3	1.43	1.00
1:B:602:SER:HB3	1:B:661:ASP:HB3	1.44	0.97
1:B:606:ILE:HG22	1:B:607:THR:H	1.41	0.85
1:A:606:ILE:HG22	1:A:607:THR:H	1.43	0.83
1:A:115:ILE:HG22	4:A:2049:HOH:O	1.77	0.82
1:A:112:PHE:HD1	4:A:2137:HOH:O	1.63	0.80
1:A:341:MET:HB2	1:A:406:ARG:NH1	1.97	0.79
1:B:4:ASN:ND2	1:B:6:LYS:HB2	2.00	0.77
1:A:4:ASN:ND2	1:A:6:LYS:HB2	2.00	0.76
1:B:341:MET:HB2	1:B:406:ARG:NH1	2.00	0.76
1:B:132:MET:HE2	1:B:136:ILE:HG13	1.66	0.76
1:B:4:ASN:HD21	1:B:6:LYS:HB2	1.50	0.75
1:A:4:ASN:HD21	1:A:6:LYS:HB2	1.51	0.75
1:A:132:MET:HE2	1:A:136:ILE:HG13	1.70	0.74
1:A:420:VAL:HG23	1:A:662:GLY:HA3	1.68	0.74
1:A:40:GLU:HG2	1:A:386:PHE:CD1	2.23	0.74
1:B:40:GLU:HG2	1:B:386:PHE:CD1	2.22	0.73
1:A:333:TRP:HE1	1:A:735:TYR:HB3	1.53	0.73
1:B:420:VAL:HG23	1:B:662:GLY:HA3	1.70	0.73
1:A:564:PRO:HB2	1:A:573:VAL:HG22	1.71	0.73
1:B:720:GLU:C	1:B:722:PRO:HD3	2.13	0.73
1:A:720:GLU:C	1:A:722:PRO:HD3	2.14	0.73
1:A:39:ASP:HB3	1:A:382:ASN:ND2	2.04	0.71
1:B:564:PRO:HB2	1:B:573:VAL:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:THR:HA	1:B:706:ASN:HB2	1.72	0.71
1:B:39:ASP:HB3	1:B:382:ASN:ND2	2.04	0.71
1:A:328:SER:HB3	1:A:746:GLN:NE2	2.04	0.71
1:B:333:TRP:HE1	1:B:735:TYR:HB3	1.56	0.70
1:B:328:SER:HB3	1:B:746:GLN:NE2	2.06	0.70
1:A:666:THR:HA	1:A:706:ASN:HB2	1.73	0.70
1:B:115:ILE:HG21	1:B:138:THR:HG22	1.74	0.70
1:A:278:ARG:HD2	4:A:2200:HOH:O	1.92	0.68
1:A:115:ILE:HG21	1:A:138:THR:HG22	1.76	0.68
1:B:40:GLU:HG2	1:B:386:PHE:CG	2.28	0.67
1:B:212:ASN:O	1:B:216:THR:HG22	1.95	0.67
1:A:526:ILE:HD11	1:A:584:PHE:CD2	2.30	0.66
1:A:212:ASN:O	1:A:216:THR:HG22	1.95	0.66
1:A:40:GLU:HG2	1:A:386:PHE:CG	2.30	0.66
1:A:743:THR:OG1	1:A:746:GLN:HG3	1.96	0.66
1:B:526:ILE:HD11	1:B:584:PHE:CD2	2.31	0.65
1:B:696:GLU:HB2	1:B:699:ILE:CG2	2.26	0.65
1:A:696:GLU:HB2	1:A:699:ILE:CG2	2.27	0.65
1:B:743:THR:OG1	1:B:746:GLN:HG3	1.97	0.65
1:B:218:ARG:O	1:B:222:GLU:HG3	1.97	0.64
1:A:623:ARG:NH1	1:A:627:ALA:O	2.32	0.63
1:A:218:ARG:O	1:A:222:GLU:HG3	1.98	0.63
1:B:749:ASP:O	1:B:753:ARG:HG3	1.98	0.63
1:A:333:TRP:NE1	1:A:735:TYR:HB3	2.14	0.62
1:A:423:MET:HE2	1:A:430:GLN:NE2	2.14	0.62
1:B:706:ASN:HD21	1:B:734:GLY:N	1.98	0.62
1:A:725:TYR:HB3	1:A:728:LEU:HB2	1.82	0.62
1:B:602:SER:HB3	1:B:661:ASP:CB	2.27	0.62
1:A:743:THR:O	1:A:747:GLN:HG3	1.99	0.62
1:B:623:ARG:NH1	1:B:627:ALA:O	2.33	0.61
1:A:605:THR:O	1:A:608:SER:HB2	2.00	0.61
1:B:725:TYR:HB3	1:B:728:LEU:HB2	1.82	0.61
1:B:696:GLU:HB2	1:B:699:ILE:HG23	1.82	0.61
1:A:696:GLU:HB2	1:A:699:ILE:HG23	1.82	0.61
1:A:656:PHE:O	1:A:660:LYS:HD2	2.00	0.61
1:A:706:ASN:HD21	1:A:734:GLY:N	1.99	0.61
1:A:749:ASP:O	1:A:753:ARG:HG3	2.01	0.61
1:B:333:TRP:NE1	1:B:735:TYR:HB3	2.16	0.61
1:B:423:MET:HE2	1:B:430:GLN:NE2	2.17	0.60
1:A:420:VAL:CG2	1:A:662:GLY:HA3	2.31	0.60
1:B:75:THR:HG21	4:B:2241:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:THR:O	1:B:747:GLN:HG3	2.01	0.60
1:A:678:ASP:O	1:A:682:LYS:HG3	2.02	0.59
1:B:420:VAL:CG2	1:B:662:GLY:HA3	2.32	0.59
1:B:670:VAL:HG13	1:B:711:ASN:ND2	2.16	0.59
1:A:670:VAL:HG13	1:A:711:ASN:ND2	2.16	0.59
1:B:605:THR:O	1:B:608:SER:HB2	2.02	0.59
1:B:559:ILE:N	1:B:559:ILE:HD12	2.17	0.59
1:B:656:PHE:O	1:B:660:LYS:HD2	2.02	0.59
1:B:115:ILE:HG21	1:B:138:THR:CG2	2.33	0.59
1:B:644:ALA:HB2	1:B:756:THR:HG21	1.84	0.59
1:B:678:ASP:O	1:B:682:LYS:HG3	2.03	0.58
1:A:559:ILE:HD12	1:A:559:ILE:N	2.17	0.58
1:A:115:ILE:HG21	1:A:138:THR:CG2	2.34	0.58
1:B:39:ASP:HB3	1:B:382:ASN:HD22	1.68	0.58
1:A:15:THR:HB	1:A:31:LYS:O	2.04	0.58
1:B:606:ILE:HG22	1:B:607:THR:N	2.14	0.58
1:A:644:ALA:HB2	1:A:756:THR:HG21	1.85	0.58
1:A:39:ASP:HB3	1:A:382:ASN:HD22	1.68	0.58
1:B:548:ARG:HH11	1:B:548:ARG:HG3	1.69	0.58
1:B:15:THR:HB	1:B:31:LYS:O	2.04	0.58
1:B:566:PHE:O	1:B:635:PRO:HB3	2.04	0.58
1:B:278:ARG:HD2	4:B:2091:HOH:O	2.04	0.57
1:A:606:ILE:HG22	1:A:607:THR:N	2.16	0.56
1:A:110:ILE:HG13	1:A:270:ASN:HB3	1.87	0.56
1:A:431:PHE:CZ	1:A:520:ARG:HD3	2.40	0.56
1:B:402:ASP:OD2	1:B:406:ARG:NH1	2.38	0.56
1:A:341:MET:O	1:A:406:ARG:HD3	2.05	0.56
1:A:656:PHE:CD1	1:A:703:GLN:HG3	2.40	0.56
1:B:712:ARG:HH12	1:B:751:ILE:HB	1.70	0.56
1:B:431:PHE:CZ	1:B:520:ARG:HD3	2.41	0.56
1:A:548:ARG:HG3	1:A:548:ARG:HH11	1.71	0.56
1:B:110:ILE:HG13	1:B:270:ASN:HB3	1.87	0.56
1:A:402:ASP:OD2	1:A:406:ARG:NH1	2.40	0.55
1:B:341:MET:O	1:B:406:ARG:HD3	2.06	0.55
1:B:284:ASP:HB2	1:B:352:ASN:HB2	1.88	0.55
1:B:720:GLU:O	1:B:722:PRO:HD3	2.06	0.55
1:B:656:PHE:CD1	1:B:703:GLN:HG3	2.41	0.55
1:B:677:ASP:O	1:B:681:ARG:HG3	2.07	0.55
1:A:284:ASP:HB2	1:A:352:ASN:HB2	1.89	0.55
1:A:602:SER:HB3	1:A:661:ASP:CB	2.26	0.55
1:B:357:LEU:O	1:B:360:LEU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:GLU:O	1:A:722:PRO:HD3	2.07	0.54
1:B:409:PHE:HE2	1:B:422:PRO:HB2	1.72	0.54
1:A:222:GLU:CD	1:A:595:ARG:HH22	2.15	0.54
1:A:566:PHE:O	1:A:635:PRO:HB3	2.06	0.54
1:B:158:ARG:HG2	1:B:456:MET:HE1	1.89	0.54
1:A:712:ARG:HH12	1:A:751:ILE:HB	1.72	0.54
1:A:677:ASP:O	1:A:681:ARG:HG3	2.07	0.54
1:B:595:ARG:HD3	4:B:2119:HOH:O	2.07	0.54
1:B:708:ASN:HB3	1:B:710:MET:HE1	1.89	0.54
1:A:290:ASP:HB3	1:A:296:ILE:HG12	1.89	0.54
1:B:290:ASP:HB3	1:B:296:ILE:HG12	1.89	0.53
1:A:33:TYR:CE1	1:A:35:PRO:HG3	2.43	0.53
1:A:158:ARG:HG2	1:A:456:MET:HE1	1.91	0.53
1:A:708:ASN:HB3	1:A:710:MET:HE1	1.90	0.53
1:A:357:LEU:O	1:A:360:LEU:HB2	2.08	0.53
1:A:712:ARG:O	1:A:716:LEU:HD13	2.08	0.53
1:B:222:GLU:CD	1:B:595:ARG:HH22	2.16	0.53
1:B:712:ARG:NH1	1:B:751:ILE:HB	2.24	0.53
1:A:488:LYS:HD2	1:B:208:GLU:O	2.09	0.53
1:A:189:ILE:HG21	1:A:234:LYS:HG3	1.91	0.53
1:B:651:VAL:HG11	1:B:665:TYR:HB2	1.90	0.53
1:B:712:ARG:O	1:B:716:LEU:HD13	2.08	0.53
1:A:409:PHE:HE2	1:A:422:PRO:HB2	1.73	0.52
1:A:372:THR:HG21	1:A:400:GLU:HG3	1.90	0.52
1:A:418:CYS:SG	3:A:2001:PYR:CA	2.97	0.52
1:A:330:ASP:N	1:A:331:PRO:CD	2.73	0.52
1:B:372:THR:HG21	1:B:400:GLU:HG3	1.91	0.52
1:B:189:ILE:HG21	1:B:234:LYS:HG3	1.92	0.52
1:B:330:ASP:N	1:B:331:PRO:CD	2.73	0.52
1:A:385:LYS:NZ	1:A:683:THR:HG22	2.25	0.52
1:A:165:LEU:HD11	1:A:490:TYR:HA	1.92	0.51
1:A:180:ASP:HB3	1:A:183:ARG:HG3	1.91	0.51
1:A:651:VAL:HG11	1:A:665:TYR:HB2	1.91	0.51
1:B:165:LEU:HD11	1:B:490:TYR:HA	1.92	0.51
1:A:208:GLU:O	1:B:488:LYS:HD2	2.10	0.51
1:A:550:GLU:HA	1:A:550:GLU:OE1	2.11	0.51
1:A:677:ASP:OD2	1:A:679:GLU:HB2	2.11	0.51
1:B:704:HIS:CG	1:B:705:LEU:N	2.79	0.51
1:B:385:LYS:NZ	1:B:683:THR:HG22	2.26	0.51
1:A:704:HIS:CG	1:A:705:LEU:N	2.79	0.51
1:B:677:ASP:OD2	1:B:679:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:GLY:HA3	1:B:759:MET:OXT	2.11	0.51
1:B:685:LEU:HG	1:B:689:MET:HE2	1.93	0.50
1:A:643:GLY:HA3	1:A:759:MET:OXT	2.12	0.50
1:A:132:MET:HE2	1:A:136:ILE:CG1	2.40	0.50
1:A:146:GLN:HG2	4:A:2074:HOH:O	2.11	0.50
1:B:445:ALA:HA	1:B:482:PHE:CE2	2.46	0.50
1:A:685:LEU:HG	1:A:689:MET:HE2	1.94	0.50
1:B:186:LEU:HD13	1:B:187:TYR:CE1	2.47	0.50
1:B:420:VAL:O	1:B:422:PRO:HD3	2.11	0.50
1:A:712:ARG:NH1	1:A:751:ILE:HB	2.26	0.50
1:B:648:LEU:HD23	1:B:665:TYR:HE2	1.77	0.50
1:A:328:SER:CB	1:A:746:GLN:NE2	2.73	0.50
1:A:393:ASP:HA	4:A:2108:HOH:O	2.12	0.49
1:A:649:THR:O	1:A:653:LYS:HG3	2.12	0.49
1:A:66:ARG:HD2	4:A:2207:HOH:O	2.12	0.49
1:A:445:ALA:HA	1:A:482:PHE:CE2	2.48	0.49
1:B:649:THR:O	1:B:653:LYS:HG3	2.12	0.49
1:A:112:PHE:HE1	4:A:2141:HOH:O	1.95	0.49
1:A:420:VAL:O	1:A:422:PRO:HD3	2.12	0.49
1:B:158:ARG:HG2	1:B:456:MET:CE	2.42	0.49
1:A:471:ASN:HD22	1:A:472:TYR:N	2.11	0.49
1:A:222:GLU:OE2	1:A:595:ARG:NH2	2.46	0.49
1:A:696:GLU:HB2	1:A:699:ILE:HG22	1.95	0.49
1:A:19:TRP:HD1	1:A:27:ASP:OD1	1.95	0.49
1:A:648:LEU:HD23	1:A:665:TYR:HE2	1.78	0.48
1:B:696:GLU:HB2	1:B:699:ILE:HG22	1.94	0.48
1:B:60:GLY:O	1:B:64:GLU:HG3	2.12	0.48
1:B:490:TYR:CE2	1:B:524:CYS:HB3	2.47	0.48
1:B:471:ASN:HD22	1:B:472:TYR:N	2.10	0.48
1:A:186:LEU:HD13	1:A:187:TYR:CE1	2.48	0.48
1:B:186:LEU:HD13	1:B:187:TYR:CZ	2.48	0.48
1:B:550:GLU:HA	1:B:550:GLU:OE1	2.12	0.48
1:A:165:LEU:HD22	1:A:168:LEU:HD11	1.95	0.48
1:B:33:TYR:CE1	1:B:35:PRO:HG3	2.48	0.48
1:B:381:LEU:HD22	1:B:384:LYS:HD2	1.95	0.48
1:B:180:ASP:HB3	1:B:183:ARG:HG3	1.95	0.48
1:B:748:GLN:O	1:B:752:THR:HG23	2.13	0.48
1:A:158:ARG:HG2	1:A:456:MET:CE	2.44	0.48
1:B:33:TYR:HA	1:B:285:VAL:HG22	1.96	0.48
1:B:468:ASP:O	1:B:545:LYS:HG3	2.14	0.48
1:A:372:THR:CG2	1:A:400:GLU:HG3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLU:OE2	1:A:704:HIS:HD2	1.97	0.48
1:A:719:MET:SD	1:A:751:ILE:HD13	2.54	0.47
1:B:236:MET:HE1	1:B:260:PHE:O	2.13	0.47
1:A:381:LEU:HD22	1:A:384:LYS:HD2	1.96	0.47
1:A:548:ARG:HG3	1:A:548:ARG:NH1	2.29	0.47
1:B:445:ALA:HA	1:B:482:PHE:CD2	2.50	0.47
1:A:526:ILE:CG1	1:A:601:GLN:HE21	2.28	0.47
1:B:406:ARG:N	1:B:407:PRO:HD2	2.29	0.47
1:A:526:ILE:HG13	1:A:601:GLN:NE2	2.29	0.47
1:B:19:TRP:HD1	1:B:27:ASP:OD1	1.96	0.47
1:B:313:ARG:HG2	1:B:368:GLU:O	2.14	0.47
1:A:112:PHE:HD2	1:A:141:ARG:CZ	2.26	0.47
1:A:468:ASP:O	1:A:545:LYS:HG3	2.15	0.47
1:A:748:GLN:O	1:A:752:THR:HG23	2.15	0.47
1:B:333:TRP:CD1	1:B:418:CYS:HG	2.33	0.47
1:B:526:ILE:HG13	1:B:601:GLN:NE2	2.30	0.47
1:B:636:MET:HB2	1:B:639:ARG:HD2	1.97	0.47
1:A:33:TYR:HA	1:A:285:VAL:HG22	1.97	0.47
1:A:60:GLY:O	1:A:64:GLU:HG3	2.15	0.47
1:A:110:ILE:C	4:A:2137:HOH:O	2.58	0.47
1:B:468:ASP:O	1:B:546:PRO:HD2	2.15	0.47
1:A:186:LEU:HD13	1:A:187:TYR:CZ	2.50	0.46
1:B:16:LYS:O	1:B:31:LYS:HD3	2.15	0.46
1:B:372:THR:CG2	1:B:400:GLU:HG3	2.45	0.46
1:A:490:TYR:CE2	1:A:524:CYS:HB3	2.50	0.46
1:B:719:MET:SD	1:B:751:ILE:HD13	2.55	0.46
1:B:132:MET:HE2	1:B:136:ILE:CG1	2.39	0.46
1:B:328:SER:CB	1:B:746:GLN:NE2	2.76	0.46
1:B:386:PHE:O	1:B:390:VAL:HG23	2.16	0.46
1:B:710:MET:HB2	1:B:714:MET:HE3	1.97	0.46
1:A:636:MET:HB2	1:A:639:ARG:HD2	1.96	0.46
1:A:17:GLY:HA3	1:A:31:LYS:HD2	1.98	0.46
1:A:406:ARG:N	1:A:407:PRO:HD2	2.31	0.46
1:A:720:GLU:C	1:A:721:ASN:HD22	2.23	0.46
1:B:409:PHE:CE2	1:B:422:PRO:HB2	2.49	0.46
1:B:537:SER:OG	1:B:564:PRO:HG2	2.16	0.46
1:A:159:CYS:HB3	1:A:165:LEU:HB2	1.98	0.46
1:B:159:CYS:HB3	1:B:165:LEU:HB2	1.97	0.46
1:B:360:LEU:HD23	1:B:390:VAL:CG1	2.46	0.46
1:A:236:MET:HE1	1:A:260:PHE:O	2.16	0.46
1:B:134:LYS:O	1:B:138:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LYS:HG2	1:B:553:LEU:CD2	2.46	0.46
1:A:442:MET:HE1	1:A:536:LEU:HG	1.98	0.46
1:B:414:TYR:HA	1:B:424:ILE:HA	1.98	0.46
1:A:38:GLY:C	1:A:382:ASN:HD22	2.24	0.45
1:A:710:MET:HB2	1:A:714:MET:HE3	1.98	0.45
1:B:278:ARG:HG3	4:B:2208:HOH:O	2.15	0.45
1:B:548:ARG:HG3	1:B:548:ARG:NH1	2.27	0.45
1:B:720:GLU:C	1:B:721:ASN:HD22	2.24	0.45
1:A:313:ARG:HG2	1:A:368:GLU:O	2.15	0.45
1:B:159:CYS:HB3	1:B:164:VAL:HG13	1.99	0.45
1:A:386:PHE:O	1:A:390:VAL:HG23	2.16	0.45
1:A:601:GLN:HG2	1:A:602:SER:N	2.32	0.45
1:B:112:PHE:HD2	1:B:141:ARG:CZ	2.28	0.45
1:B:442:MET:HE1	1:B:536:LEU:HG	1.98	0.45
1:A:445:ALA:HA	1:A:482:PHE:CD2	2.52	0.45
1:A:537:SER:OG	1:A:564:PRO:HG2	2.16	0.45
1:B:222:GLU:OE2	1:B:595:ARG:NH2	2.50	0.45
1:B:400:GLU:OE2	1:B:704:HIS:HD2	2.00	0.45
1:B:526:ILE:CG1	1:B:601:GLN:HE21	2.29	0.45
1:A:159:CYS:HB3	1:A:164:VAL:HG13	1.97	0.45
1:A:230:LEU:O	1:A:233:MET:HB2	2.16	0.45
1:A:538:ALA:O	1:A:542:ALA:HB3	2.17	0.45
1:B:160:ARG:HA	1:B:165:LEU:O	2.17	0.45
1:B:265:ALA:HB1	1:B:510:LEU:HD11	1.99	0.45
1:B:17:GLY:HA3	1:B:31:LYS:HD2	1.99	0.45
1:A:414:TYR:HA	1:A:424:ILE:HA	1.98	0.45
1:B:165:LEU:HD22	1:B:168:LEU:HD11	1.98	0.45
1:A:353:SER:O	1:A:357:LEU:HD13	2.17	0.44
1:A:409:PHE:CE2	1:A:422:PRO:HB2	2.50	0.44
1:B:79:SER:HB3	1:B:110:ILE:HD13	2.00	0.44
1:B:151:VAL:HG21	1:B:500:MET:HE3	1.99	0.44
1:A:16:LYS:O	1:A:31:LYS:HD3	2.17	0.44
1:A:112:PHE:CD1	4:A:2137:HOH:O	2.49	0.44
1:B:601:GLN:HG2	1:B:602:SER:N	2.32	0.44
1:A:309:VAL:O	1:A:313:ARG:HG3	2.18	0.44
1:B:538:ALA:O	1:B:542:ALA:HB3	2.17	0.44
1:A:360:LEU:HD23	1:A:390:VAL:CG1	2.48	0.44
1:A:368:GLU:HA	1:A:369:PRO:C	2.43	0.44
1:B:73:PHE:CZ	1:B:127:ARG:HG3	2.52	0.44
1:B:353:SER:O	1:B:357:LEU:HD13	2.17	0.44
1:A:73:PHE:CZ	1:A:127:ARG:HG3	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:HA	1:A:165:LEU:O	2.18	0.44
1:A:713:GLU:OE1	1:A:713:GLU:N	2.50	0.44
1:B:114:GLY:HA2	1:B:143:THR:CB	2.48	0.44
1:B:481:HIS:O	1:B:484:ASP:HB2	2.17	0.44
1:B:610:VAL:HA	1:B:628:PRO:HB3	1.99	0.44
1:B:677:ASP:OD1	1:B:680:VAL:HG23	2.18	0.44
1:A:241:GLY:HA3	2:A:1001:PGE:H4	1.99	0.44
1:A:468:ASP:O	1:A:546:PRO:HD2	2.17	0.44
1:B:526:ILE:HD11	1:B:584:PHE:CE2	2.52	0.44
1:B:578:VAL:O	1:B:582:GLU:HG3	2.18	0.44
1:A:151:VAL:HG21	1:A:500:MET:HE3	2.00	0.44
1:A:526:ILE:HD11	1:A:584:PHE:CE2	2.53	0.44
1:A:712:ARG:HH11	1:A:712:ARG:HG3	1.83	0.44
1:B:310:MET:O	1:B:313:ARG:HB2	2.18	0.44
1:A:427:LYS:HG2	1:A:515:ASP:OD1	2.18	0.43
1:A:677:ASP:OD1	1:A:680:VAL:HG23	2.18	0.43
1:B:132:MET:CE	1:B:136:ILE:HG13	2.43	0.43
1:B:556:ASP:OD1	1:B:557:PHE:N	2.51	0.43
1:A:132:MET:CE	1:A:136:ILE:HG13	2.44	0.43
1:B:116:LYS:HB2	1:B:117:MET:HE3	1.99	0.43
1:B:710:MET:HB2	1:B:714:MET:CE	2.49	0.43
1:A:265:ALA:HB1	1:A:510:LEU:HD11	2.01	0.43
1:B:414:TYR:CD1	1:B:414:TYR:C	2.96	0.43
1:A:578:VAL:O	1:A:582:GLU:HG3	2.18	0.43
1:B:713:GLU:N	1:B:713:GLU:OE1	2.51	0.43
1:A:54:TRP:HE1	1:A:727:GLN:HE22	1.67	0.43
1:A:114:GLY:HA2	1:A:143:THR:CB	2.48	0.43
1:A:414:TYR:CD1	1:A:414:TYR:C	2.96	0.43
1:B:559:ILE:HD12	1:B:559:ILE:H	1.84	0.43
1:A:455:LYS:HG2	1:A:553:LEU:CD2	2.49	0.43
1:A:640:ASP:OD1	1:A:754:THR:HG21	2.19	0.43
1:A:710:MET:HB2	1:A:714:MET:CE	2.49	0.43
1:A:733:SER:HB2	4:A:2076:HOH:O	2.18	0.43
1:B:368:GLU:HA	1:B:369:PRO:C	2.43	0.43
1:A:610:VAL:HA	1:A:628:PRO:HB3	2.00	0.43
1:A:481:HIS:O	1:A:484:ASP:HB2	2.18	0.43
1:B:230:LEU:O	1:B:233:MET:HB2	2.19	0.43
1:A:134:LYS:O	1:A:138:THR:HG23	2.18	0.43
1:A:650:SER:O	1:A:653:LYS:HB2	2.19	0.43
1:A:559:ILE:HD12	1:A:559:ILE:H	1.83	0.42
1:A:732:VAL:HG23	1:A:735:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:VAL:O	1:B:313:ARG:HG3	2.18	0.42
1:A:526:ILE:CG1	1:A:601:GLN:NE2	2.82	0.42
1:B:360:LEU:HD12	1:B:360:LEU:HA	1.90	0.42
1:B:471:ASN:ND2	1:B:471:ASN:C	2.76	0.42
1:B:146:GLN:HG2	4:B:2158:HOH:O	2.19	0.42
1:A:230:LEU:HD23	1:A:233:MET:HE3	2.00	0.42
1:B:86:ALA:HA	1:B:240:TYR:CZ	2.55	0.42
1:B:158:ARG:NH1	4:B:2179:HOH:O	2.51	0.42
1:B:64:GLU:O	1:B:68:HIS:N	2.53	0.42
1:B:531:VAL:HG12	1:B:636:MET:CG	2.50	0.42
1:B:640:ASP:OD1	1:B:754:THR:HG21	2.19	0.42
1:B:333:TRP:HB3	1:B:418:CYS:HA	2.00	0.42
1:A:385:LYS:HE3	1:A:683:THR:HG23	2.02	0.42
1:A:333:TRP:HB3	1:A:418:CYS:HA	2.01	0.42
1:B:230:LEU:HD23	1:B:233:MET:HE3	2.02	0.42
1:B:650:SER:O	1:B:653:LYS:HB2	2.19	0.42
1:B:712:ARG:HH11	1:B:712:ARG:HG3	1.85	0.42
1:A:116:LYS:HB2	1:A:117:MET:HE3	2.01	0.42
1:A:748:GLN:NE2	1:A:751:ILE:HD11	2.34	0.42
1:B:732:VAL:HG23	1:B:735:TYR:CE2	2.55	0.42
1:B:342:GLY:HA3	4:B:2172:HOH:O	2.19	0.41
1:B:421:SER:HA	1:B:422:PRO:HD2	1.93	0.41
1:A:79:SER:HB3	1:A:110:ILE:HD13	2.02	0.41
1:A:471:ASN:C	1:A:471:ASN:ND2	2.77	0.41
1:A:212:ASN:O	1:A:213:LEU:C	2.63	0.41
1:A:435:ARG:HE	1:A:435:ARG:HB3	1.72	0.41
1:B:748:GLN:NE2	1:B:751:ILE:HD11	2.35	0.41
1:B:117:MET:HG2	1:B:171:ALA:O	2.21	0.41
1:A:86:ALA:HA	1:A:240:TYR:CZ	2.55	0.41
1:B:548:ARG:HD3	1:B:552:GLY:O	2.21	0.41
1:A:281:THR:HB	4:A:2005:HOH:O	2.20	0.41
1:A:548:ARG:HD3	1:A:552:GLY:O	2.20	0.41
1:B:38:GLY:C	1:B:382:ASN:HD22	2.27	0.41
1:B:165:LEU:HA	1:B:165:LEU:HD23	1.79	0.41
1:B:196:LYS:HA	1:B:196:LYS:HD3	1.88	0.41
1:B:472:TYR:OH	1:B:476:MET:HE2	2.21	0.41
1:A:211:VAL:O	1:A:216:THR:HG21	2.20	0.41
1:B:427:LYS:HG2	1:B:515:ASP:OD1	2.21	0.41
1:A:556:ASP:OD1	1:A:557:PHE:N	2.50	0.40
1:B:526:ILE:CG1	1:B:601:GLN:NE2	2.84	0.40
1:A:47:THR:HG23	4:A:2054:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:NZ	4:A:2117:HOH:O	2.49	0.40
1:A:388:ALA:O	1:A:392:ILE:HG13	2.22	0.40
1:A:531:VAL:HG12	1:A:636:MET:CG	2.51	0.40
1:B:211:VAL:O	1:B:216:THR:HG21	2.20	0.40
1:B:398:GLN:HB3	1:B:731:ARG:NH2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1001:PGE:C1	2:A:1001:PGE:O1[8_776]	1.46	0.74

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	754/759 (99%)	708 (94%)	44 (6%)	2 (0%)	36	60
1	B	754/759 (99%)	706 (94%)	46 (6%)	2 (0%)	36	60
All	All	1508/1518 (99%)	1414 (94%)	90 (6%)	4 (0%)	36	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	606	ILE
1	A	733	SER
1	B	606	ILE
1	B	733	SER

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	635/638 (100%)	613 (96%)	22 (4%)	32	61
1	B	635/638 (100%)	613 (96%)	22 (4%)	32	61
All	All	1270/1276 (100%)	1226 (96%)	44 (4%)	32	61

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	75	THR
1	A	152	TYR
1	A	186	LEU
1	A	207	LEU
1	A	216	THR
1	A	278	ARG
1	A	326	LEU
1	A	348	LEU
1	A	360	LEU
1	A	381	LEU
1	A	400	GLU
1	A	435	ARG
1	A	438	LEU
1	A	479	MET
1	A	550	GLU
1	A	559	ILE
1	A	573	VAL
1	A	595	ARG
1	A	699	ILE
1	A	710	MET
1	A	735	TYR
1	B	40	GLU
1	B	75	THR
1	B	152	TYR
1	B	186	LEU
1	B	207	LEU

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Mol	Chain	Res	Type
1	B	216	THR
1	B	278	ARG
1	B	326	LEU
1	B	348	LEU
1	B	360	LEU
1	B	381	LEU
1	B	400	GLU
1	B	435	ARG
1	B	438	LEU
1	B	479	MET
1	B	550	GLU
1	B	559	ILE
1	B	573	VAL
1	B	595	ARG
1	B	699	ILE
1	B	710	MET
1	B	735	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	92	GLN
1	A	126	ASN
1	A	144	HIS
1	A	252	GLN
1	A	358	ASN
1	A	382	ASN
1	A	410	ASN
1	A	471	ASN
1	A	589	GLN
1	A	601	GLN
1	A	684	ASN
1	A	706	ASN
1	A	711	ASN
1	A	721	ASN
1	A	727	GLN
1	A	748	GLN
1	B	4	ASN
1	B	68	HIS
1	B	92	GLN
1	B	126	ASN

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Mol	Chain	Res	Type
1	B	144	HIS
1	B	252	GLN
1	B	358	ASN
1	B	382	ASN
1	B	410	ASN
1	B	471	ASN
1	B	589	GLN
1	B	601	GLN
1	B	684	ASN
1	B	706	ASN
1	B	711	ASN
1	B	721	ASN
1	B	727	GLN
1	B	748	GLN
1	B	757	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	PYR	B	2002	-	5,5,5	1.76	2 (40%)	3,6,6	1.58	1 (33%)
2	PGE	A	1001	-	9,9,9	0.83	0	8,8,8	0.75	0
3	PYR	A	2001	-	5,5,5	1.98	3 (60%)	3,6,6	1.31	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
3	PYR	B	2002	-	-	0/4/4/4	-
2	PGE	A	1001	-	-	2/7/7/7	-
3	PYR	A	2001	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	PYR	CA-C	-2.63	1.45	1.54
3	A	2001	PYR	CB-CA	-2.41	1.45	1.50
3	B	2002	PYR	CA-C	-2.21	1.47	1.54
3	A	2001	PYR	OXT-C	-2.04	1.25	1.30
3	B	2002	PYR	CB-CA	-2.03	1.46	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	PYR	OXT-C-CA	2.12	119.47	113.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	PYR	OXT-C-CA-CB
2	A	1001	PGE	O2-C3-C4-O3
2	A	1001	PGE	O1-C1-C2-O2
3	A	2001	PYR	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	PGE	1	1
3	A	2001	PYR	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	756/759 (99%)	-0.24	3 (0%) 88 87	25, 43, 74, 96	0
1	B	756/759 (99%)	-0.17	1 (0%) 92 91	25, 45, 74, 95	0
All	All	1512/1518 (99%)	-0.20	4 (0%) 90 89	25, 44, 74, 96	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	561	GLY	2.5
1	B	553	LEU	2.3
1	A	7	LEU	2.2
1	A	6	LYS	2.1

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	PGE	A	1001	10/10	0.87	0.12	46,55,61,63	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PYR	B	2002	6/6	0.92	0.12	46,47,50,50	0
3	PYR	A	2001	6/6	0.96	0.06	32,33,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.