



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:05 PM UTC

PDB ID : 1AW1 / pdb_00001aw1
Title : TRIOSEPHOSPHATE ISOMERASE OF VIBRIO MARINUS COMPLEXED
WITH 2-PHOSPHOGLYCOLATE
Authors : Maes, D.; Zeelen, J.P.; Wierenga, R.K.
Deposited on : 1997-10-09
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

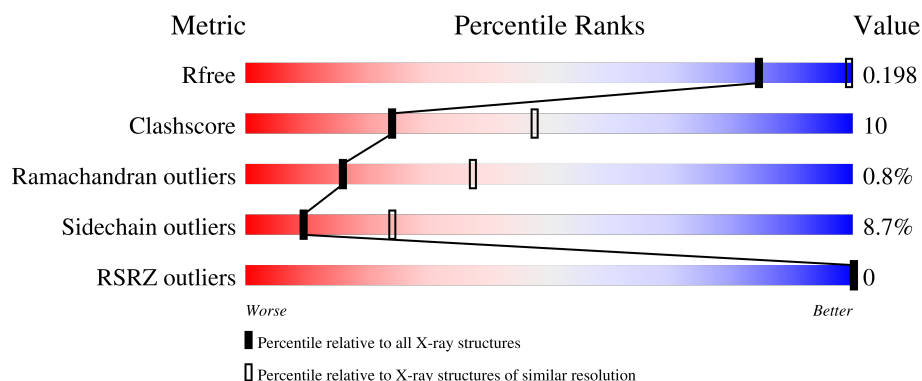
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

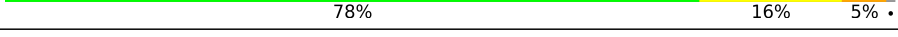
The reported resolution of this entry is 2.70 Å.

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	256	 73% 23% ..
1	B	256	 78% 16% 5% .
1	D	256	 74% 23% ..
1	E	256	 78% 16% 5% .
1	G	256	 74% 23% ..

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Mol	Chain	Length	Quality of chain
1	H	256	79% 16% 5%
1	J	256	74% 23% • •
1	K	256	79% 15% 5%

2 Entry composition

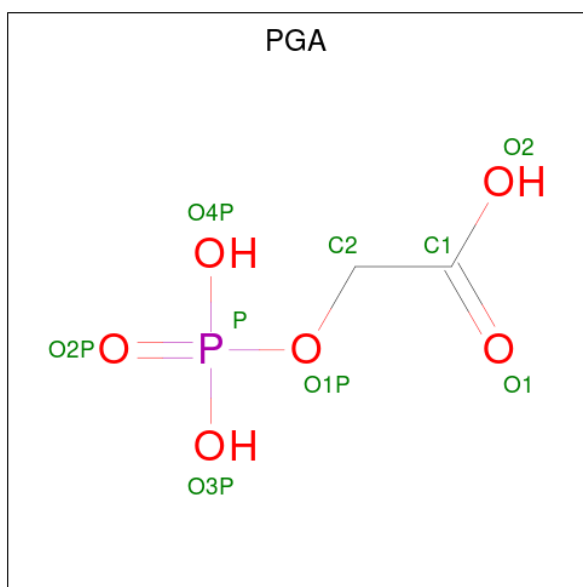
There are 3 unique types of molecules in this entry. The entry contains 15324 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	2	0	0
			1871	1172	323	369	7			
1	B	254	Total	C	N	O	S	1	0	0
			1865	1169	322	367	7			
1	D	255	Total	C	N	O	S	2	0	0
			1871	1172	323	369	7			
1	E	254	Total	C	N	O	S	1	0	0
			1865	1169	322	367	7			
1	G	255	Total	C	N	O	S	2	0	0
			1871	1172	323	369	7			
1	H	254	Total	C	N	O	S	1	0	0
			1865	1169	322	367	7			
1	J	255	Total	C	N	O	S	2	0	0
			1871	1172	323	369	7			
1	K	254	Total	C	N	O	S	1	0	0
			1865	1169	322	367	7			

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (CCD ID: PGA) (formula: C₂H₅O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		
2	D	1	Total	C	O	P	0	0
			9	2	6	1		
2	E	1	Total	C	O	P	0	0
			9	2	6	1		
2	G	1	Total	C	O	P	0	0
			9	2	6	1		
2	H	1	Total	C	O	P	0	0
			9	2	6	1		
2	J	1	Total	C	O	P	0	0
			9	2	6	1		
2	K	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	34	Total	O	0	0
			34	34		
3	D	42	Total	O	0	0
			42	42		
3	E	33	Total	O	0	0
			33	33		

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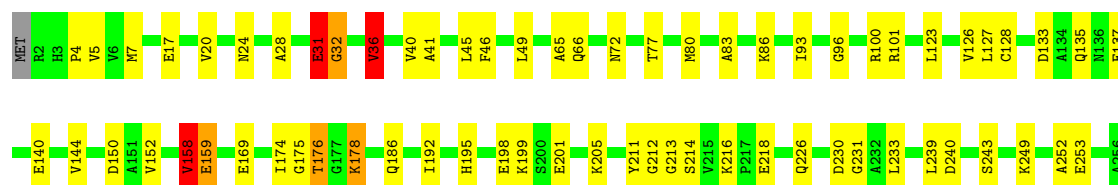
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	44	Total 44	O 44	0	0
3	H	34	Total 34	O 34	0	0
3	J	44	Total 44	O 44	0	0
3	K	33	Total 33	O 33	0	0

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 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.

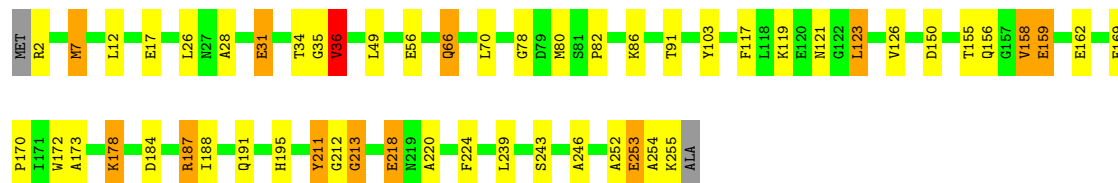
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A: 



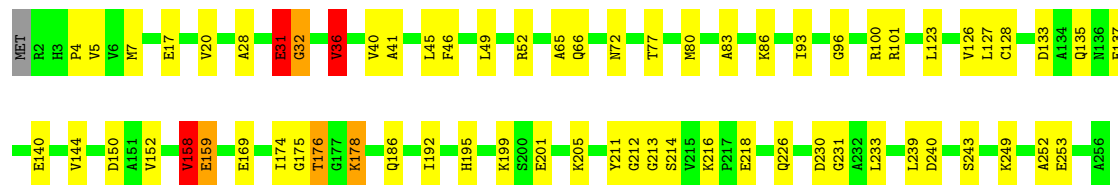
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B: 



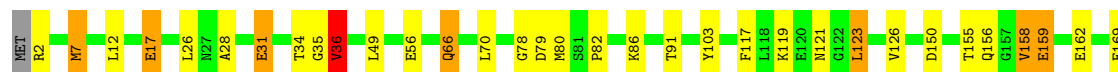
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain D: 



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

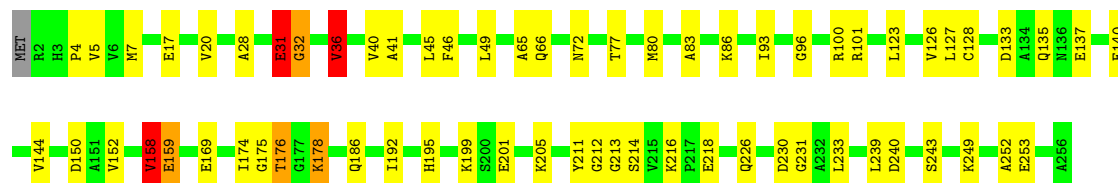
Chain E: 





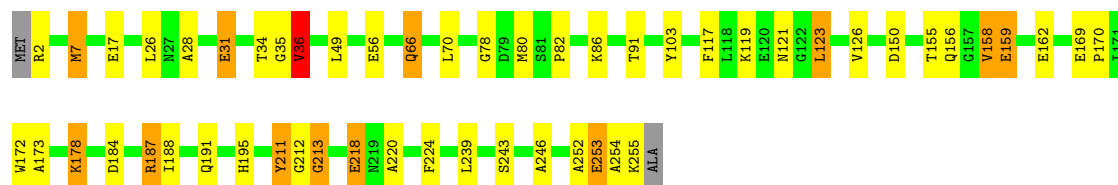
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain G: 74% 23% ..



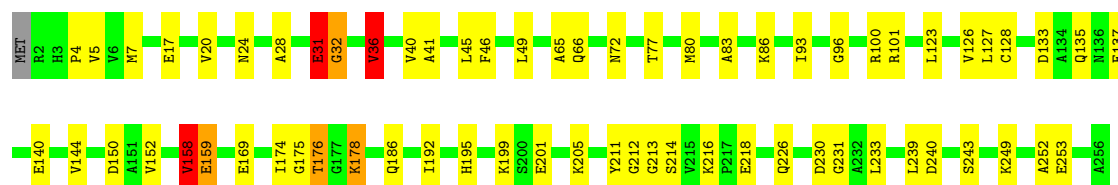
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain H: 79% 16% 5% .



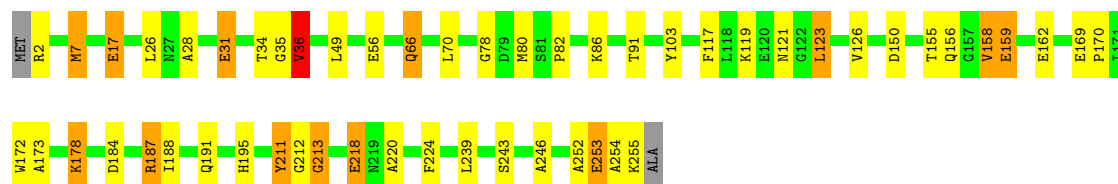
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain J: 74% 23% ..



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain K: 79% 15% 5% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.51Å 138.08Å 89.52Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70 8.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (8.00-2.70) 99.9 (8.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.49 (at 2.71Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.192 , 0.215 0.176 , 0.198	Depositor DCC
R_{free} test set	2980 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 7.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.188 for l,k,-h 0.187 for h,-k,-l 0.479 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15324	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: PGA

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	0.90	0/1900	1.10	7/2576 (0.3%)
1	B	0.86	0/1894	1.12	6/2569 (0.2%)
1	D	0.89	0/1900	1.10	7/2576 (0.3%)
1	E	0.86	0/1894	1.12	7/2569 (0.3%)
1	G	0.89	0/1900	1.10	7/2576 (0.3%)
1	H	0.86	0/1894	1.12	6/2569 (0.2%)
1	J	0.90	0/1900	1.10	7/2576 (0.3%)
1	K	0.86	0/1894	1.12	6/2569 (0.2%)
All	All	0.88	0/15176	1.11	53/20580 (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
1	E	0	1
1	H	0	1
1	K	0	1
All	All	0	4

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	VAL	CB-CA-C	-7.69	96.95	110.71
1	J	36	VAL	CB-CA-C	-7.68	96.96	110.71
1	A	36	VAL	CB-CA-C	-7.66	96.99	110.71
1	G	36	VAL	CB-CA-C	-7.66	97.00	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	103	TYR	N-CA-C	6.84	118.81	111.36
1	B	103	TYR	N-CA-C	6.79	118.76	111.36
1	H	103	TYR	N-CA-C	6.79	118.76	111.36
1	E	103	TYR	N-CA-C	6.78	118.75	111.36
1	H	70	LEU	N-CA-C	6.40	120.10	112.93
1	B	70	LEU	N-CA-C	6.39	120.08	112.93
1	H	66	GLN	N-CA-C	6.39	121.08	113.16
1	B	66	GLN	N-CA-C	6.38	121.07	113.16
1	K	70	LEU	N-CA-C	6.37	120.07	112.93
1	K	66	GLN	N-CA-C	6.37	121.05	113.16
1	D	158	VAL	CB-CA-C	-6.35	102.77	112.05
1	E	66	GLN	N-CA-C	6.35	121.04	113.16
1	A	158	VAL	CB-CA-C	-6.35	102.78	112.05
1	G	158	VAL	CB-CA-C	-6.34	102.79	112.05
1	J	158	VAL	CB-CA-C	-6.34	102.79	112.05
1	E	70	LEU	N-CA-C	6.33	120.02	112.93
1	E	158	VAL	CB-CA-C	-5.97	104.08	112.14
1	D	31	GLU	N-CA-C	5.96	123.50	110.80
1	G	31	GLU	N-CA-C	5.96	123.49	110.80
1	B	158	VAL	CB-CA-C	-5.95	104.10	112.14
1	J	31	GLU	N-CA-C	5.95	123.47	110.80
1	A	31	GLU	N-CA-C	5.95	123.47	110.80
1	K	158	VAL	CB-CA-C	-5.95	104.11	112.14
1	H	158	VAL	CB-CA-C	-5.94	104.12	112.14
1	D	192	ILE	N-CA-C	-5.93	104.57	110.62
1	G	192	ILE	N-CA-C	-5.90	104.60	110.62
1	A	192	ILE	N-CA-C	-5.90	104.61	110.62
1	J	192	ILE	N-CA-C	-5.89	104.61	110.62
1	E	36	VAL	CB-CA-C	-5.54	101.05	111.30
1	K	36	VAL	CB-CA-C	-5.53	101.07	111.30
1	H	36	VAL	CB-CA-C	-5.53	101.08	111.30
1	B	36	VAL	CB-CA-C	-5.52	101.09	111.30
1	D	126	VAL	N-CA-C	-5.49	98.78	106.53
1	G	126	VAL	N-CA-C	-5.49	98.79	106.53
1	A	126	VAL	N-CA-C	-5.49	98.79	106.53
1	J	126	VAL	N-CA-C	-5.47	98.82	106.53
1	G	233	LEU	N-CA-C	-5.22	98.75	107.99
1	A	233	LEU	N-CA-C	-5.21	98.77	107.99
1	J	233	LEU	N-CA-C	-5.21	98.77	107.99
1	D	233	LEU	N-CA-C	-5.19	98.80	107.99
1	G	176	THR	N-CA-C	5.13	118.80	112.54
1	A	176	THR	N-CA-C	5.13	118.79	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	THR	N-CA-C	5.12	118.78	112.54
1	J	176	THR	N-CA-C	5.09	118.75	112.54
1	B	220	ALA	N-CA-C	5.05	116.79	111.28
1	K	220	ALA	N-CA-C	5.05	116.79	111.28
1	H	220	ALA	N-CA-C	5.03	116.76	111.28
1	E	220	ALA	N-CA-C	5.02	116.75	111.28
1	E	79	ASP	N-CA-C	5.02	117.33	110.55

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	TYR	Sidechain
1	E	211	TYR	Sidechain
1	H	211	TYR	Sidechain
1	K	211	TYR	Sidechain

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	1871	0	1848	38	3
1	B	1865	0	1843	40	0
1	D	1871	0	1848	44	0
1	E	1865	0	1843	42	0
1	G	1871	0	1848	36	3
1	H	1865	0	1843	40	0
1	J	1871	0	1848	44	0
1	K	1865	0	1843	40	0
2	A	9	0	2	1	0
2	B	9	0	2	0	0
2	D	9	0	2	1	0
2	E	9	0	2	0	0
2	G	9	0	2	1	0
2	H	9	0	2	0	0
2	J	9	0	2	1	0
2	K	9	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	0	3	0
3	B	34	0	0	0	0
3	D	42	0	0	3	0
3	E	33	0	0	0	0
3	G	44	0	0	3	0
3	H	34	0	0	0	0
3	J	44	0	0	3	0
3	K	33	0	0	0	0
All	All	15324	0	14780	297	3

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 10.

All (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:GLY:HA2	1:J:253:GLU:OE2	1.26	1.32
1:D:32:GLY:CA	1:J:253:GLU:OE2	1.87	1.23
1:D:253:GLU:OE2	1:J:32:GLY:HA2	1.42	1.18
1:H:169:GLU:HG2	1:H:212:GLY:HA3	1.31	1.12
1:B:169:GLU:HG2	1:B:212:GLY:HA3	1.31	1.12
1:E:169:GLU:HG2	1:E:212:GLY:HA3	1.31	1.10
1:K:169:GLU:HG2	1:K:212:GLY:HA3	1.31	1.10
1:D:253:GLU:OE2	1:J:32:GLY:CA	2.14	0.96
1:A:66:GLN:HE21	1:B:78:GLY:H	1.21	0.89
1:G:66:GLN:HE21	1:H:78:GLY:H	1.21	0.88
1:D:169:GLU:HG2	1:D:212:GLY:HA3	1.55	0.87
1:J:66:GLN:HE21	1:K:78:GLY:H	1.21	0.87
1:J:169:GLU:HG2	1:J:212:GLY:HA3	1.55	0.86
1:D:66:GLN:HE21	1:E:78:GLY:H	1.21	0.86
1:G:169:GLU:HG2	1:G:212:GLY:HA3	1.55	0.86
1:A:169:GLU:HG2	1:A:212:GLY:HA3	1.55	0.86
1:D:66:GLN:NE2	1:E:78:GLY:H	1.74	0.85
1:D:32:GLY:N	1:J:253:GLU:OE2	2.09	0.84
1:J:66:GLN:NE2	1:K:78:GLY:H	1.74	0.84
1:G:66:GLN:NE2	1:H:78:GLY:H	1.74	0.84
1:A:66:GLN:NE2	1:B:78:GLY:H	1.74	0.83
1:K:211:TYR:OH	1:K:213:GLY:HA3	1.79	0.83
1:E:211:TYR:OH	1:E:213:GLY:HA3	1.79	0.83
1:H:211:TYR:OH	1:H:213:GLY:HA3	1.79	0.81
1:B:211:TYR:OH	1:B:213:GLY:HA3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG22	1:A:252:ALA:HB2	1.66	0.77
1:G:36:VAL:HG22	1:G:252:ALA:HB2	1.66	0.76
1:D:36:VAL:HG22	1:D:252:ALA:HB2	1.66	0.75
1:J:36:VAL:HG22	1:J:252:ALA:HB2	1.66	0.75
1:E:169:GLU:CG	1:E:212:GLY:HA3	2.18	0.69
1:H:169:GLU:CG	1:H:212:GLY:HA3	2.18	0.69
1:K:169:GLU:CG	1:K:212:GLY:HA3	2.18	0.69
1:B:169:GLU:CG	1:B:212:GLY:HA3	2.18	0.68
1:D:201:GLU:O	1:D:205:LYS:HG2	1.94	0.67
1:B:159:GLU:O	1:B:162:GLU:HG2	1.94	0.67
1:A:174:ILE:O	1:A:176:THR:HG23	1.95	0.67
1:H:159:GLU:O	1:H:162:GLU:HG2	1.95	0.67
1:G:174:ILE:O	1:G:176:THR:HG23	1.95	0.67
1:G:201:GLU:O	1:G:205:LYS:HG2	1.94	0.66
1:J:201:GLU:O	1:J:205:LYS:HG2	1.94	0.66
1:A:201:GLU:O	1:A:205:LYS:HG2	1.94	0.66
1:J:174:ILE:O	1:J:176:THR:HG23	1.95	0.66
1:D:174:ILE:O	1:D:176:THR:HG23	1.95	0.66
1:K:159:GLU:O	1:K:162:GLU:HG2	1.95	0.66
1:E:159:GLU:O	1:E:162:GLU:HG2	1.94	0.65
1:H:155:THR:HG23	1:H:156:GLN:HG3	1.81	0.63
1:K:253:GLU:HG2	1:K:254:ALA:N	2.14	0.63
1:B:155:THR:HG23	1:B:156:GLN:HG3	1.81	0.63
1:E:253:GLU:HG2	1:E:254:ALA:N	2.14	0.63
1:B:253:GLU:HG2	1:B:254:ALA:N	2.14	0.62
1:E:155:THR:HG23	1:E:156:GLN:HG3	1.81	0.62
1:K:155:THR:HG23	1:K:156:GLN:HG3	1.81	0.62
1:H:253:GLU:HG2	1:H:254:ALA:N	2.14	0.62
1:A:133:ASP:O	1:A:137:GLU:HG3	2.00	0.62
1:G:133:ASP:O	1:G:137:GLU:HG3	2.00	0.62
1:D:133:ASP:O	1:D:137:GLU:HG3	2.00	0.61
1:J:133:ASP:O	1:J:137:GLU:HG3	2.00	0.61
1:B:28:ALA:O	1:B:31:GLU:HB2	2.01	0.60
1:H:28:ALA:O	1:H:31:GLU:HB2	2.01	0.60
1:K:28:ALA:O	1:K:31:GLU:HB2	2.01	0.60
1:B:243:SER:O	1:B:246:ALA:HB3	2.02	0.60
1:H:243:SER:O	1:H:246:ALA:HB3	2.02	0.60
1:E:243:SER:O	1:E:246:ALA:HB3	2.02	0.60
1:E:28:ALA:O	1:E:31:GLU:HB2	2.01	0.59
1:K:243:SER:O	1:K:246:ALA:HB3	2.02	0.59
1:A:17:GLU:CD	1:A:17:GLU:H	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PHE:HA	3:A:306:HOH:O	2.02	0.59
1:D:46:PHE:HA	3:D:305:HOH:O	2.02	0.59
1:G:17:GLU:H	1:G:17:GLU:CD	2.10	0.59
1:G:46:PHE:HA	3:G:306:HOH:O	2.02	0.59
1:J:46:PHE:HA	3:J:307:HOH:O	2.02	0.59
1:D:17:GLU:H	1:D:17:GLU:CD	2.10	0.58
1:J:17:GLU:CD	1:J:17:GLU:H	2.10	0.58
1:J:159:GLU:CD	1:J:159:GLU:H	2.12	0.58
1:D:159:GLU:H	1:D:159:GLU:CD	2.12	0.58
1:K:150:ASP:OD1	1:K:195:HIS:HE1	1.87	0.57
1:G:66:GLN:HE21	1:H:78:GLY:N	1.98	0.57
1:B:150:ASP:OD1	1:B:195:HIS:HE1	1.87	0.57
1:E:150:ASP:OD1	1:E:195:HIS:HE1	1.88	0.57
1:A:66:GLN:HE21	1:B:78:GLY:N	1.97	0.56
1:G:159:GLU:H	1:G:159:GLU:CD	2.12	0.56
1:H:150:ASP:OD1	1:H:195:HIS:HE1	1.88	0.56
1:A:159:GLU:CD	1:A:159:GLU:H	2.12	0.56
1:A:198:GLU:OE2	1:D:52:ARG:NH2	2.34	0.55
1:J:66:GLN:HE21	1:K:78:GLY:N	1.97	0.55
1:H:34:THR:HG22	1:H:35:GLY:N	2.22	0.55
1:A:77:THR:HG23	1:B:66:GLN:HB3	1.89	0.55
1:B:34:THR:HG22	1:B:35:GLY:N	2.22	0.55
1:D:77:THR:HG23	1:E:66:GLN:HB3	1.89	0.55
1:G:77:THR:HG23	1:H:66:GLN:HB3	1.89	0.55
1:D:66:GLN:HE21	1:E:78:GLY:N	1.97	0.54
1:J:77:THR:HG23	1:K:66:GLN:HB3	1.89	0.54
1:E:34:THR:HG22	1:E:35:GLY:N	2.22	0.54
1:K:34:THR:HG22	1:K:35:GLY:N	2.22	0.54
1:J:240:ASP:HB3	1:J:243:SER:HB2	1.90	0.53
1:D:178:LYS:HD3	1:D:178:LYS:C	2.34	0.52
1:D:240:ASP:HB3	1:D:243:SER:HB2	1.91	0.52
1:A:240:ASP:HB3	1:A:243:SER:HB2	1.91	0.52
1:G:240:ASP:HB3	1:G:243:SER:HB2	1.90	0.52
1:G:178:LYS:C	1:G:178:LYS:HD3	2.34	0.52
1:J:178:LYS:HD3	1:J:178:LYS:C	2.34	0.52
1:H:211:TYR:CZ	1:H:213:GLY:HA3	2.44	0.52
1:A:178:LYS:HD3	1:A:178:LYS:C	2.34	0.52
1:B:211:TYR:CZ	1:B:213:GLY:HA3	2.44	0.52
1:D:249:LYS:O	1:D:253:GLU:HG2	2.10	0.52
1:E:211:TYR:CZ	1:E:213:GLY:HA3	2.44	0.52
1:B:36:VAL:HG22	1:B:252:ALA:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:211:TYR:CZ	1:K:213:GLY:HA3	2.44	0.51
1:K:36:VAL:HG22	1:K:252:ALA:HB2	1.91	0.51
1:E:36:VAL:HG22	1:E:252:ALA:HB2	1.91	0.51
1:J:249:LYS:O	1:J:253:GLU:HG2	2.10	0.51
1:A:249:LYS:O	1:A:253:GLU:HG2	2.10	0.51
1:D:5:VAL:O	1:D:231:GLY:HA3	2.11	0.51
1:H:36:VAL:HG22	1:H:252:ALA:HB2	1.91	0.51
1:J:5:VAL:O	1:J:231:GLY:HA3	2.11	0.51
1:A:5:VAL:O	1:A:231:GLY:HA3	2.11	0.51
1:B:7:MET:HE1	1:B:126:VAL:HG21	1.93	0.51
1:G:249:LYS:O	1:G:253:GLU:HG2	2.10	0.51
1:K:218:GLU:CD	1:K:218:GLU:H	2.19	0.51
1:E:218:GLU:CD	1:E:218:GLU:H	2.19	0.51
1:G:5:VAL:O	1:G:231:GLY:HA3	2.11	0.51
1:B:218:GLU:CD	1:B:218:GLU:H	2.19	0.50
1:H:7:MET:HE1	1:H:126:VAL:HG21	1.93	0.50
1:K:184:ASP:O	1:K:188:ILE:HG13	2.12	0.50
1:E:184:ASP:O	1:E:188:ILE:HG13	2.12	0.50
1:K:7:MET:HE1	1:K:126:VAL:HG21	1.93	0.50
1:B:212:GLY:O	1:B:213:GLY:O	2.30	0.50
1:E:7:MET:HE1	1:E:126:VAL:HG21	1.93	0.50
1:H:218:GLU:CD	1:H:218:GLU:H	2.19	0.49
1:K:172:TRP:CZ3	1:K:178:LYS:HD3	2.47	0.49
1:K:187:ARG:HG3	1:K:187:ARG:HH11	1.77	0.49
1:E:172:TRP:CZ3	1:E:178:LYS:HD3	2.47	0.49
1:E:187:ARG:O	1:E:191:GLN:HG3	2.12	0.49
1:H:212:GLY:O	1:H:213:GLY:O	2.30	0.49
1:K:187:ARG:O	1:K:191:GLN:HG3	2.12	0.49
1:G:211:TYR:OH	1:G:213:GLY:HA3	2.12	0.49
1:A:211:TYR:OH	1:A:213:GLY:HA3	2.12	0.49
1:J:211:TYR:OH	1:J:213:GLY:HA3	2.12	0.49
1:B:172:TRP:CZ3	1:B:178:LYS:HD3	2.47	0.49
1:B:212:GLY:O	1:B:213:GLY:C	2.55	0.49
1:K:212:GLY:O	1:K:213:GLY:O	2.30	0.49
1:D:211:TYR:OH	1:D:213:GLY:HA3	2.12	0.49
1:H:172:TRP:CZ3	1:H:178:LYS:HD3	2.47	0.49
1:E:187:ARG:HG3	1:E:187:ARG:HH11	1.77	0.49
1:H:86:LYS:HE2	1:H:121:ASN:O	2.13	0.49
1:H:187:ARG:O	1:H:191:GLN:HG3	2.12	0.49
1:B:86:LYS:HE2	1:B:121:ASN:O	2.13	0.48
1:E:212:GLY:O	1:E:213:GLY:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:212:GLY:O	1:K:213:GLY:C	2.55	0.48
1:B:253:GLU:CG	1:B:254:ALA:N	2.76	0.48
1:E:212:GLY:O	1:E:213:GLY:O	2.30	0.48
1:B:184:ASP:O	1:B:188:ILE:HG13	2.12	0.48
1:B:187:ARG:HG3	1:B:187:ARG:HH11	1.77	0.48
1:B:187:ARG:O	1:B:191:GLN:HG3	2.12	0.48
1:H:212:GLY:O	1:H:213:GLY:C	2.55	0.48
1:H:187:ARG:HH11	1:H:187:ARG:HG3	1.77	0.48
1:H:253:GLU:CG	1:H:254:ALA:N	2.76	0.48
1:D:150:ASP:OD1	1:D:195:HIS:HE1	1.97	0.48
1:H:224:PHE:O	1:H:255:LYS:HE2	2.14	0.48
1:H:184:ASP:O	1:H:188:ILE:HG13	2.12	0.47
1:D:7:MET:HE2	1:D:41:ALA:HB2	1.96	0.47
1:J:150:ASP:OD1	1:J:195:HIS:HE1	1.97	0.47
1:J:7:MET:HE2	1:J:41:ALA:HB2	1.96	0.47
1:K:253:GLU:CG	1:K:254:ALA:N	2.76	0.47
1:B:224:PHE:O	1:B:255:LYS:HE2	2.14	0.47
1:E:86:LYS:HE2	1:E:121:ASN:O	2.13	0.47
1:A:7:MET:HE2	1:A:41:ALA:HB2	1.96	0.47
1:G:150:ASP:OD1	1:G:195:HIS:HE1	1.97	0.47
1:E:253:GLU:CG	1:E:254:ALA:N	2.76	0.47
1:K:86:LYS:HE2	1:K:121:ASN:O	2.13	0.47
1:A:169:GLU:HG2	1:A:212:GLY:CA	2.38	0.47
1:A:86:LYS:HG3	1:A:123:LEU:HD21	1.96	0.46
1:G:7:MET:HE2	1:G:41:ALA:HB2	1.96	0.46
1:H:91:THR:HA	1:H:123:LEU:HD12	1.97	0.46
1:K:91:THR:HA	1:K:123:LEU:HD12	1.97	0.46
1:K:224:PHE:O	1:K:255:LYS:HE2	2.14	0.46
1:A:150:ASP:OD1	1:A:195:HIS:HE1	1.97	0.46
1:B:91:THR:HA	1:B:123:LEU:HD12	1.97	0.46
1:D:86:LYS:HG3	1:D:123:LEU:HD21	1.97	0.46
1:D:186:GLN:HB2	1:D:226:GLN:HG3	1.98	0.46
1:E:91:THR:HA	1:E:123:LEU:HD12	1.97	0.46
1:E:224:PHE:O	1:E:255:LYS:HE2	2.14	0.46
1:G:86:LYS:HG3	1:G:123:LEU:HD21	1.97	0.46
1:B:218:GLU:CD	1:B:218:GLU:N	2.74	0.46
1:J:86:LYS:HG3	1:J:123:LEU:HD21	1.96	0.46
1:G:72:ASN:ND2	1:G:83:ALA:H	2.14	0.46
1:E:170:PRO:HG2	1:E:173:ALA:HB3	1.98	0.46
1:K:170:PRO:HG2	1:K:173:ALA:HB3	1.98	0.46
1:A:72:ASN:ND2	1:A:83:ALA:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:72:ASN:ND2	1:J:83:ALA:H	2.14	0.45
1:J:186:GLN:HB2	1:J:226:GLN:HG3	1.98	0.45
1:B:170:PRO:HG2	1:B:173:ALA:HB3	1.98	0.45
1:D:72:ASN:ND2	1:D:83:ALA:H	2.14	0.45
1:E:218:GLU:CD	1:E:218:GLU:N	2.74	0.45
1:H:170:PRO:HG2	1:H:173:ALA:HB3	1.98	0.45
1:H:218:GLU:CD	1:H:218:GLU:N	2.74	0.45
1:K:187:ARG:HH11	1:K:187:ARG:CG	2.30	0.45
1:K:218:GLU:CD	1:K:218:GLU:N	2.74	0.45
1:D:135:GLN:CD	1:D:144:VAL:HG21	2.42	0.45
1:E:187:ARG:HH11	1:E:187:ARG:CG	2.30	0.45
1:J:135:GLN:CD	1:J:144:VAL:HG21	2.42	0.45
1:A:135:GLN:CD	1:A:144:VAL:HG21	2.42	0.45
1:G:135:GLN:CD	1:G:144:VAL:HG21	2.42	0.45
1:D:169:GLU:HG2	1:D:212:GLY:CA	2.38	0.45
1:H:187:ARG:HH11	1:H:187:ARG:CG	2.30	0.45
1:J:169:GLU:HG2	1:J:212:GLY:CA	2.38	0.45
1:A:186:GLN:HB2	1:A:226:GLN:HG3	1.98	0.44
1:D:31:GLU:C	1:J:253:GLU:OE2	2.60	0.44
1:B:187:ARG:HH11	1:B:187:ARG:CG	2.30	0.44
1:J:24:ASN:HD22	1:J:24:ASN:HA	1.68	0.44
1:G:169:GLU:HG2	1:G:212:GLY:CA	2.38	0.44
1:G:186:GLN:HB2	1:G:226:GLN:HG3	1.98	0.44
1:H:169:GLU:HG2	1:H:212:GLY:CA	2.23	0.44
1:K:253:GLU:OE2	1:K:254:ALA:HB2	2.18	0.44
1:E:159:GLU:H	1:E:159:GLU:HG2	1.64	0.43
1:E:253:GLU:OE2	1:E:254:ALA:HB2	2.19	0.43
1:J:28:ALA:O	1:J:31:GLU:HB2	2.18	0.43
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.89	0.43
1:D:28:ALA:O	1:D:31:GLU:HB2	2.19	0.43
1:D:96:GLY:O	1:D:101:ARG:HD2	2.18	0.43
1:G:214:SER:HB3	1:G:216:LYS:HE2	1.99	0.43
1:A:214:SER:HB3	1:A:216:LYS:HE2	1.99	0.43
1:B:172:TRP:CD1	1:B:172:TRP:H	2.36	0.43
1:D:77:THR:CG2	1:E:66:GLN:HB3	2.48	0.43
1:D:101:ARG:NH2	3:D:296:HOH:O	2.52	0.43
1:G:28:ALA:O	1:G:31:GLU:HB2	2.18	0.43
1:J:77:THR:CG2	1:K:66:GLN:HB3	2.48	0.43
1:J:96:GLY:O	1:J:101:ARG:HD2	2.18	0.43
1:A:28:ALA:O	1:A:31:GLU:HB2	2.18	0.43
1:A:101:ARG:NH2	3:A:297:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:101:ARG:NH2	3:J:298:HOH:O	2.52	0.43
1:D:214:SER:HB3	1:D:216:LYS:HE2	1.99	0.43
1:A:96:GLY:O	1:A:101:ARG:HD2	2.18	0.43
1:A:158:VAL:HG11	1:A:199:LYS:HB2	2.01	0.43
1:G:77:THR:CG2	1:H:66:GLN:HB3	2.48	0.43
1:G:96:GLY:O	1:G:101:ARG:HD2	2.18	0.43
1:H:172:TRP:CD1	1:H:172:TRP:H	2.36	0.43
1:A:77:THR:CG2	1:B:66:GLN:HB3	2.48	0.42
1:A:169:GLU:OE2	2:A:290:PGA:O1	2.37	0.42
1:G:101:ARG:NH2	3:G:297:HOH:O	2.52	0.42
1:J:65:ALA:HB3	1:J:93:ILE:HD12	2.01	0.42
1:J:214:SER:HB3	1:J:216:LYS:HE2	2.00	0.42
1:K:119:LYS:HD2	1:K:119:LYS:HA	1.82	0.42
1:K:172:TRP:CD1	1:K:172:TRP:H	2.36	0.42
1:G:169:GLU:OE2	2:G:290:PGA:O1	2.37	0.42
1:J:169:GLU:OE2	2:J:290:PGA:O1	2.37	0.42
1:B:253:GLU:OE2	1:B:254:ALA:HB2	2.18	0.42
1:D:65:ALA:HB3	1:D:93:ILE:HD12	2.01	0.42
1:G:158:VAL:HG11	1:G:199:LYS:HB2	2.01	0.42
1:H:253:GLU:OE2	1:H:254:ALA:HB2	2.18	0.42
1:E:172:TRP:CD1	1:E:172:TRP:H	2.36	0.42
1:B:169:GLU:HG2	1:B:212:GLY:CA	2.23	0.42
1:D:31:GLU:C	3:D:307:HOH:O	2.63	0.42
1:E:169:GLU:HG2	1:E:212:GLY:CA	2.23	0.42
1:K:17:GLU:H	1:K:17:GLU:HG3	1.62	0.42
1:J:31:GLU:C	3:J:309:HOH:O	2.63	0.42
1:G:65:ALA:HB3	1:G:93:ILE:HD12	2.01	0.42
1:G:101:ARG:NH1	1:G:128:CYS:O	2.53	0.42
1:D:169:GLU:OE2	2:D:290:PGA:O1	2.37	0.42
1:A:65:ALA:HB3	1:A:93:ILE:HD12	2.01	0.42
1:A:101:ARG:NH1	1:A:128:CYS:O	2.53	0.42
1:E:172:TRP:HZ3	1:E:178:LYS:HD3	1.84	0.42
1:G:31:GLU:C	3:G:308:HOH:O	2.63	0.41
1:J:17:GLU:CD	1:J:17:GLU:N	2.78	0.41
1:A:4:PRO:HA	1:A:230:ASP:O	2.20	0.41
1:J:4:PRO:HA	1:J:230:ASP:O	2.20	0.41
1:B:119:LYS:HD2	1:B:119:LYS:HA	1.82	0.41
1:D:4:PRO:HA	1:D:230:ASP:O	2.20	0.41
1:J:158:VAL:HG11	1:J:199:LYS:HB2	2.01	0.41
1:G:4:PRO:HA	1:G:230:ASP:O	2.20	0.41
1:H:82:PRO:HG2	1:H:117:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:LYS:HD2	1:H:119:LYS:HA	1.82	0.41
1:D:72:ASN:HD22	1:D:72:ASN:HA	1.70	0.41
1:D:158:VAL:HG11	1:D:199:LYS:HB2	2.01	0.41
1:E:17:GLU:H	1:E:17:GLU:HG3	1.62	0.41
1:K:7:MET:CE	1:K:126:VAL:HG21	2.50	0.41
1:D:17:GLU:CD	1:D:17:GLU:N	2.78	0.41
1:E:7:MET:CE	1:E:126:VAL:HG21	2.50	0.41
1:E:12:LEU:HD12	1:E:12:LEU:HA	1.89	0.41
1:H:7:MET:CE	1:H:126:VAL:HG21	2.50	0.41
1:A:31:GLU:C	3:A:308:HOH:O	2.63	0.41
1:B:82:PRO:HG2	1:B:117:PHE:CE2	2.55	0.41
1:D:101:ARG:NH1	1:D:128:CYS:O	2.53	0.41
1:J:101:ARG:NH1	1:J:128:CYS:O	2.53	0.41
1:K:172:TRP:HZ3	1:K:178:LYS:HD3	1.84	0.41
1:B:7:MET:CE	1:B:126:VAL:HG21	2.50	0.41
1:E:82:PRO:HG2	1:E:117:PHE:CE2	2.55	0.41
1:G:17:GLU:CD	1:G:17:GLU:N	2.78	0.41
1:H:159:GLU:H	1:H:159:GLU:HG2	1.64	0.41
1:K:82:PRO:HG2	1:K:117:PHE:CE2	2.55	0.41
1:A:24:ASN:HD22	1:A:24:ASN:HA	1.68	0.41
1:K:169:GLU:HG2	1:K:212:GLY:CA	2.23	0.41
1:E:119:LYS:HD2	1:E:119:LYS:HA	1.82	0.40
1:A:17:GLU:CD	1:A:17:GLU:N	2.78	0.40
1:B:172:TRP:HZ3	1:B:178:LYS:HD3	1.84	0.40
1:J:72:ASN:HD22	1:J:72:ASN:HA	1.69	0.40
1:H:172:TRP:HZ3	1:H:178:LYS:HD3	1.84	0.40

All (3) 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)
1:A:253:GLU:OE2	1:G:32:GLY:CA[2_646]	1.87	0.33
1:A:253:GLU:OE2	1:G:32:GLY:N[2_646]	2.08	0.12
1:A:32:GLY:CA	1:G:253:GLU:OE2[2_646]	2.14	0.06

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	253/256 (99%)	244 (96%)	6 (2%)	3 (1%)	10	27
1	B	252/256 (98%)	238 (94%)	13 (5%)	1 (0%)	30	54
1	D	253/256 (99%)	244 (96%)	6 (2%)	3 (1%)	10	27
1	E	252/256 (98%)	238 (94%)	13 (5%)	1 (0%)	30	54
1	G	253/256 (99%)	244 (96%)	6 (2%)	3 (1%)	10	27
1	H	252/256 (98%)	238 (94%)	13 (5%)	1 (0%)	30	54
1	J	253/256 (99%)	244 (96%)	6 (2%)	3 (1%)	10	27
1	K	252/256 (98%)	238 (94%)	13 (5%)	1 (0%)	30	54
All	All	2020/2048 (99%)	1928 (95%)	76 (4%)	16 (1%)	16	37

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	D	31	GLU
1	G	31	GLU
1	J	31	GLU
1	B	213	GLY
1	E	213	GLY
1	H	213	GLY
1	K	213	GLY
1	A	32	GLY
1	D	32	GLY
1	G	32	GLY
1	J	32	GLY
1	A	175	GLY
1	D	175	GLY
1	G	175	GLY
1	J	175	GLY

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	184/185 (100%)	169 (92%)	15 (8%)	10	27
1	B	184/185 (100%)	167 (91%)	17 (9%)	8	22
1	D	184/185 (100%)	169 (92%)	15 (8%)	10	27
1	E	184/185 (100%)	167 (91%)	17 (9%)	8	22
1	G	184/185 (100%)	169 (92%)	15 (8%)	10	27
1	H	184/185 (100%)	167 (91%)	17 (9%)	8	22
1	J	184/185 (100%)	169 (92%)	15 (8%)	10	27
1	K	184/185 (100%)	167 (91%)	17 (9%)	8	22
All	All	1472/1480 (100%)	1344 (91%)	128 (9%)	9	24

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	36	VAL
1	A	40	VAL
1	A	45	LEU
1	A	49	LEU
1	A	80	MET
1	A	100	ARG
1	A	127	LEU
1	A	140	GLU
1	A	152	VAL
1	A	158	VAL
1	A	159	GLU
1	A	178	LYS
1	A	218	GLU
1	A	239	LEU
1	B	2	ARG
1	B	7	MET
1	B	17	GLU
1	B	26	LEU

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Mol	Chain	Res	Type
1	B	31	GLU
1	B	36	VAL
1	B	49	LEU
1	B	56	GLU
1	B	80	MET
1	B	123	LEU
1	B	158	VAL
1	B	159	GLU
1	B	178	LYS
1	B	187	ARG
1	B	218	GLU
1	B	239	LEU
1	B	253	GLU
1	D	20	VAL
1	D	36	VAL
1	D	40	VAL
1	D	45	LEU
1	D	49	LEU
1	D	80	MET
1	D	100	ARG
1	D	127	LEU
1	D	140	GLU
1	D	152	VAL
1	D	158	VAL
1	D	159	GLU
1	D	178	LYS
1	D	218	GLU
1	D	239	LEU
1	E	2	ARG
1	E	7	MET
1	E	17	GLU
1	E	26	LEU
1	E	31	GLU
1	E	36	VAL
1	E	49	LEU
1	E	56	GLU
1	E	80	MET
1	E	123	LEU
1	E	158	VAL
1	E	159	GLU
1	E	178	LYS
1	E	187	ARG

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Mol	Chain	Res	Type
1	E	218	GLU
1	E	239	LEU
1	E	253	GLU
1	G	20	VAL
1	G	36	VAL
1	G	40	VAL
1	G	45	LEU
1	G	49	LEU
1	G	80	MET
1	G	100	ARG
1	G	127	LEU
1	G	140	GLU
1	G	152	VAL
1	G	158	VAL
1	G	159	GLU
1	G	178	LYS
1	G	218	GLU
1	G	239	LEU
1	H	2	ARG
1	H	7	MET
1	H	17	GLU
1	H	26	LEU
1	H	31	GLU
1	H	36	VAL
1	H	49	LEU
1	H	56	GLU
1	H	80	MET
1	H	123	LEU
1	H	158	VAL
1	H	159	GLU
1	H	178	LYS
1	H	187	ARG
1	H	218	GLU
1	H	239	LEU
1	H	253	GLU
1	J	20	VAL
1	J	36	VAL
1	J	40	VAL
1	J	45	LEU
1	J	49	LEU
1	J	80	MET
1	J	100	ARG

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Mol	Chain	Res	Type
1	J	127	LEU
1	J	140	GLU
1	J	152	VAL
1	J	158	VAL
1	J	159	GLU
1	J	178	LYS
1	J	218	GLU
1	J	239	LEU
1	K	2	ARG
1	K	7	MET
1	K	17	GLU
1	K	26	LEU
1	K	31	GLU
1	K	36	VAL
1	K	49	LEU
1	K	56	GLU
1	K	80	MET
1	K	123	LEU
1	K	158	VAL
1	K	159	GLU
1	K	178	LYS
1	K	187	ARG
1	K	218	GLU
1	K	239	LEU
1	K	253	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	66	GLN
1	A	72	ASN
1	A	121	ASN
1	A	191	GLN
1	A	195	HIS
1	A	206	ASN
1	A	210	GLN
1	B	3	HIS
1	B	92	HIS
1	B	136	ASN
1	B	154	ASN
1	B	191	GLN

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Mol	Chain	Res	Type
1	B	195	HIS
1	B	206	ASN
1	D	24	ASN
1	D	66	GLN
1	D	72	ASN
1	D	121	ASN
1	D	191	GLN
1	D	195	HIS
1	D	206	ASN
1	D	210	GLN
1	E	3	HIS
1	E	92	HIS
1	E	136	ASN
1	E	154	ASN
1	E	191	GLN
1	E	195	HIS
1	E	206	ASN
1	G	24	ASN
1	G	66	GLN
1	G	72	ASN
1	G	121	ASN
1	G	191	GLN
1	G	195	HIS
1	G	206	ASN
1	G	210	GLN
1	H	3	HIS
1	H	92	HIS
1	H	136	ASN
1	H	154	ASN
1	H	191	GLN
1	H	195	HIS
1	H	206	ASN
1	J	24	ASN
1	J	66	GLN
1	J	72	ASN
1	J	121	ASN
1	J	191	GLN
1	J	195	HIS
1	J	206	ASN
1	J	210	GLN
1	K	92	HIS
1	K	136	ASN

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Mol	Chain	Res	Type
1	K	154	ASN
1	K	191	GLN
1	K	195	HIS
1	K	206	ASN

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 ⓘ

8 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	PGA	B	290	-	8,8,8	1.44	2 (25%)	10,11,11	1.17	1 (10%)
2	PGA	A	290	-	8,8,8	1.50	1 (12%)	10,11,11	1.66	1 (10%)
2	PGA	E	290	-	8,8,8	1.44	2 (25%)	10,11,11	1.16	1 (10%)
2	PGA	J	290	-	8,8,8	1.50	1 (12%)	10,11,11	1.66	1 (10%)
2	PGA	D	290	-	8,8,8	1.50	1 (12%)	10,11,11	1.66	1 (10%)
2	PGA	H	290	-	8,8,8	1.44	2 (25%)	10,11,11	1.16	1 (10%)
2	PGA	G	290	-	8,8,8	1.50	1 (12%)	10,11,11	1.67	1 (10%)
2	PGA	K	290	-	8,8,8	1.44	2 (25%)	10,11,11	1.16	1 (10%)

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	PGA	B	290	-	-	3/6/6/6	-
2	PGA	A	290	-	-	2/6/6/6	-
2	PGA	E	290	-	-	3/6/6/6	-
2	PGA	J	290	-	-	2/6/6/6	-
2	PGA	D	290	-	-	2/6/6/6	-
2	PGA	H	290	-	-	3/6/6/6	-
2	PGA	G	290	-	-	2/6/6/6	-
2	PGA	K	290	-	-	3/6/6/6	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	290	PGA	O2-C1	-3.38	1.19	1.30
2	G	290	PGA	O2-C1	-3.37	1.19	1.30
2	D	290	PGA	O2-C1	-3.37	1.19	1.30
2	J	290	PGA	O2-C1	-3.37	1.19	1.30
2	H	290	PGA	O2-C1	-2.82	1.21	1.30
2	E	290	PGA	O2-C1	-2.82	1.21	1.30
2	B	290	PGA	O2-C1	-2.80	1.21	1.30
2	K	290	PGA	O2-C1	-2.80	1.21	1.30
2	H	290	PGA	O1-C1	2.40	1.29	1.22
2	K	290	PGA	O1-C1	2.39	1.29	1.22
2	E	290	PGA	O1-C1	2.38	1.29	1.22
2	B	290	PGA	O1-C1	2.37	1.29	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	290	PGA	O1P-C2-C1	4.31	117.03	110.54
2	D	290	PGA	O1P-C2-C1	4.28	116.99	110.54
2	J	290	PGA	O1P-C2-C1	4.27	116.98	110.54
2	A	290	PGA	O1P-C2-C1	4.27	116.97	110.54
2	K	290	PGA	O1P-C2-C1	2.39	114.13	110.54
2	B	290	PGA	O1P-C2-C1	2.38	114.13	110.54
2	E	290	PGA	O1P-C2-C1	2.37	114.11	110.54
2	H	290	PGA	O1P-C2-C1	2.36	114.09	110.54

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	290	PGA	C2-O1P-P-O2P
2	B	290	PGA	C2-O1P-P-O3P
2	B	290	PGA	C2-O1P-P-O4P
2	E	290	PGA	C2-O1P-P-O2P
2	E	290	PGA	C2-O1P-P-O3P
2	E	290	PGA	C2-O1P-P-O4P
2	H	290	PGA	C2-O1P-P-O2P
2	H	290	PGA	C2-O1P-P-O3P
2	H	290	PGA	C2-O1P-P-O4P
2	K	290	PGA	C2-O1P-P-O2P
2	K	290	PGA	C2-O1P-P-O3P
2	K	290	PGA	C2-O1P-P-O4P
2	A	290	PGA	O1-C1-C2-O1P
2	D	290	PGA	O1-C1-C2-O1P
2	G	290	PGA	O1-C1-C2-O1P
2	J	290	PGA	O1-C1-C2-O1P
2	A	290	PGA	O2-C1-C2-O1P
2	G	290	PGA	O2-C1-C2-O1P
2	J	290	PGA	O2-C1-C2-O1P
2	D	290	PGA	O2-C1-C2-O1P

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	290	PGA	1	0
2	J	290	PGA	1	0
2	D	290	PGA	1	0
2	G	290	PGA	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	255/256 (99%)	-1.97	0 100 100	2, 8, 26, 42	1 (0%)
1	B	254/256 (99%)	-1.94	0 100 100	3, 12, 30, 45	1 (0%)
1	D	255/256 (99%)	-1.97	0 100 100	2, 8, 26, 42	1 (0%)
1	E	254/256 (99%)	-1.92	0 100 100	3, 12, 30, 45	1 (0%)
1	G	255/256 (99%)	-1.97	0 100 100	2, 8, 26, 42	1 (0%)
1	H	254/256 (99%)	-1.93	0 100 100	3, 12, 30, 45	1 (0%)
1	J	255/256 (99%)	-1.97	0 100 100	2, 8, 26, 42	1 (0%)
1	K	254/256 (99%)	-1.93	0 100 100	3, 12, 30, 45	1 (0%)
All	All	2036/2048 (99%)	-1.95	0 100 100	2, 10, 30, 45	8 (0%)

There are no RSRZ outliers to report.

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($\text{\AA}^2$)	Q<0.9
2	PGA	A	290	9/9	1.00	0.02	26,28,30,30	0
2	PGA	B	290	9/9	1.00	0.02	22,24,29,29	0
2	PGA	D	290	9/9	1.00	0.04	26,28,30,30	0
2	PGA	E	290	9/9	1.00	0.02	22,24,29,29	0
2	PGA	G	290	9/9	1.00	0.04	26,28,30,30	0
2	PGA	H	290	9/9	1.00	0.02	22,24,29,29	0
2	PGA	J	290	9/9	1.00	0.02	26,28,30,30	0
2	PGA	K	290	9/9	1.00	0.02	22,24,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.