



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 04:42 PM EST

PDB ID : 1LZO  
Title : Plasmodium Falciparum Triosephosphate Isomerase-Phosphoglycolate Complex  
Authors : Parthasarathy, S.; Balaram, H.; Balaram, P.; Murthy, M.R.  
Deposited on : 2002-06-11  
Resolution : 2.80 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

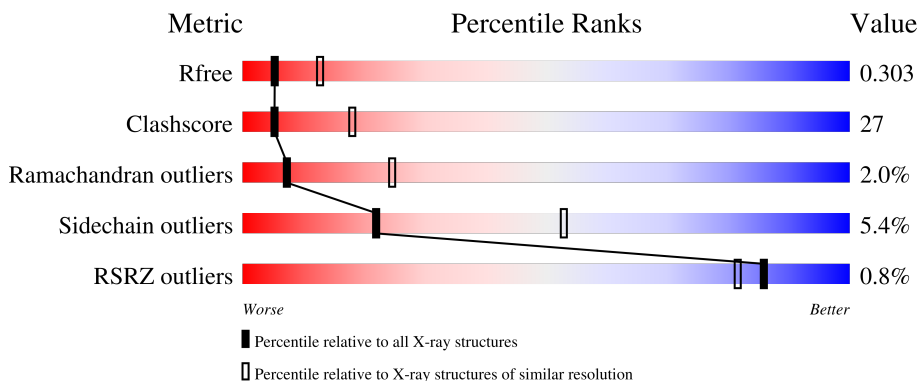
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	248	
1	B	248	
1	C	248	
1	D	248	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7996 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.

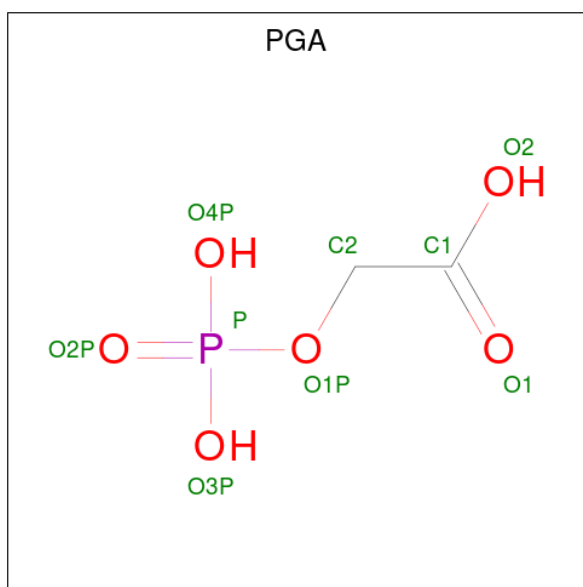
- Molecule 1 is a protein called Triosephosphate Isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	246	1957	1239	333	380	5	0	0	0
1	B	246	1957	1239	333	380	5	0	0	0
1	C	246	1957	1239	333	380	5	0	0	0
1	D	246	1957	1239	333	380	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	VAL	ALA	conflict	UNP Q07412
B	163	VAL	ALA	conflict	UNP Q07412
C	163	VAL	ALA	conflict	UNP Q07412
D	163	VAL	ALA	conflict	UNP Q07412

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: C<sub>2</sub>H<sub>5</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

- Molecule 3 is water.

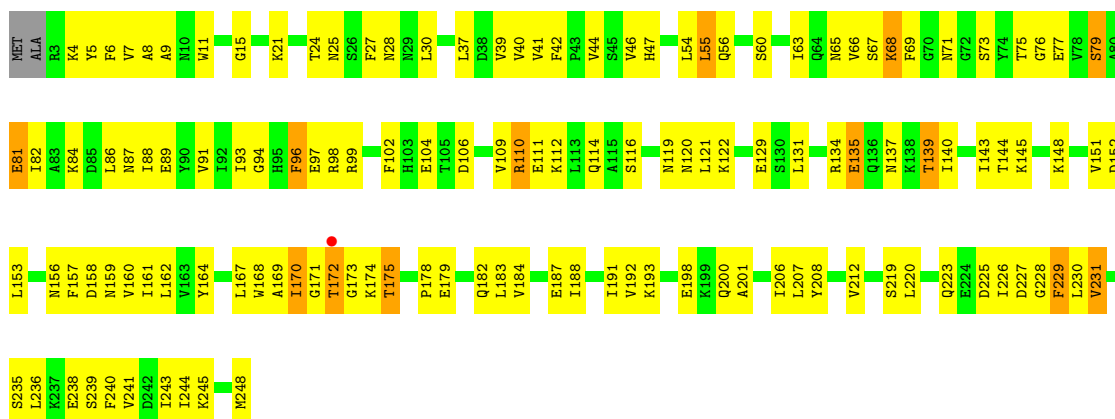
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	42	Total	O	0	0
			42	42		
3	C	25	Total	O	0	0
			25	25		
3	D	39	Total	O	0	0
			39	39		

### 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.

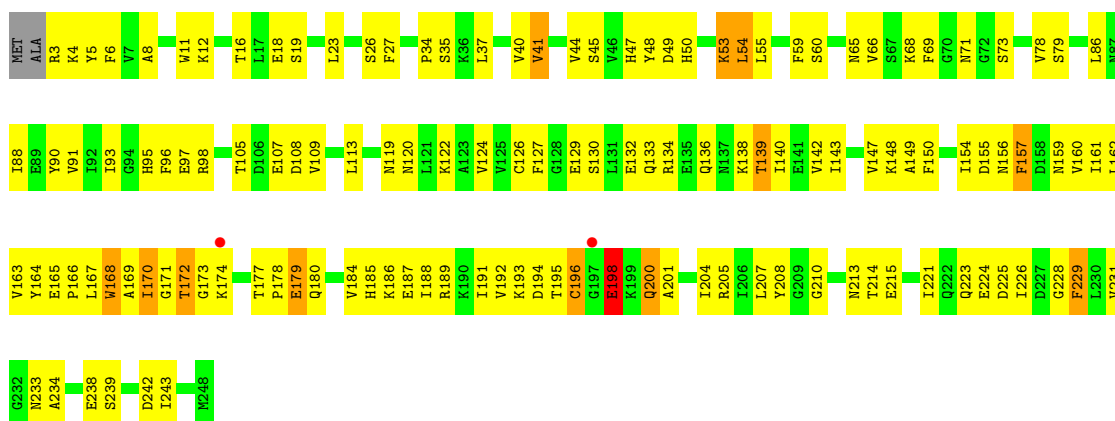
- Molecule 1: Triosephosphate Isomerase

Chain A: 



- Molecule 1: Triosephosphate Isomerase

Chain B: 

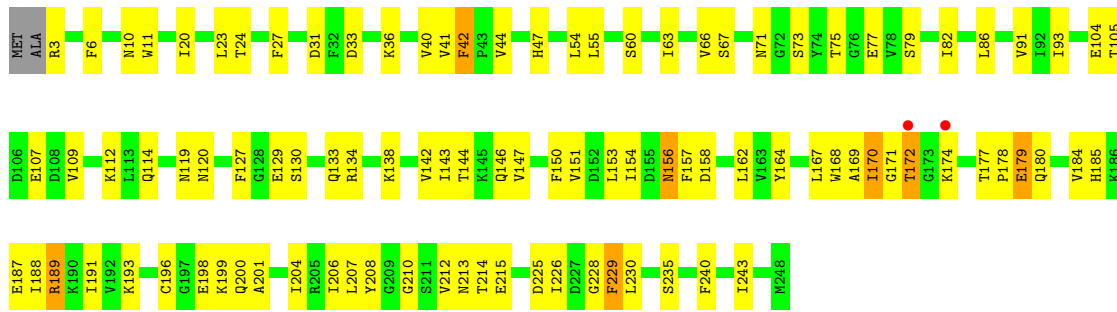


- Molecule 1: Triosephosphate Isomerase

Chain C: 



● Molecule 1: Triosephosphate Isomerase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.82Å 106.77Å 181.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (20.00-2.80) 94.2 (19.80-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.71 (at 2.79Å)	Xtrriage
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.232 , 0.311 0.225 , 0.303	Depositor DCC
$R_{free}$ test set	2330 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtrriage
Anisotropy	0.101	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 25.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0837e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.39	0/1989	0.65	0/2682
1	B	0.40	0/1989	0.65	0/2682
1	C	0.44	1/1989 (0.1%)	0.65	0/2682
1	D	0.45	0/1989	0.66	0/2682
All	All	0.42	1/7956 (0.0%)	0.65	0/10728

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	ILE	CA-CB	5.54	1.67	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1957	0	1953	111	0
1	B	1957	0	1953	113	0
1	C	1957	0	1953	110	0
1	D	1957	0	1953	97	0
2	B	9	0	2	0	0
2	D	9	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	0	2	1
3	B	42	0	0	7	1
3	C	25	0	0	2	0
3	D	39	0	0	4	0
All	All	7996	0	7817	416	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 27.

All (416) 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:B:6:PHE:HB3	1:B:207:LEU:HD21	1.43	0.99
1:C:173:GLY:HA2	3:C:555:HOH:O	1.67	0.94
1:C:207:LEU:HB3	1:C:229:PHE:HA	1.49	0.94
1:D:114:GLN:HE21	1:D:153:LEU:HD21	1.37	0.90
1:D:179:GLU:CD	1:D:179:GLU:H	1.73	0.89
1:D:156:ASN:HD22	1:D:157:PHE:N	1.71	0.89
1:B:165:GLU:OE2	3:B:642:HOH:O	1.90	0.89
1:C:6:PHE:HB3	1:C:207:LEU:HD21	1.59	0.85
1:D:156:ASN:HD22	1:D:156:ASN:C	1.79	0.84
1:D:82:ILE:O	1:D:86:LEU:HD13	1.78	0.83
1:D:189:ARG:HH11	1:D:189:ARG:HB2	1.43	0.83
1:A:207:LEU:HB3	1:A:229:PHE:HA	1.60	0.82
1:B:132:GLU:O	1:B:136:GLN:HG2	1.79	0.82
1:A:131:LEU:O	1:A:135:GLU:HB3	1.80	0.81
1:A:63:ILE:HG12	1:A:91:VAL:HG12	1.62	0.81
1:D:114:GLN:HB2	1:D:153:LEU:HD11	1.61	0.81
1:D:114:GLN:NE2	1:D:153:LEU:HD21	1.98	0.79
1:C:175:THR:HG21	3:C:595:HOH:O	1.84	0.77
1:A:21:LYS:HA	1:A:54:LEU:HD13	1.65	0.77
1:C:245:LYS:HA	1:C:248:MET:HG2	1.66	0.76
1:D:40:VAL:HG22	1:D:60:SER:HB2	1.68	0.76
1:C:30:LEU:HD21	1:C:248:MET:HE1	1.68	0.75
1:C:67:SER:HB2	1:C:77:GLU:HB3	1.67	0.74
1:A:140:ILE:HG12	1:A:187:GLU:HG2	1.69	0.73
1:A:6:PHE:O	1:A:228:GLY:HA3	1.88	0.73
1:B:188:ILE:HA	1:B:191:ILE:HD12	1.70	0.72
1:D:3:ARG:CZ	1:D:189:ARG:HH21	2.02	0.71
1:D:6:PHE:HD2	1:D:207:LEU:HD11	1.55	0.71
1:C:84:LYS:HE3	1:C:119:ASN:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:N	1:A:161:ILE:HD12	2.06	0.70
1:D:156:ASN:ND2	1:D:158:ASP:H	1.90	0.70
1:B:233:ASN:HB3	3:B:585:HOH:O	1.91	0.70
1:B:136:GLN:HB2	1:B:138:LYS:HG3	1.73	0.70
1:A:84:LYS:HE3	1:A:119:ASN:O	1.92	0.69
1:B:41:VAL:HG11	1:B:55:LEU:CD1	2.22	0.69
1:A:25:ASN:HA	1:A:28:ASN:HD22	1.56	0.69
1:B:167:LEU:HA	1:B:170:ILE:HG12	1.74	0.69
1:C:64:GLN:HB3	1:D:75:THR:HG23	1.73	0.69
1:D:230:LEU:HD23	3:D:568:HOH:O	1.93	0.68
1:C:182:GLN:OE1	1:C:223:GLN:HB3	1.94	0.67
1:A:63:ILE:CG1	1:A:91:VAL:HG12	2.24	0.67
1:A:9:ALA:HB1	1:A:235:SER:HB2	1.75	0.67
1:A:98:ARG:O	1:A:102:PHE:O	2.13	0.67
1:A:245:LYS:HA	1:A:248:MET:HG2	1.77	0.67
1:C:102:PHE:O	1:C:104:GLU:N	2.27	0.66
1:D:134:ARG:HD2	1:D:168:TRP:CG	2.30	0.66
1:A:76:GLY:HA3	1:B:98:ARG:NH1	2.11	0.66
1:A:134:ARG:HD2	1:A:168:TRP:CG	2.31	0.66
1:B:40:VAL:HG22	1:B:60:SER:HB2	1.78	0.66
1:A:40:VAL:HG22	1:A:60:SER:HB2	1.78	0.65
1:C:131:LEU:HD22	1:C:172:THR:HG21	1.76	0.65
1:C:187:GLU:O	1:C:191:ILE:HG13	1.97	0.65
1:C:37:LEU:HD22	1:C:248:MET:HB3	1.79	0.65
1:A:182:GLN:HE22	1:A:225:ASP:HB2	1.60	0.65
1:C:138:LYS:O	1:C:142:VAL:HG23	1.97	0.65
1:D:41:VAL:HG11	1:D:55:LEU:CD1	2.28	0.64
1:C:160:VAL:C	1:C:161:ILE:HD12	2.18	0.64
1:A:200:GLN:CD	1:A:200:GLN:H	2.01	0.64
1:A:230:LEU:HD23	3:A:567:HOH:O	1.97	0.64
1:D:3:ARG:NE	1:D:189:ARG:HH21	1.96	0.64
1:B:140:ILE:HG12	1:B:187:GLU:HG2	1.78	0.63
1:D:6:PHE:CD2	1:D:207:LEU:HD11	2.34	0.63
1:C:30:LEU:HD21	1:C:248:MET:CE	2.29	0.63
1:C:182:GLN:HE22	1:C:225:ASP:HB2	1.63	0.63
1:D:156:ASN:C	1:D:156:ASN:ND2	2.52	0.63
1:C:185:HIS:CE1	1:C:226:ILE:HG12	2.34	0.62
1:D:179:GLU:CD	1:D:179:GLU:N	2.51	0.62
1:B:193:LYS:HD2	1:B:194:ASP:OD2	2.00	0.62
1:A:131:LEU:HD13	1:A:172:THR:HG21	1.81	0.62
1:B:161:ILE:HD12	1:B:161:ILE:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:GLU:OE2	1:D:134:ARG:NH1	2.33	0.62
1:D:171:GLY:O	1:D:172:THR:HG23	2.00	0.62
1:A:93:ILE:HG22	1:A:109:VAL:HG22	1.82	0.62
1:C:193:LYS:HD2	1:C:198:GLU:HG2	1.82	0.61
1:B:177:THR:HG23	1:B:180:GLN:OE1	2.00	0.61
1:D:177:THR:OG1	1:D:180:GLN:HG3	2.00	0.61
1:C:177:THR:HG23	1:C:180:GLN:OE1	2.00	0.61
1:B:71:ASN:ND2	1:B:79:SER:OG	2.33	0.60
1:B:187:GLU:O	1:B:191:ILE:HG13	2.00	0.60
1:C:162:LEU:HB2	1:C:206:ILE:HG23	1.84	0.60
2:D:9251:PGA:O3P	3:D:645:HOH:O	2.16	0.60
1:C:9:ALA:HB1	1:C:235:SER:HB2	1.84	0.60
1:C:188:ILE:O	1:C:192:VAL:HG23	2.01	0.60
1:A:73:SER:HA	1:B:12:LYS:HD3	1.84	0.60
1:B:188:ILE:O	1:B:192:VAL:HG23	2.02	0.60
1:B:186:LYS:NZ	1:B:186:LYS:HB3	2.17	0.59
1:D:200:GLN:OE1	1:D:200:GLN:N	2.35	0.59
1:C:147:VAL:O	1:C:151:VAL:HB	2.02	0.59
1:A:171:GLY:O	1:A:173:GLY:N	2.31	0.59
1:C:12:LYS:HD3	1:D:73:SER:HA	1.84	0.59
1:A:187:GLU:O	1:A:191:ILE:HG13	2.02	0.58
1:A:238:GLU:O	1:A:241:VAL:HG22	2.02	0.58
1:D:167:LEU:HA	1:D:170:ILE:HG12	1.82	0.58
1:B:171:GLY:O	1:B:172:THR:HG23	2.03	0.58
1:D:189:ARG:NH1	1:D:206:ILE:HD12	2.18	0.58
1:A:6:PHE:CD2	1:A:207:LEU:HD11	2.38	0.58
1:A:97:GLU:OE1	1:B:73:SER:HB3	2.03	0.58
1:A:179:GLU:CD	1:A:179:GLU:H	2.07	0.58
1:D:164:TYR:CZ	1:D:184:VAL:HG11	2.39	0.58
1:A:44:VAL:CG1	1:B:78:VAL:HG22	2.34	0.58
1:B:105:THR:O	1:B:109:VAL:HG23	2.04	0.58
1:D:188:ILE:HG22	1:D:206:ILE:HD13	1.85	0.58
1:B:207:LEU:HD22	1:B:229:PHE:N	2.19	0.57
1:B:66:VAL:HG11	1:B:91:VAL:HG11	1.86	0.57
1:C:164:TYR:CZ	1:C:184:VAL:HG11	2.40	0.57
1:C:94:GLY:O	1:C:99:ARG:NE	2.36	0.57
1:A:164:TYR:O	1:A:208:TYR:O	2.21	0.57
1:D:20:ILE:O	1:D:24:THR:HG23	2.05	0.57
1:A:96:PHE:HA	1:A:99:ARG:HD2	1.87	0.56
1:A:5:TYR:O	1:A:37:LEU:HD12	2.04	0.56
1:C:171:GLY:O	1:C:173:GLY:N	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:SER:OG	1:A:81:GLU:HG2	2.06	0.56
1:C:130:SER:OG	1:C:133:GLN:HG3	2.06	0.56
1:A:67:SER:HB2	1:A:77:GLU:HB3	1.88	0.56
1:B:164:TYR:CE1	1:B:184:VAL:HG11	2.40	0.56
1:C:51:THR:HG22	1:C:55:LEU:HD22	1.87	0.56
1:B:185:HIS:HD2	1:B:225:ASP:O	1.89	0.56
1:B:41:VAL:HG11	1:B:55:LEU:HD13	1.87	0.56
1:B:213:ASN:HA	1:B:243:ILE:HD11	1.88	0.56
1:C:84:LYS:CE	1:C:119:ASN:O	2.54	0.56
1:A:71:ASN:HD21	1:A:82:ILE:HG13	1.71	0.55
1:C:169:ALA:HA	1:C:172:THR:OG1	2.06	0.55
1:A:8:ALA:HB1	1:A:42:PHE:HE1	1.72	0.55
1:A:208:TYR:CD2	1:A:220:LEU:HD13	2.40	0.55
1:C:154:ILE:HG12	1:C:160:VAL:HG21	1.89	0.55
1:D:187:GLU:O	1:D:191:ILE:HG13	2.07	0.55
1:A:68:LYS:HE2	1:A:69:PHE:CZ	2.42	0.55
1:B:160:VAL:C	1:B:161:ILE:HD12	2.27	0.55
1:B:169:ALA:O	1:B:171:GLY:N	2.40	0.55
1:B:221:ILE:HD13	1:B:228:GLY:HA2	1.87	0.55
1:C:164:TYR:CE1	1:C:184:VAL:HG11	2.41	0.55
1:A:160:VAL:C	1:A:161:ILE:HD12	2.26	0.55
1:C:38:ASP:OD2	1:C:205:ARG:NH2	2.39	0.55
1:B:156:ASN:HD22	1:B:159:ASN:CG	2.10	0.55
1:B:156:ASN:HD22	1:B:159:ASN:ND2	2.05	0.55
1:A:144:THR:HA	1:A:191:ILE:HD13	1.89	0.55
1:C:15:GLY:O	1:C:47:HIS:HE1	1.89	0.54
1:D:105:THR:O	1:D:109:VAL:HG23	2.07	0.54
1:D:172:THR:C	1:D:174:LYS:H	2.10	0.54
1:B:41:VAL:HG11	1:B:55:LEU:HD11	1.90	0.54
1:D:11:TRP:CZ2	1:D:23:LEU:HD23	2.42	0.54
1:A:223:GLN:HB2	1:A:226:ILE:HD12	1.89	0.54
1:D:185:HIS:CD2	1:D:206:ILE:HG22	2.42	0.54
1:B:178:PRO:O	1:B:223:GLN:HG3	2.08	0.54
1:C:245:LYS:CG	1:C:248:MET:HE3	2.38	0.54
1:B:196:CYS:O	1:B:200:GLN:NE2	2.41	0.54
1:C:113:LEU:HD13	1:C:117:LEU:HD13	1.89	0.54
1:B:134:ARG:HD2	1:B:168:TRP:CG	2.43	0.53
1:D:40:VAL:HG22	1:D:60:SER:CB	2.37	0.53
1:B:126:CYS:HB3	1:B:165:GLU:OE1	2.08	0.53
1:D:130:SER:OG	1:D:133:GLN:HG3	2.09	0.53
1:D:24:THR:O	1:D:27:PHE:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLY:CA	3:B:641:HOH:O	2.56	0.53
1:B:172:THR:C	1:B:174:LYS:H	2.12	0.53
1:C:107:GLU:N	1:C:107:GLU:OE1	2.42	0.52
1:A:24:THR:HB	1:A:55:LEU:HD13	1.91	0.52
1:D:33:ASP:OD1	1:D:36:LYS:HG3	2.10	0.52
1:D:189:ARG:HD2	1:D:225:ASP:OD1	2.09	0.52
1:D:213:ASN:HA	1:D:243:ILE:HD11	1.91	0.52
1:A:207:LEU:HB3	1:A:229:PHE:CA	2.35	0.52
1:A:44:VAL:HG12	1:B:78:VAL:HG22	1.91	0.52
1:D:157:PHE:CD1	1:D:200:GLN:HB3	2.45	0.52
1:C:78:VAL:HG22	1:D:44:VAL:CG1	2.39	0.52
1:A:106:ASP:OD2	1:A:145:LYS:HE2	2.10	0.51
1:B:207:LEU:HB3	1:B:229:PHE:HA	1.91	0.51
1:B:215:GLU:N	1:B:215:GLU:CD	2.63	0.51
1:C:71:ASN:ND2	1:C:79:SER:OG	2.43	0.51
1:D:3:ARG:CZ	1:D:189:ARG:NH2	2.73	0.51
1:B:5:TYR:CD1	1:B:221:ILE:HD11	2.46	0.51
1:C:161:ILE:HD12	1:C:161:ILE:N	2.26	0.51
1:A:30:LEU:HD21	1:A:248:MET:CE	2.41	0.51
1:C:200:GLN:HA	1:C:203:GLN:HG2	1.91	0.51
1:D:10:ASN:HB2	1:D:230:LEU:HD11	1.93	0.51
1:B:189:ARG:HG3	1:B:201:ALA:HB1	1.93	0.51
1:D:127:PHE:HB2	1:D:146:GLN:OE1	2.11	0.51
1:D:235:SER:HA	1:D:240:PHE:CD1	2.45	0.51
1:C:150:PHE:O	1:C:153:LEU:HB2	2.11	0.51
1:D:6:PHE:O	1:D:228:GLY:HA3	2.11	0.51
1:D:71:ASN:HD21	1:D:82:ILE:HG13	1.75	0.51
1:C:131:LEU:O	1:C:135:GLU:HG2	2.11	0.50
1:A:129:GLU:O	1:A:167:LEU:HB2	2.11	0.50
1:B:223:GLN:HB2	1:B:226:ILE:HD12	1.93	0.50
1:B:177:THR:OG1	1:B:179:GLU:HG2	2.12	0.50
1:D:162:LEU:HG	1:D:204:ILE:HD11	1.93	0.50
1:D:170:ILE:O	1:D:170:ILE:HG22	2.11	0.50
1:B:8:ALA:HA	1:B:40:VAL:O	2.11	0.50
1:D:93:ILE:HG22	1:D:109:VAL:HG13	1.92	0.50
1:B:184:VAL:O	1:B:188:ILE:HG13	2.12	0.50
1:A:24:THR:HG22	1:A:55:LEU:HD13	1.94	0.49
1:A:66:VAL:O	1:A:112:LYS:HD3	2.12	0.49
1:C:10:ASN:HB2	1:C:230:LEU:HD11	1.94	0.49
1:D:23:LEU:HG	1:D:27:PHE:CE1	2.47	0.49
1:D:143:ILE:HG22	1:D:191:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:TYR:CE1	1:D:184:VAL:HG11	2.47	0.49
1:B:130:SER:OG	1:B:133:GLN:HG3	2.12	0.49
1:C:80:ALA:HB1	1:C:121:LEU:HD11	1.94	0.49
1:C:193:LYS:CD	1:C:198:GLU:HG2	2.43	0.49
1:A:110:ARG:HG3	1:A:111:GLU:N	2.26	0.49
1:A:11:TRP:CD1	1:A:236:LEU:HD13	2.48	0.49
1:D:144:THR:HA	1:D:191:ILE:HD13	1.95	0.49
1:C:134:ARG:HA	1:C:139:THR:HG22	1.93	0.49
1:B:170:ILE:O	1:B:170:ILE:HG22	2.12	0.49
1:C:245:LYS:HA	1:C:248:MET:CG	2.40	0.49
1:D:67:SER:HB2	1:D:77:GLU:HB3	1.95	0.49
1:A:134:ARG:HD2	1:A:168:TRP:CD2	2.48	0.48
1:A:182:GLN:NE2	1:A:225:ASP:HB2	2.24	0.48
1:B:53:LYS:HD2	1:B:54:LEU:HD13	1.95	0.48
1:C:24:THR:HB	1:C:55:LEU:HD13	1.94	0.48
1:D:66:VAL:HG23	1:D:112:LYS:HB3	1.95	0.48
1:B:44:VAL:O	1:B:45:SER:C	2.51	0.48
1:C:245:LYS:HG3	1:C:248:MET:HE3	1.94	0.48
1:D:119:ASN:O	1:D:120:ASN:HB2	2.13	0.48
1:B:3:ARG:N	3:B:591:HOH:O	2.46	0.48
1:C:129:GLU:O	1:C:167:LEU:HB2	2.13	0.48
1:C:139:THR:O	1:C:143:ILE:HG12	2.13	0.48
1:D:185:HIS:CD2	1:D:226:ILE:HG12	2.49	0.48
1:C:56:GLN:O	1:C:58:LYS:N	2.47	0.48
1:A:63:ILE:HD12	1:A:65:ASN:O	2.13	0.48
1:B:124:VAL:HG12	1:B:124:VAL:O	2.13	0.48
1:B:113:LEU:HD22	1:B:150:PHE:CD1	2.49	0.48
1:C:132:GLU:O	1:C:136:GLN:HG2	2.14	0.48
1:B:44:VAL:O	1:B:47:HIS:N	2.35	0.48
1:B:154:ILE:HG23	1:B:160:VAL:HG21	1.96	0.48
1:C:40:VAL:HG22	1:C:60:SER:HB2	1.96	0.48
1:C:164:TYR:O	1:C:208:TYR:O	2.31	0.48
1:A:9:ALA:CB	1:A:235:SER:HB2	2.43	0.47
1:B:193:LYS:HG3	1:B:198:GLU:HA	1.95	0.47
1:C:40:VAL:HA	1:C:60:SER:O	2.15	0.47
1:B:105:THR:H	1:B:108:ASP:HB2	1.79	0.47
1:C:3:ARG:HD2	1:C:227:ASP:CG	2.35	0.47
1:C:131:LEU:HD22	1:C:172:THR:CG2	2.42	0.47
1:D:138:LYS:O	1:D:142:VAL:HG23	2.15	0.47
1:A:5:TYR:CE2	1:A:227:ASP:HA	2.50	0.47
1:A:129:GLU:OE2	1:A:134:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:N	1:A:161:ILE:CD1	2.75	0.47
1:C:129:GLU:OE2	1:C:139:THR:HB	2.14	0.47
1:C:80:ALA:HB1	1:C:121:LEU:CD1	2.44	0.47
1:C:155:ASP:CG	1:C:156:ASN:H	2.18	0.47
1:A:24:THR:CG2	1:A:55:LEU:HD13	2.45	0.47
1:B:127:PHE:CE1	1:B:143:ILE:HG23	2.50	0.47
1:A:139:THR:O	1:A:143:ILE:HG12	2.16	0.46
1:A:192:VAL:CG1	1:A:201:ALA:HA	2.44	0.46
1:B:208:TYR:CZ	1:B:210:GLY:HA3	2.50	0.46
1:B:239:SER:O	1:B:242:ASP:HB2	2.15	0.46
1:A:122:LYS:HG2	1:A:159:ASN:HB3	1.97	0.46
1:C:4:LYS:HE2	1:C:38:ASP:OD2	2.15	0.46
1:B:26:SER:OG	1:B:238:GLU:HB3	2.16	0.46
1:B:195:THR:O	1:B:196:CYS:SG	2.69	0.46
1:C:64:GLN:HB3	1:D:75:THR:CG2	2.44	0.46
1:A:24:THR:CB	1:A:55:LEU:HD13	2.45	0.46
1:B:16:THR:OG1	1:B:18:GLU:CD	2.54	0.46
1:B:177:THR:OG1	1:B:180:GLN:HG3	2.16	0.46
1:B:231:VAL:CG1	1:B:234:ALA:HB3	2.45	0.46
1:B:129:GLU:OE2	1:B:134:ARG:NH1	2.48	0.46
1:A:46:VAL:HB	1:B:86:LEU:CD2	2.46	0.46
1:D:134:ARG:HG3	1:D:134:ARG:HH11	1.80	0.46
1:A:30:LEU:HD21	1:A:248:MET:HE3	1.97	0.46
1:D:114:GLN:HG3	1:D:153:LEU:HD21	1.98	0.46
1:B:185:HIS:CD2	1:B:226:ILE:HA	2.51	0.46
1:D:3:ARG:NE	1:D:189:ARG:NH2	2.63	0.46
1:D:189:ARG:HH11	1:D:189:ARG:CB	2.21	0.46
1:A:73:SER:HB3	1:B:97:GLU:OE2	2.16	0.45
1:D:41:VAL:HG11	1:D:55:LEU:HD11	1.98	0.45
1:D:150:PHE:O	1:D:153:LEU:HB2	2.15	0.45
1:B:93:ILE:HG22	1:B:109:VAL:HG13	1.99	0.45
1:C:162:LEU:HG	1:C:204:ILE:HD11	1.98	0.45
1:C:32:PHE:CD1	1:C:32:PHE:C	2.90	0.45
1:C:157:PHE:HB3	1:C:203:GLN:HG3	1.99	0.45
1:A:156:ASN:OD1	1:A:158:ASP:HB2	2.16	0.45
1:B:18:GLU:HG2	1:B:19:SER:N	2.32	0.45
1:B:167:LEU:HA	1:B:170:ILE:CG1	2.45	0.45
1:B:90:TYR:HA	1:B:122:LYS:O	2.17	0.45
1:D:193:LYS:HA	1:D:201:ALA:HB2	1.98	0.45
1:A:75:THR:O	1:B:98:ARG:NH1	2.46	0.45
1:B:167:LEU:C	1:B:169:ALA:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ASN:ND2	1:D:79:SER:OG	2.49	0.45
1:C:9:ALA:CB	1:C:235:SER:HB2	2.47	0.45
1:A:178:PRO:HG2	1:A:219:SER:HB3	1.98	0.45
1:C:151:VAL:HG13	1:C:152:ASP:N	2.32	0.45
1:A:46:VAL:HB	1:B:86:LEU:HD21	1.99	0.45
1:A:244:ILE:HG22	1:A:248:MET:HE2	1.99	0.45
1:D:6:PHE:HB3	1:D:207:LEU:HD21	1.98	0.45
1:B:200:GLN:N	1:B:200:GLN:OE1	2.50	0.44
1:D:199:LYS:HB3	1:D:200:GLN:OE1	2.16	0.44
1:B:119:ASN:O	1:B:120:ASN:HB2	2.18	0.44
1:B:177:THR:HG1	1:B:179:GLU:HG2	1.81	0.44
1:C:208:TYR:CZ	1:C:210:GLY:HA3	2.52	0.44
1:C:96:PHE:HA	1:C:99:ARG:HD2	1.99	0.44
1:C:200:GLN:O	1:C:203:GLN:N	2.50	0.44
1:A:109:VAL:HG12	1:A:110:ARG:N	2.32	0.44
1:B:95:HIS:ND1	1:B:97:GLU:HB2	2.32	0.44
1:D:207:LEU:HB3	1:D:229:PHE:HA	1.98	0.44
1:A:114:GLN:HB2	1:A:153:LEU:HD13	1.99	0.44
1:A:152:ASP:OD2	1:A:153:LEU:N	2.51	0.44
1:C:43:PRO:HD2	1:C:62:GLY:O	2.17	0.44
1:C:199:LYS:H	1:C:199:LYS:HG3	1.62	0.44
1:D:193:LYS:HG3	1:D:198:GLU:HA	2.00	0.44
1:B:48:TYR:CZ	1:B:88:ILE:HG12	2.52	0.44
1:B:215:GLU:CD	1:B:215:GLU:H	2.21	0.44
1:C:105:THR:O	1:C:108:ASP:N	2.51	0.44
1:C:127:PHE:CZ	1:C:188:ILE:HD13	2.53	0.44
1:C:238:GLU:C	1:C:240:PHE:H	2.21	0.44
1:A:220:LEU:HB3	1:A:226:ILE:HD13	2.00	0.44
1:B:27:PHE:HB3	1:B:59:PHE:CZ	2.53	0.44
1:B:157:PHE:HD2	1:B:204:ILE:HB	1.82	0.44
1:B:162:LEU:HG	1:B:204:ILE:HD11	1.98	0.44
1:B:147:VAL:C	1:B:149:ALA:H	2.21	0.43
1:B:188:ILE:O	1:B:191:ILE:HB	2.18	0.43
1:C:236:LEU:N	1:C:236:LEU:HD22	2.33	0.43
1:D:104:GLU:OE1	1:D:112:LYS:NZ	2.50	0.43
1:A:94:GLY:HA2	1:A:104:GLU:OE1	2.18	0.43
1:A:174:LYS:C	1:A:175:THR:HG1	2.22	0.43
1:A:193:LYS:HD2	1:A:198:GLU:HG2	2.00	0.43
1:B:138:LYS:O	1:B:142:VAL:HG23	2.18	0.43
1:D:66:VAL:HG11	1:D:91:VAL:HG11	2.00	0.43
1:A:6:PHE:HD2	1:A:207:LEU:HD11	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASN:N	1:A:159:ASN:ND2	2.65	0.43
1:D:188:ILE:CG2	1:D:206:ILE:HD13	2.47	0.43
1:D:196:CYS:O	1:D:200:GLN:NE2	2.52	0.43
1:A:28:ASN:OD1	1:A:56:GLN:HG3	2.18	0.43
1:A:144:THR:O	1:A:148:LYS:HG3	2.19	0.43
1:A:212:VAL:HB	1:A:231:VAL:HG13	2.01	0.43
1:C:189:ARG:O	1:C:192:VAL:HB	2.18	0.43
1:D:134:ARG:HD2	1:D:168:TRP:CD2	2.53	0.43
1:B:90:TYR:CE2	1:B:122:LYS:HD3	2.54	0.43
1:B:163:VAL:HG22	1:B:207:LEU:HB2	2.01	0.43
1:C:63:ILE:HG23	1:C:88:ILE:HG21	2.01	0.43
1:A:63:ILE:HG23	1:A:88:ILE:HG21	2.00	0.43
1:A:71:ASN:HD22	1:A:71:ASN:HA	1.67	0.43
1:A:144:THR:HG23	1:A:148:LYS:HE3	2.01	0.43
1:A:173:GLY:HA2	3:A:649:HOH:O	2.18	0.43
1:B:35:SER:HB2	1:C:118:LYS:CG	2.48	0.43
1:D:208:TYR:CZ	1:D:210:GLY:HA3	2.54	0.43
1:C:139:THR:OG1	1:C:140:ILE:N	2.50	0.43
1:C:171:GLY:C	1:C:173:GLY:H	2.21	0.43
1:A:5:TYR:HD2	1:A:227:ASP:O	2.02	0.43
1:A:6:PHE:HB3	1:A:207:LEU:HD21	2.01	0.43
1:A:182:GLN:HE22	1:A:225:ASP:CB	2.31	0.43
1:C:41:VAL:O	1:C:43:PRO:HD3	2.19	0.43
1:A:76:GLY:HA3	1:B:98:ARG:HH11	1.83	0.42
1:A:24:THR:O	1:A:27:PHE:HB2	2.19	0.42
1:B:6:PHE:CD2	1:B:207:LEU:HD11	2.54	0.42
1:D:42:PHE:N	1:D:42:PHE:CD1	2.87	0.42
1:D:63:ILE:CG1	1:D:91:VAL:HG12	2.49	0.42
1:B:11:TRP:CZ2	1:B:23:LEU:HD23	2.54	0.42
1:A:151:VAL:HG13	1:A:152:ASP:N	2.35	0.42
1:A:240:PHE:O	1:A:243:ILE:HB	2.19	0.42
1:B:164:TYR:CZ	1:B:184:VAL:HG11	2.53	0.42
1:B:173:GLY:N	3:B:641:HOH:O	2.52	0.42
1:D:171:GLY:HA2	3:D:646:HOH:O	2.19	0.42
1:A:208:TYR:HB3	1:A:229:PHE:HB3	2.01	0.42
1:C:144:THR:HA	1:C:191:ILE:HD13	2.01	0.42
1:C:179:GLU:O	1:C:182:GLN:HB3	2.19	0.42
1:D:156:ASN:ND2	1:D:158:ASP:N	2.64	0.42
1:D:210:GLY:O	1:D:212:VAL:HG23	2.20	0.42
1:A:15:GLY:O	1:A:47:HIS:HE1	2.02	0.42
1:B:165:GLU:HG2	3:B:642:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ILE:O	1:D:91:VAL:HA	2.20	0.42
1:A:116:SER:HB3	1:A:121:LEU:HB2	2.01	0.42
1:A:162:LEU:O	1:A:206:ILE:HA	2.20	0.42
1:B:4:LYS:HB3	1:B:4:LYS:HE2	1.85	0.42
1:C:9:ALA:HB1	1:C:235:SER:CB	2.49	0.42
1:D:151:VAL:O	1:D:154:ILE:HG13	2.19	0.42
1:D:114:GLN:HE21	1:D:153:LEU:CD2	2.20	0.42
1:A:25:ASN:HA	1:A:28:ASN:ND2	2.31	0.41
1:B:186:LYS:HB3	1:B:186:LYS:HZ3	1.83	0.41
1:C:167:LEU:C	1:C:169:ALA:H	2.22	0.41
1:C:212:VAL:HG22	1:C:220:LEU:HD13	2.02	0.41
1:D:156:ASN:HD21	1:D:158:ASP:HB2	1.85	0.41
1:D:157:PHE:CG	1:D:200:GLN:HB3	2.55	0.41
1:A:60:SER:HA	1:A:89:GLU:OE1	2.20	0.41
1:A:86:LEU:O	1:A:87:ASN:HB2	2.18	0.41
1:A:169:ALA:O	1:A:170:ILE:C	2.58	0.41
1:B:129:GLU:CD	1:B:139:THR:HG23	2.41	0.41
1:C:6:PHE:HB3	1:C:207:LEU:CD2	2.38	0.41
1:B:16:THR:H	1:B:19:SER:HG	1.68	0.41
1:B:54:LEU:HD12	1:B:54:LEU:HA	1.88	0.41
1:A:134:ARG:CD	1:A:168:TRP:CD2	3.03	0.41
1:C:82:ILE:HG12	3:D:527:HOH:O	2.19	0.41
1:D:167:LEU:O	1:D:168:TRP:C	2.59	0.41
1:B:147:VAL:O	1:B:149:ALA:N	2.53	0.41
1:B:165:GLU:HA	1:B:166:PRO:HD2	1.94	0.41
1:C:82:ILE:HG23	1:D:47:HIS:NE2	2.36	0.41
1:C:221:ILE:HD13	1:C:228:GLY:HA2	2.03	0.41
1:D:147:VAL:O	1:D:151:VAL:HB	2.21	0.41
1:A:84:LYS:HE3	1:A:120:ASN:HB2	2.03	0.41
1:B:68:LYS:HE3	1:B:69:PHE:CZ	2.56	0.41
1:C:116:SER:HB3	1:C:121:LEU:HB2	2.02	0.41
1:C:116:SER:HA	1:C:121:LEU:HD12	2.02	0.41
1:C:218:SER:O	1:C:222:GLN:HB2	2.20	0.41
1:D:71:ASN:HD22	1:D:71:ASN:HA	1.63	0.41
1:D:169:ALA:O	1:D:171:GLY:N	2.54	0.41
1:A:84:LYS:CE	1:A:119:ASN:O	2.64	0.41
1:A:184:VAL:HG12	1:A:188:ILE:HD11	2.03	0.41
1:C:119:ASN:O	1:C:120:ASN:HB2	2.20	0.41
1:C:140:ILE:HG12	1:C:187:GLU:HG2	2.03	0.41
1:C:208:TYR:HB3	1:C:229:PHE:HB3	2.02	0.41
1:C:245:LYS:HG2	1:C:248:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:VAL:CG2	1:D:112:LYS:HB3	2.51	0.41
1:A:7:VAL:O	1:A:39:VAL:HA	2.21	0.40
1:B:129:GLU:OE2	1:B:139:THR:HG23	2.21	0.40
1:C:118:LYS:HE2	1:C:118:LYS:HB2	1.96	0.40
1:A:41:VAL:HG21	1:A:55:LEU:HD21	2.04	0.40
1:A:135:GLU:O	1:A:135:GLU:HG2	2.21	0.40
1:B:173:GLY:HA3	3:B:641:HOH:O	2.21	0.40
1:C:32:PHE:CE1	1:C:58:LYS:HB2	2.55	0.40
1:C:45:SER:OG	1:C:46:VAL:N	2.54	0.40
1:C:71:ASN:HD22	1:C:71:ASN:HA	1.66	0.40
1:C:179:GLU:CD	1:C:179:GLU:H	2.24	0.40
1:D:185:HIS:CG	1:D:226:ILE:HG12	2.56	0.40
1:A:193:LYS:HA	1:A:201:ALA:HB2	2.03	0.40
1:A:239:SER:O	1:A:240:PHE:C	2.59	0.40
1:C:151:VAL:C	1:C:153:LEU:H	2.24	0.40
1:B:34:PRO:HA	1:B:37:LEU:O	2.20	0.40
1:B:50:HIS:HD2	1:B:53:LYS:HE3	1.87	0.40
1:C:71:ASN:ND2	1:C:79:SER:CB	2.85	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)
3:A:649:HOH:O	3:B:509:HOH:O[1_455]	1.60	0.60

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	244/248 (98%)	209 (86%)	31 (13%)	4 (2%)	<b>9</b>   <b>31</b>
1	B	244/248 (98%)	210 (86%)	26 (11%)	8 (3%)	<b>4</b>   <b>13</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	244/248 (98%)	208 (85%)	31 (13%)	5 (2%)	7	24
1	D	244/248 (98%)	219 (90%)	22 (9%)	3 (1%)	13	39
All	All	976/992 (98%)	846 (87%)	110 (11%)	20 (2%)	7	24

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	THR
1	B	170	ILE
1	C	103	HIS
1	C	172	THR
1	C	208	TYR
1	D	170	ILE
1	A	137	ASN
1	A	170	ILE
1	C	57	SER
1	A	157	PHE
1	B	139	THR
1	B	148	LYS
1	B	157	PHE
1	B	172	THR
1	B	198	GLU
1	C	168	TRP
1	D	172	THR
1	B	168	TRP
1	B	196	CYS
1	D	214	THR

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	219/220 (100%)	206 (94%)	13 (6%)	19	49
1	B	219/220 (100%)	204 (93%)	15 (7%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	219/220 (100%)	210 (96%)	9 (4%)	30	64
1	D	219/220 (100%)	209 (95%)	10 (5%)	27	60
All	All	876/880 (100%)	829 (95%)	47 (5%)	22	53

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	55	LEU
1	A	68	LYS
1	A	79	SER
1	A	81	GLU
1	A	96	PHE
1	A	110	ARG
1	A	135	GLU
1	A	139	THR
1	A	175	THR
1	A	183	LEU
1	A	229	PHE
1	A	231	VAL
1	B	41	VAL
1	B	49	ASP
1	B	53	LYS
1	B	54	LEU
1	B	65	ASN
1	B	96	PHE
1	B	107	GLU
1	B	155	ASP
1	B	179	GLU
1	B	198	GLU
1	B	200	GLN
1	B	205	ARG
1	B	214	THR
1	B	224	GLU
1	B	229	PHE
1	C	29	ASN
1	C	49	ASP
1	C	55	LEU
1	C	81	GLU
1	C	110	ARG
1	C	139	THR

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Mol	Chain	Res	Type
1	C	175	THR
1	C	194	ASP
1	C	229	PHE
1	D	31	ASP
1	D	42	PHE
1	D	54	LEU
1	D	107	GLU
1	D	156	ASN
1	D	178	PRO
1	D	179	GLU
1	D	189	ARG
1	D	215	GLU
1	D	229	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	71	ASN
1	A	159	ASN
1	A	185	HIS
1	A	202	ASN
1	B	29	ASN
1	B	50	HIS
1	B	56	GLN
1	B	65	ASN
1	B	71	ASN
1	B	87	ASN
1	B	120	ASN
1	B	156	ASN
1	B	185	HIS
1	B	203	GLN
1	B	222	GLN
1	C	14	ASN
1	C	47	HIS
1	C	71	ASN
1	C	120	ASN
1	C	159	ASN
1	C	202	ASN
1	D	29	ASN
1	D	50	HIS
1	D	56	GLN

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Mol	Chain	Res	Type
1	D	65	ASN
1	D	71	ASN
1	D	114	GLN
1	D	120	ASN
1	D	156	ASN
1	D	159	ASN
1	D	202	ASN
1	D	222	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

2 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	7251	-	8,8,8	2.15	2 (25%)	10,11,11	3.40	3 (30%)
2	PGA	D	9251	-	8,8,8	2.18	2 (25%)	10,11,11	3.36	3 (30%)

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	7251	-	-	2/6/6/6	-
2	PGA	D	9251	-	-	2/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9251	PGA	O1-C1	4.82	1.38	1.22
2	B	7251	PGA	O1-C1	4.79	1.38	1.22
2	B	7251	PGA	O1P-C2	2.30	1.44	1.43
2	D	9251	PGA	O1P-C2	2.24	1.44	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7251	PGA	O2-C1-O1	-6.88	106.16	123.30
2	D	9251	PGA	O2-C1-O1	-6.85	106.24	123.30
2	B	7251	PGA	O1P-C2-C1	-6.67	100.49	110.54
2	D	9251	PGA	O1P-C2-C1	-6.64	100.53	110.54
2	B	7251	PGA	O2-C1-C2	2.90	126.75	113.34
2	D	9251	PGA	O2-C1-C2	2.86	126.60	113.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	9251	PGA	O1-C1-C2-O1P
2	D	9251	PGA	O2-C1-C2-O1P
2	B	7251	PGA	O2-C1-C2-O1P
2	B	7251	PGA	O1-C1-C2-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	9251	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	246/248 (99%)	-0.36	1 (0%) 92 91	5, 10, 38, 63	0
1	B	246/248 (99%)	-0.34	2 (0%) 86 81	5, 10, 40, 61	0
1	C	246/248 (99%)	-0.26	3 (1%) 79 73	5, 10, 40, 75	0
1	D	246/248 (99%)	-0.36	2 (0%) 86 81	5, 10, 42, 67	0
All	All	984/992 (99%)	-0.33	8 (0%) 86 81	5, 10, 41, 75	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	172	THR	5.2
1	C	170	ILE	5.2
1	C	174	LYS	4.2
1	D	172	THR	3.9
1	D	174	LYS	2.8
1	A	172	THR	2.7
1	B	174	LYS	2.2
1	B	197	GLY	2.2

### 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 monosaccharides 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, 95<sup>th</sup> 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	D	9251	9/9	0.92	0.24	33,33,33,33	0
2	PGA	B	7251	9/9	0.93	0.21	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.