Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:51 PM GMT

PDB ID	:	1HG3
Title	:	CRYSTAL STRUCTURE OF TETRAMERIC TIM FROM PYROCOCCUS WOESEI.
Authors	:	Walden, H.; Bell, G.S.; Russell, R.J.M.; Siebers, B.; Hensel, R.; Taylor, G.L.
Deposited on	:	2000-12-12
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

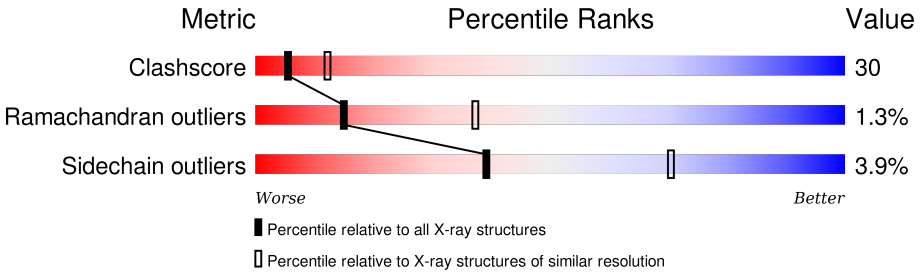
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	225	63% 33% .
1	B	225	60% 36% .
1	C	225	60% 36% .
1	D	225	62% 34% .
1	E	225	62% 34% .
1	F	225	61% 34% .
1	G	225	60% 36% .

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Mol	Chain	Length	Quality of chain
1	H	225	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3PP	A	1226	-	-	X	-
2	3PP	B	1226	-	-	X	-
2	3PP	C	1226	-	-	X	-
2	3PP	D	1226	-	-	X	-
2	3PP	E	1226	-	-	X	-
2	3PP	F	1226	-	-	X	-
2	3PP	G	1226	-	-	X	-
2	3PP	H	1226	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13650 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	224	Total	C	N	O	S	0	0	0
			1654	1055	277	316	6			
1	B	224	Total	C	N	O	S	0	0	0
			1654	1055	277	316	6			
1	C	224	Total	C	N	O	S	0	0	0
			1654	1055	277	316	6			
1	D	224	Total	C	N	O	S	0	0	0
			1654	1055	277	316	6			
1	E	224	Total	C	N	O	S	0	0	0
			1654	1055	277	316	6			
1	F	224	Total	C	N	O	S	0	0	0
			1654	1055	277	316	6			
1	G	224	Total	C	N	O	S	0	0	0
			1654	1055	277	316	6			
1	H	224	Total	C	N	O	S	0	0	0
			1654	1055	277	316	6			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	ALA	GLN	SEE REMARK 999	UNP P95583
A	212	LYS	ARG	SEE REMARK 999	UNP P95583
A	213	ASP	SER	SEE REMARK 999	UNP P95583
A	214	PRO	ARG	SEE REMARK 999	UNP P95583
A	216	LYS	GLY	SEE REMARK 999	UNP P95583
A	217	ALA	ASP	SEE REMARK 999	UNP P95583
A	218	ILE	MET	SEE REMARK 999	UNP P95583
A	219	TRP	GLY	SEE REMARK 999	UNP P95583
A	220	ASP	SER	SEE REMARK 999	UNP P95583
A	221	LEU	CYS	SEE REMARK 999	UNP P95583
A	222	VAL	PHE	SEE REMARK 999	UNP P95583
A	223	SER	GLY	SEE REMARK 999	UNP P95583
A	224	GLY	ASN	SEE REMARK 999	UNP P95583

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Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ILE	ASN	SEE REMARK 999	UNP P95583
B	211	ALA	GLN	SEE REMARK 999	UNP P95583
B	212	LYS	ARG	SEE REMARK 999	UNP P95583
B	213	ASP	SER	SEE REMARK 999	UNP P95583
B	214	PRO	ARG	SEE REMARK 999	UNP P95583
B	216	LYS	GLY	SEE REMARK 999	UNP P95583
B	217	ALA	ASP	SEE REMARK 999	UNP P95583
B	218	ILE	MET	SEE REMARK 999	UNP P95583
B	219	TRP	GLY	SEE REMARK 999	UNP P95583
B	220	ASP	SER	SEE REMARK 999	UNP P95583
B	221	LEU	CYS	SEE REMARK 999	UNP P95583
B	222	VAL	PHE	SEE REMARK 999	UNP P95583
B	223	SER	GLY	SEE REMARK 999	UNP P95583
B	224	GLY	ASN	SEE REMARK 999	UNP P95583
B	225	ILE	ASN	SEE REMARK 999	UNP P95583
C	211	ALA	GLN	SEE REMARK 999	UNP P95583
C	212	LYS	ARG	SEE REMARK 999	UNP P95583
C	213	ASP	SER	SEE REMARK 999	UNP P95583
C	214	PRO	ARG	SEE REMARK 999	UNP P95583
C	216	LYS	GLY	SEE REMARK 999	UNP P95583
C	217	ALA	ASP	SEE REMARK 999	UNP P95583
C	218	ILE	MET	SEE REMARK 999	UNP P95583
C	219	TRP	GLY	SEE REMARK 999	UNP P95583
C	220	ASP	SER	SEE REMARK 999	UNP P95583
C	221	LEU	CYS	SEE REMARK 999	UNP P95583
C	222	VAL	PHE	SEE REMARK 999	UNP P95583
C	223	SER	GLY	SEE REMARK 999	UNP P95583
C	224	GLY	ASN	SEE REMARK 999	UNP P95583
C	225	ILE	ASN	SEE REMARK 999	UNP P95583
D	211	ALA	GLN	SEE REMARK 999	UNP P95583
D	212	LYS	ARG	SEE REMARK 999	UNP P95583
D	213	ASP	SER	SEE REMARK 999	UNP P95583
D	214	PRO	ARG	SEE REMARK 999	UNP P95583
D	216	LYS	GLY	SEE REMARK 999	UNP P95583
D	217	ALA	ASP	SEE REMARK 999	UNP P95583
D	218	ILE	MET	SEE REMARK 999	UNP P95583
D	219	TRP	GLY	SEE REMARK 999	UNP P95583
D	220	ASP	SER	SEE REMARK 999	UNP P95583
D	221	LEU	CYS	SEE REMARK 999	UNP P95583
D	222	VAL	PHE	SEE REMARK 999	UNP P95583
D	223	SER	GLY	SEE REMARK 999	UNP P95583
D	224	GLY	ASN	SEE REMARK 999	UNP P95583

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Chain	Residue	Modelled	Actual	Comment	Reference
D	225	ILE	ASN	SEE REMARK 999	UNP P95583
E	211	ALA	GLN	SEE REMARK 999	UNP P95583
E	212	LYS	ARG	SEE REMARK 999	UNP P95583
E	213	ASP	SER	SEE REMARK 999	UNP P95583
E	214	PRO	ARG	SEE REMARK 999	UNP P95583
E	216	LYS	GLY	SEE REMARK 999	UNP P95583
E	217	ALA	ASP	SEE REMARK 999	UNP P95583
E	218	ILE	MET	SEE REMARK 999	UNP P95583
E	219	TRP	GLY	SEE REMARK 999	UNP P95583
E	220	ASP	SER	SEE REMARK 999	UNP P95583
E	221	LEU	CYS	SEE REMARK 999	UNP P95583
E	222	VAL	PHE	SEE REMARK 999	UNP P95583
E	223	SER	GLY	SEE REMARK 999	UNP P95583
E	224	GLY	ASN	SEE REMARK 999	UNP P95583
E	225	ILE	ASN	SEE REMARK 999	UNP P95583
F	211	ALA	GLN	SEE REMARK 999	UNP P95583
F	212	LYS	ARG	SEE REMARK 999	UNP P95583
F	213	ASP	SER	SEE REMARK 999	UNP P95583
F	214	PRO	ARG	SEE REMARK 999	UNP P95583
F	216	LYS	GLY	SEE REMARK 999	UNP P95583
F	217	ALA	ASP	SEE REMARK 999	UNP P95583
F	218	ILE	MET	SEE REMARK 999	UNP P95583
F	219	TRP	GLY	SEE REMARK 999	UNP P95583
F	220	ASP	SER	SEE REMARK 999	UNP P95583
F	221	LEU	CYS	SEE REMARK 999	UNP P95583
F	222	VAL	PHE	SEE REMARK 999	UNP P95583
F	223	SER	GLY	SEE REMARK 999	UNP P95583
F	224	GLY	ASN	SEE REMARK 999	UNP P95583
F	225	ILE	ASN	SEE REMARK 999	UNP P95583
G	211	ALA	GLN	SEE REMARK 999	UNP P95583
G	212	LYS	ARG	SEE REMARK 999	UNP P95583
G	213	ASP	SER	SEE REMARK 999	UNP P95583
G	214	PRO	ARG	SEE REMARK 999	UNP P95583
G	216	LYS	GLY	SEE REMARK 999	UNP P95583
G	217	ALA	ASP	SEE REMARK 999	UNP P95583
G	218	ILE	MET	SEE REMARK 999	UNP P95583
G	219	TRP	GLY	SEE REMARK 999	UNP P95583
G	220	ASP	SER	SEE REMARK 999	UNP P95583
G	221	LEU	CYS	SEE REMARK 999	UNP P95583
G	222	VAL	PHE	SEE REMARK 999	UNP P95583
G	223	SER	GLY	SEE REMARK 999	UNP P95583
G	224	GLY	ASN	SEE REMARK 999	UNP P95583

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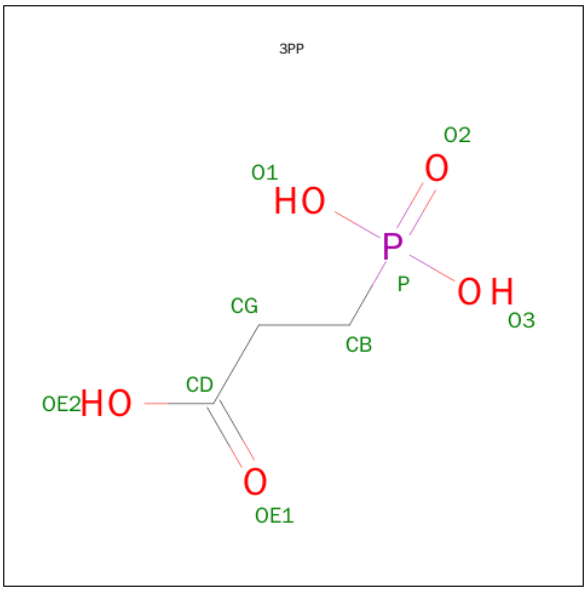
Chain	Residue	Modelled	Actual	Comment	Reference
G	225	ILE	ASN	SEE REMARK 999	UNP P95583
H	211	ALA	GLN	SEE REMARK 999	UNP P95583
H	212	LYS	ARG	SEE REMARK 999	UNP P95583
H	213	ASP	SER	SEE REMARK 999	UNP P95583
H	214	PRO	ARG	SEE REMARK 999	UNP P95583
H	216	LYS	GLY	SEE REMARK 999	UNP P95583
H	217	ALA	ASP	SEE REMARK 999	UNP P95583
H	218	ILE	MET	SEE REMARK 999	UNP P95583
H	219	TRP	GLY	SEE REMARK 999	UNP P95583
H	220	ASP	SER	SEE REMARK 999	UNP P95583
H	221	LEU	CYS	SEE REMARK 999	UNP P95583
H	222	VAL	PHE	SEE REMARK 999	UNP P95583
H	223	SER	GLY	SEE REMARK 999	UNP P95583
H	224	GLY	ASN	SEE REMARK 999	UNP P95583
H	225	ILE	ASN	SEE REMARK 999	UNP P95583

- Molecule 2 is 3-PHOSPHONOPROPANOIC ACID (three-letter code: 3PP) (formula: $C_3H_7O_5P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	3	5	1		
2	B	1	Total	C	O	P	0	0
			9	3	5	1		
2	C	1	Total	C	O	P	0	0
			9	3	5	1		
2	D	1	Total	C	O	P	0	0
			9	3	5	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O P 9 3 5 1	0	0
2	F	1	Total C O P 9 3 5 1	0	0
2	G	1	Total C O P 9 3 5 1	0	0
2	H	1	Total C O P 9 3 5 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0
3	B	36	Total O 36 36	0	0
3	C	52	Total O 52 52	0	0
3	D	46	Total O 46 46	0	0
3	E	43	Total O 43 43	0	0
3	F	41	Total O 41 41	0	0
3	G	46	Total O 46 46	0	0
3	H	44	Total O 44 44	0	0

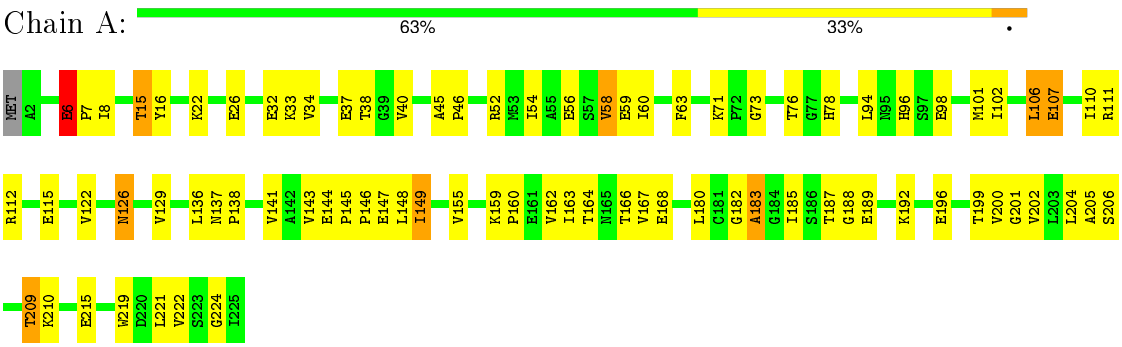
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

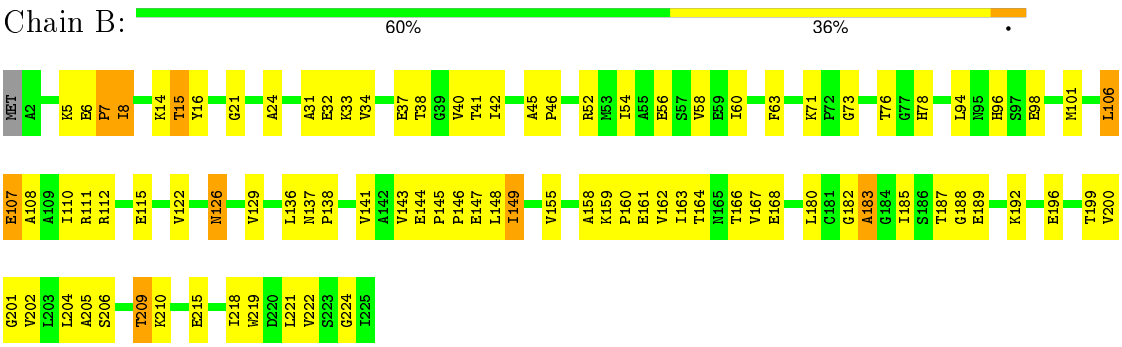
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A:



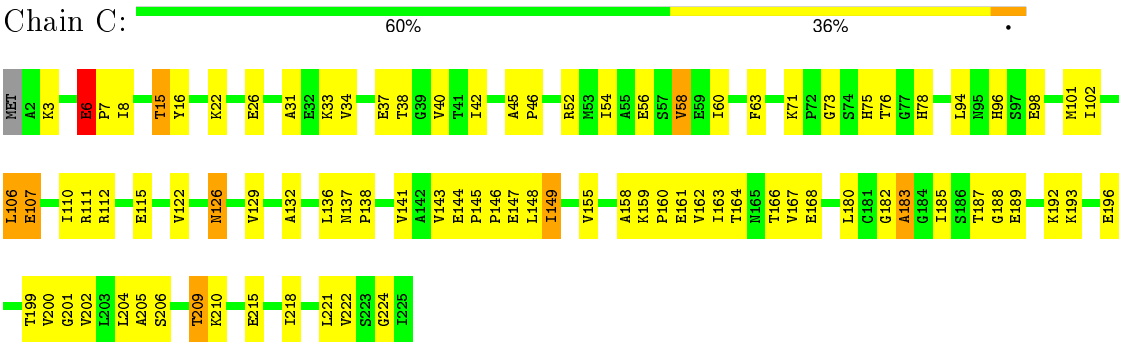
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B:



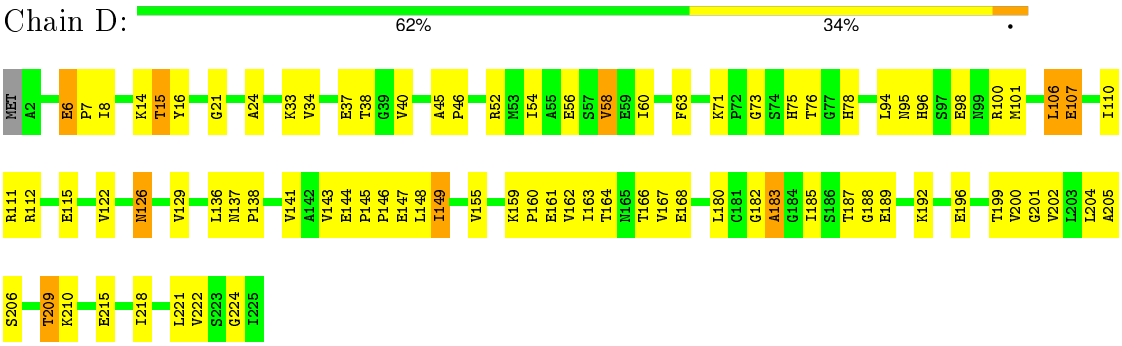
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain C:



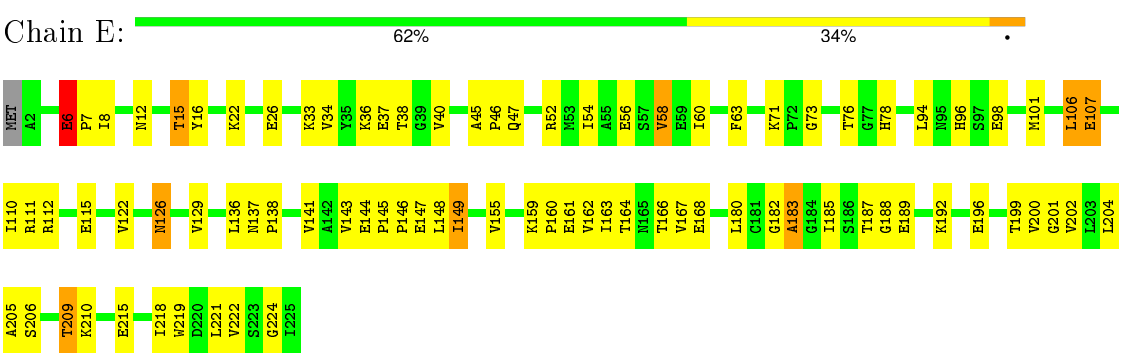
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain D:



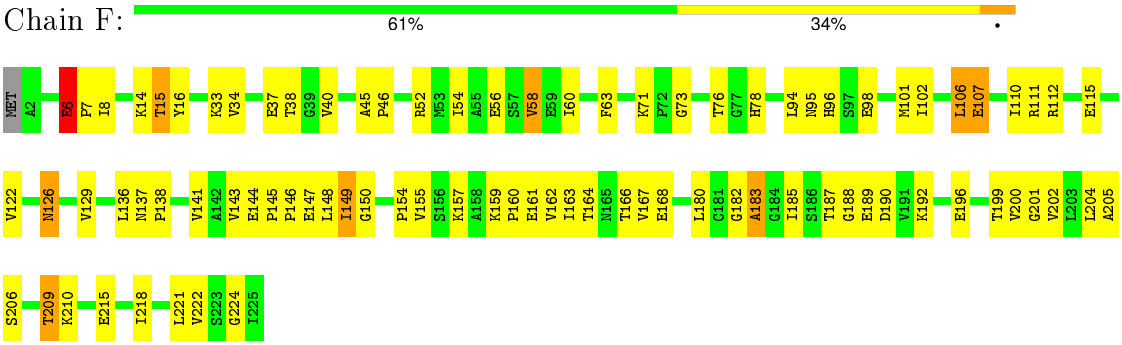
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain E:



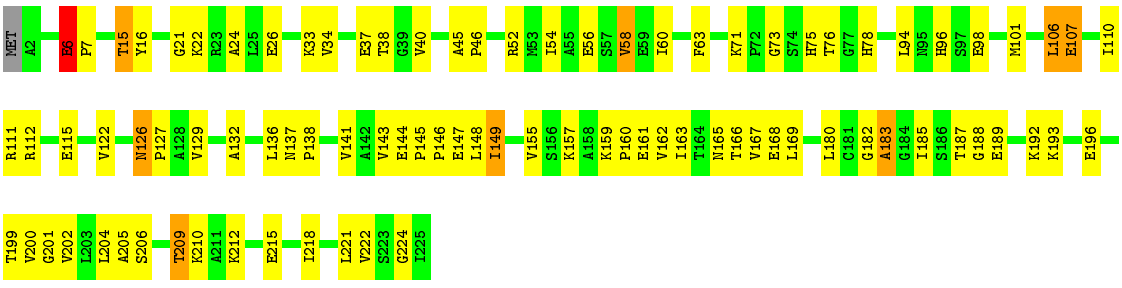
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain F:



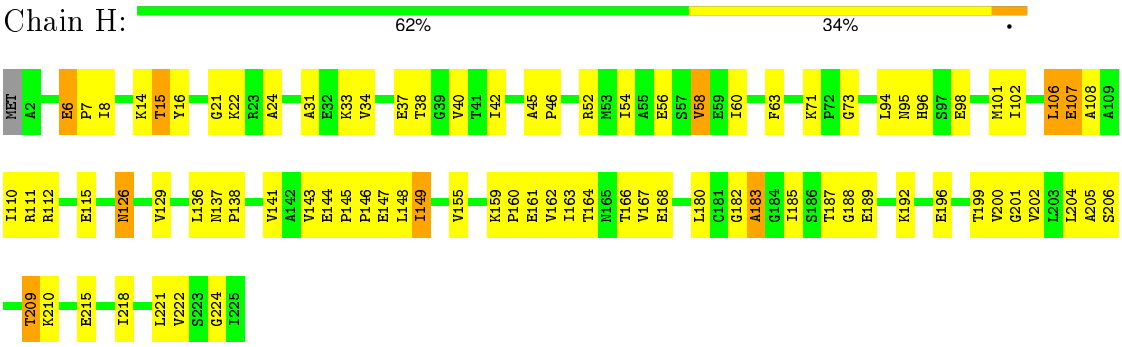
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain G:



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.00Å 89.10Å 145.10Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.1 (6.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.254 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13650	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PP

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	0.35	0/1678	0.64	1/2282 (0.0%)
1	B	0.39	1/1678 (0.1%)	0.68	1/2282 (0.0%)
1	C	0.35	0/1678	0.64	1/2282 (0.0%)
1	D	0.34	0/1678	0.64	0/2282
1	E	0.34	0/1678	0.64	1/2282 (0.0%)
1	F	0.34	0/1678	0.65	1/2282 (0.0%)
1	G	0.36	0/1678	0.66	0/2282
1	H	0.34	0/1678	0.64	0/2282
All	All	0.35	1/13424 (0.0%)	0.65	5/18256 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	PRO	N-CD	5.37	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	8	ILE	N-CA-C	6.12	127.52	111.00
1	A	6	GLU	N-CA-C	5.15	124.91	111.00
1	C	6	GLU	N-CA-C	5.12	124.83	111.00
1	E	6	GLU	N-CA-C	5.12	124.82	111.00
1	F	6	GLU	N-CA-C	5.00	124.51	111.00

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	1654	0	1744	110	1
1	B	1654	0	1744	126	0
1	C	1654	0	1744	100	1
1	D	1654	0	1744	96	0
1	E	1654	0	1744	120	1
1	F	1654	0	1744	87	2
1	G	1654	0	1744	102	3
1	H	1654	0	1744	92	0
2	A	9	0	4	8	0
2	B	9	0	4	5	0
2	C	9	0	4	6	0
2	D	9	0	4	4	0
2	E	9	0	4	7	0
2	F	9	0	4	4	0
2	G	9	0	4	6	0
2	H	9	0	4	4	0
3	A	38	0	0	0	0
3	B	36	0	0	0	0
3	C	52	0	0	4	0
3	D	46	0	0	5	0
3	E	43	0	0	2	0
3	F	41	0	0	2	0
3	G	46	0	0	5	0
3	H	44	0	0	3	0
All	All	13650	0	13984	808	4

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 30.

All (808) 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:E:34:VAL:HG22	1:E:219:TRP:CE2	1.53	1.43
1:A:34:VAL:HG22	1:A:219:TRP:CE2	1.54	1.42
1:B:34:VAL:HG22	1:B:219:TRP:CE2	1.54	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLU:HG2	1:A:219:TRP:NE1	1.44	1.32
1:B:215:GLU:HG2	1:B:219:TRP:NE1	1.44	1.31
1:E:215:GLU:HG2	1:E:219:TRP:NE1	1.45	1.31
1:E:34:VAL:HA	1:E:219:TRP:CH2	1.75	1.21
1:B:34:VAL:HA	1:B:219:TRP:CH2	1.74	1.20
1:B:215:GLU:CG	1:B:219:TRP:HE1	1.55	1.19
1:A:34:VAL:HA	1:A:219:TRP:CH2	1.77	1.19
1:A:215:GLU:CG	1:A:219:TRP:HE1	1.55	1.18
1:E:215:GLU:CG	1:E:219:TRP:HE1	1.56	1.17
1:F:187:THR:HG22	1:F:189:GLU:H	1.19	1.06
1:E:37:GLU:CG	1:E:219:TRP:HH2	1.68	1.05
1:B:37:GLU:CG	1:B:219:TRP:HH2	1.69	1.03
1:E:187:THR:HG22	1:E:189:GLU:H	1.23	1.03
1:D:187:THR:HG22	1:D:189:GLU:H	1.19	1.03
1:A:187:THR:HG22	1:A:189:GLU:H	1.23	1.03
1:B:187:THR:HG22	1:B:189:GLU:H	1.23	1.02
1:H:187:THR:HG22	1:H:189:GLU:H	1.22	1.01
1:C:187:THR:HG22	1:C:189:GLU:H	1.22	1.01
1:B:162:VAL:O	1:B:166:THR:HG23	1.60	1.01
1:G:187:THR:HG22	1:G:189:GLU:H	1.23	1.00
1:E:34:VAL:CG2	1:E:219:TRP:CE2	2.47	0.98
1:A:34:VAL:CG2	1:A:219:TRP:CE2	2.48	0.97
1:E:215:GLU:O	1:E:219:TRP:CD1	2.21	0.94
1:A:34:VAL:HG22	1:A:219:TRP:CD2	2.01	0.94
1:E:34:VAL:HG22	1:E:219:TRP:CD2	2.02	0.94
1:E:37:GLU:HG3	1:E:219:TRP:CH2	2.03	0.94
1:E:34:VAL:HG22	1:E:219:TRP:CZ2	2.03	0.93
1:B:34:VAL:CG2	1:B:219:TRP:CE2	2.49	0.93
1:B:34:VAL:HG22	1:B:219:TRP:CD2	2.03	0.92
1:F:199:THR:HG22	1:F:201:GLY:H	1.33	0.92
1:E:199:THR:HG22	1:E:201:GLY:H	1.34	0.92
1:B:199:THR:HG22	1:B:201:GLY:H	1.35	0.92
1:A:199:THR:HG22	1:A:201:GLY:H	1.34	0.92
1:B:37:GLU:HG3	1:B:219:TRP:CH2	2.05	0.92
1:A:34:VAL:HG22	1:A:219:TRP:CZ2	2.04	0.92
1:E:37:GLU:CG	1:E:219:TRP:CH2	2.53	0.91
1:B:34:VAL:HG22	1:B:219:TRP:CZ2	2.05	0.91
1:C:199:THR:HG22	1:C:201:GLY:H	1.34	0.91
1:B:37:GLU:CG	1:B:219:TRP:CH2	2.54	0.91
1:H:199:THR:HG22	1:H:201:GLY:H	1.33	0.90
1:D:199:THR:HG22	1:D:201:GLY:H	1.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:THR:HG22	1:G:201:GLY:H	1.35	0.90
1:B:215:GLU:HG2	1:B:219:TRP:HE1	0.75	0.89
1:A:215:GLU:HG2	1:A:219:TRP:HE1	0.75	0.89
1:A:215:GLU:O	1:A:219:TRP:CD1	2.27	0.88
1:E:215:GLU:HG2	1:E:219:TRP:HE1	0.75	0.88
1:B:37:GLU:HG3	1:B:219:TRP:HH2	1.38	0.87
1:E:38:THR:HG22	1:E:40:VAL:H	1.39	0.87
1:A:38:THR:HG22	1:A:40:VAL:H	1.40	0.87
1:C:96:HIS:HE1	2:C:1226:3PP:OE1	1.56	0.87
1:B:215:GLU:O	1:B:219:TRP:CD1	2.27	0.86
1:A:34:VAL:HG13	1:A:219:TRP:CE3	2.11	0.86
1:B:38:THR:HG22	1:B:40:VAL:H	1.40	0.85
1:F:38:THR:HG22	1:F:40:VAL:H	1.40	0.85
1:G:38:THR:HG22	1:G:40:VAL:H	1.40	0.85
1:C:6:GLU:O	1:C:8:ILE:HG13	1.77	0.85
1:E:34:VAL:HG13	1:E:219:TRP:CE3	2.12	0.85
1:H:38:THR:HG22	1:H:40:VAL:H	1.40	0.85
1:B:5:LYS:HB2	1:B:41:THR:OG1	1.76	0.84
1:E:6:GLU:O	1:E:8:ILE:HG13	1.78	0.84
1:E:37:GLU:HG3	1:E:219:TRP:HH2	1.36	0.84
1:C:38:THR:HG22	1:C:40:VAL:H	1.42	0.84
1:H:6:GLU:O	1:H:8:ILE:HG13	1.79	0.83
1:B:34:VAL:HG13	1:B:219:TRP:CE3	2.13	0.83
1:D:38:THR:HG22	1:D:40:VAL:H	1.43	0.83
1:B:96:HIS:HD2	1:B:98:GLU:H	1.26	0.82
1:A:6:GLU:O	1:A:8:ILE:HG13	1.79	0.82
1:H:205:ALA:N	2:H:1226:3PP:HCB1	1.95	0.82
1:G:96:HIS:HD2	1:G:98:GLU:H	1.26	0.82
1:B:37:GLU:CD	1:B:219:TRP:CH2	2.53	0.81
1:H:96:HIS:HD2	1:H:98:GLU:H	1.29	0.81
1:C:96:HIS:HD2	1:C:98:GLU:H	1.27	0.81
1:E:37:GLU:CD	1:E:219:TRP:CH2	2.54	0.81
1:F:6:GLU:O	1:F:8:ILE:HG13	1.81	0.81
1:D:6:GLU:O	1:D:8:ILE:HG13	1.81	0.81
1:G:126:ASN:ND2	1:G:129:VAL:H	1.79	0.81
1:F:143:VAL:HG21	1:F:166:THR:HG21	1.64	0.80
1:H:58:VAL:CG1	1:H:60:ILE:HG12	2.12	0.80
1:E:96:HIS:HD2	1:E:98:GLU:H	1.28	0.79
1:B:126:ASN:ND2	1:B:129:VAL:H	1.79	0.79
1:H:126:ASN:ND2	1:H:129:VAL:H	1.81	0.79
1:F:96:HIS:HD2	1:F:98:GLU:H	1.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:HIS:HD2	1:D:98:GLU:H	1.30	0.79
1:F:126:ASN:ND2	1:F:129:VAL:H	1.80	0.79
1:A:126:ASN:ND2	1:A:129:VAL:H	1.80	0.79
1:D:58:VAL:CG1	1:D:60:ILE:HG12	2.13	0.79
1:D:126:ASN:ND2	1:D:129:VAL:H	1.81	0.79
1:C:126:ASN:ND2	1:C:129:VAL:H	1.81	0.79
1:F:187:THR:HG22	1:F:189:GLU:N	1.98	0.79
1:E:58:VAL:CG1	1:E:60:ILE:HG12	2.13	0.79
1:A:96:HIS:HD2	1:A:98:GLU:H	1.30	0.79
1:D:143:VAL:HG21	1:D:166:THR:HG21	1.65	0.78
1:E:126:ASN:ND2	1:E:129:VAL:H	1.81	0.78
1:G:58:VAL:CG1	1:G:60:ILE:HG12	2.14	0.77
1:A:58:VAL:CG1	1:A:60:ILE:HG12	2.15	0.77
1:C:187:THR:HG22	1:C:189:GLU:N	1.99	0.77
1:C:58:VAL:CG1	1:C:60:ILE:HG12	2.15	0.77
1:B:187:THR:HG22	1:B:189:GLU:N	2.01	0.76
1:A:187:THR:HG22	1:A:189:GLU:N	1.99	0.76
1:B:192:LYS:O	1:B:196:GLU:HG3	1.86	0.76
1:H:146:PRO:HA	1:H:149:ILE:HG12	1.67	0.76
1:H:143:VAL:HG21	1:H:166:THR:HG21	1.67	0.76
1:E:187:THR:HG22	1:E:189:GLU:N	2.00	0.76
1:B:146:PRO:HA	1:B:149:ILE:HG12	1.66	0.76
1:D:146:PRO:HA	1:D:149:ILE:HG12	1.67	0.76
1:G:187:THR:HG22	1:G:189:GLU:N	2.00	0.76
1:C:146:PRO:HA	1:C:149:ILE:HG12	1.66	0.75
1:E:143:VAL:HG21	1:E:166:THR:HG21	1.67	0.75
1:E:215:GLU:O	1:E:219:TRP:HD1	1.67	0.75
1:F:58:VAL:CG1	1:F:60:ILE:HG12	2.16	0.75
1:F:38:THR:HG21	1:F:222:VAL:HG11	1.68	0.75
1:F:143:VAL:CG2	1:F:166:THR:HG21	2.16	0.75
1:A:146:PRO:HA	1:A:149:ILE:HG12	1.67	0.75
1:E:143:VAL:CG2	1:E:166:THR:HG21	2.17	0.75
1:D:187:THR:HG22	1:D:189:GLU:N	1.97	0.75
1:B:205:ALA:N	2:B:1226:3PP:HCB1	2.02	0.75
1:D:143:VAL:CG2	1:D:166:THR:HG21	2.16	0.75
1:A:143:VAL:CG2	1:A:166:THR:HG21	2.17	0.75
1:A:38:THR:HG21	1:A:222:VAL:HG11	1.69	0.74
1:G:38:THR:HG21	1:G:222:VAL:HG11	1.68	0.74
1:B:162:VAL:O	1:B:166:THR:CG2	2.35	0.74
1:D:38:THR:HG21	1:D:222:VAL:HG11	1.69	0.74
1:C:192:LYS:O	1:C:196:GLU:HG3	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG21	1:A:166:THR:HG21	1.68	0.74
1:F:146:PRO:HA	1:F:149:ILE:HG12	1.68	0.74
1:B:38:THR:HG21	1:B:222:VAL:HG11	1.69	0.74
1:B:209:THR:HG22	1:B:210:LYS:HG2	1.69	0.74
1:E:38:THR:HG21	1:E:222:VAL:HG11	1.70	0.74
1:C:143:VAL:HG21	1:C:166:THR:HG21	1.68	0.74
1:E:146:PRO:HA	1:E:149:ILE:HG12	1.68	0.74
1:G:146:PRO:HA	1:G:149:ILE:HG12	1.68	0.74
1:D:126:ASN:HD22	1:D:126:ASN:C	1.91	0.74
1:H:38:THR:HG21	1:H:222:VAL:HG11	1.70	0.74
1:D:209:THR:HG22	1:D:210:LYS:HG2	1.69	0.74
1:F:209:THR:HG22	1:F:210:LYS:HG2	1.70	0.74
1:H:192:LYS:O	1:H:196:GLU:HG3	1.87	0.74
1:H:209:THR:HG22	1:H:210:LYS:HG2	1.69	0.74
1:G:192:LYS:O	1:G:196:GLU:HG3	1.86	0.74
1:B:143:VAL:HG11	1:B:166:THR:HG21	1.68	0.73
1:B:126:ASN:C	1:B:126:ASN:HD22	1.91	0.73
1:C:143:VAL:CG2	1:C:166:THR:HG21	2.17	0.73
1:C:38:THR:HG21	1:C:222:VAL:HG11	1.69	0.73
1:H:143:VAL:CG2	1:H:166:THR:HG21	2.18	0.73
1:E:205:ALA:N	2:E:1226:3PP:HCB1	2.03	0.73
1:H:126:ASN:C	1:H:126:ASN:HD22	1.92	0.73
1:F:205:ALA:N	2:F:1226:3PP:HCB1	2.03	0.73
1:B:215:GLU:HG2	1:B:219:TRP:CD1	2.24	0.73
1:E:126:ASN:C	1:E:126:ASN:HD22	1.92	0.73
1:D:192:LYS:O	1:D:196:GLU:HG3	1.89	0.73
1:H:187:THR:HG22	1:H:189:GLU:N	2.00	0.73
1:F:192:LYS:O	1:F:196:GLU:HG3	1.89	0.73
1:A:209:THR:HG22	1:A:210:LYS:HG2	1.70	0.72
1:A:96:HIS:HE1	2:A:1226:3PP:OE1	1.71	0.72
1:G:165:ASN:O	1:G:168:GLU:HG2	1.89	0.72
1:B:5:LYS:HB2	1:B:41:THR:HG1	1.51	0.72
1:E:192:LYS:O	1:E:196:GLU:HG3	1.89	0.72
1:G:96:HIS:HE1	2:G:1226:3PP:OE1	1.73	0.72
1:E:209:THR:HG22	1:E:210:LYS:HG2	1.71	0.72
1:B:215:GLU:O	1:B:219:TRP:HD1	1.73	0.71
1:A:126:ASN:C	1:A:126:ASN:HD22	1.93	0.71
1:G:143:VAL:CG2	1:G:166:THR:HG21	2.19	0.71
1:B:96:HIS:CD2	1:B:98:GLU:H	2.08	0.71
1:E:34:VAL:HA	1:E:219:TRP:CZ2	2.24	0.71
1:F:126:ASN:HD22	1:F:126:ASN:C	1.92	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:THR:HG22	1:G:210:LYS:HG2	1.71	0.71
1:A:215:GLU:HG2	1:A:219:TRP:CD1	2.24	0.71
1:G:143:VAL:HG21	1:G:166:THR:HG21	1.70	0.71
1:B:34:VAL:HA	1:B:219:TRP:CZ2	2.25	0.71
1:D:46:PRO:HB3	1:D:54:ILE:HD12	1.73	0.71
1:B:6:GLU:O	1:B:200:VAL:O	2.08	0.71
1:G:46:PRO:HB3	1:G:54:ILE:HD12	1.73	0.71
1:A:192:LYS:O	1:A:196:GLU:HG3	1.90	0.71
1:H:46:PRO:HB3	1:H:54:ILE:HD12	1.73	0.71
1:F:159:LYS:N	1:F:160:PRO:HD3	2.06	0.71
1:H:96:HIS:CD2	1:H:98:GLU:H	2.09	0.71
1:E:215:GLU:HG2	1:E:219:TRP:CD1	2.25	0.71
1:G:96:HIS:CD2	1:G:98:GLU:H	2.08	0.71
1:B:159:LYS:N	1:B:160:PRO:HD3	2.06	0.70
1:C:96:HIS:CD2	1:C:98:GLU:H	2.08	0.70
1:C:193:LYS:HD2	3:C:2049:HOH:O	1.90	0.70
1:A:159:LYS:N	1:A:160:PRO:HD3	2.06	0.70
1:E:46:PRO:HB3	1:E:54:ILE:HD12	1.72	0.70
1:E:96:HIS:CD2	1:E:98:GLU:H	2.08	0.70
1:E:159:LYS:N	1:E:160:PRO:HD3	2.06	0.70
1:D:96:HIS:CD2	1:D:98:GLU:H	2.10	0.70
1:A:46:PRO:HB3	1:A:54:ILE:HD12	1.73	0.70
1:G:126:ASN:C	1:G:126:ASN:HD22	1.94	0.70
1:G:126:ASN:HD21	1:G:129:VAL:H	1.40	0.70
1:C:126:ASN:C	1:C:126:ASN:HD22	1.94	0.70
1:D:159:LYS:N	1:D:160:PRO:HD3	2.06	0.70
1:B:58:VAL:CG1	1:B:60:ILE:HG12	2.22	0.69
1:B:46:PRO:HB3	1:B:54:ILE:HD12	1.73	0.69
1:C:46:PRO:HB3	1:C:54:ILE:HD12	1.74	0.69
1:A:34:VAL:HA	1:A:219:TRP:CZ2	2.26	0.69
1:H:159:LYS:N	1:H:160:PRO:HD3	2.07	0.69
1:F:96:HIS:CD2	1:F:98:GLU:H	2.10	0.69
1:F:46:PRO:HB3	1:F:54:ILE:HD12	1.73	0.69
1:C:209:THR:HG22	1:C:210:LYS:HG2	1.74	0.69
1:A:96:HIS:CD2	1:A:98:GLU:H	2.09	0.69
1:A:126:ASN:HD21	1:A:129:VAL:H	1.40	0.69
1:B:126:ASN:HD21	1:B:129:VAL:H	1.38	0.69
1:E:204:LEU:HA	2:E:1226:3PP:HCB2	1.75	0.68
1:C:73:GLY:O	1:D:15:THR:HG22	1.93	0.68
1:E:107:GLU:HG2	1:G:129:VAL:HG23	1.75	0.68
1:E:126:ASN:HD21	1:E:129:VAL:H	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLU:O	1:A:219:TRP:HD1	1.72	0.68
1:D:205:ALA:N	2:D:1226:3PP:HCB1	2.08	0.68
1:A:107:GLU:HG2	1:C:129:VAL:HG23	1.76	0.68
1:C:126:ASN:HD21	1:C:129:VAL:H	1.43	0.67
1:A:205:ALA:CB	2:A:1226:3PP:HCB1	2.24	0.67
1:E:15:THR:HG22	1:F:73:GLY:O	1.95	0.67
1:G:159:LYS:N	1:G:160:PRO:HD3	2.10	0.67
1:C:159:LYS:N	1:C:160:PRO:HD3	2.10	0.66
1:A:15:THR:HG22	1:B:73:GLY:O	1.96	0.66
1:A:34:VAL:HG13	1:A:219:TRP:CZ3	2.29	0.66
1:B:6:GLU:O	1:B:200:VAL:HG13	1.95	0.66
1:F:126:ASN:HD21	1:F:129:VAL:H	1.41	0.66
1:H:126:ASN:HD21	1:H:129:VAL:H	1.41	0.66
1:E:73:GLY:O	1:F:15:THR:HG22	1.95	0.65
1:E:34:VAL:HG13	1:E:219:TRP:CZ3	2.31	0.65
1:H:162:VAL:HG13	3:H:2038:HOH:O	1.96	0.65
1:D:126:ASN:HD21	1:D:129:VAL:H	1.43	0.64
1:D:58:VAL:HG13	1:D:60:ILE:HG12	1.79	0.63
1:G:73:GLY:O	1:H:15:THR:HG22	1.98	0.63
1:G:94:LEU:HB3	1:G:101:MET:CE	2.28	0.63
1:E:180:LEU:HA	1:E:199:THR:HG23	1.80	0.63
1:B:180:LEU:HA	1:B:199:THR:HG23	1.80	0.63
1:H:58:VAL:HG13	1:H:60:ILE:HG12	1.80	0.63
1:C:15:THR:HG22	1:D:73:GLY:O	1.98	0.63
1:G:7:PRO:HB2	3:G:2002:HOH:O	1.98	0.63
1:G:180:LEU:HA	1:G:199:THR:HG23	1.80	0.63
1:C:180:LEU:HA	1:C:199:THR:HG23	1.80	0.63
1:A:205:ALA:N	2:A:1226:3PP:HCB1	2.13	0.63
1:F:58:VAL:HG13	1:F:60:ILE:HG12	1.79	0.63
1:B:58:VAL:HG12	1:B:60:ILE:HG12	1.80	0.63
1:A:180:LEU:HA	1:A:199:THR:HG23	1.81	0.62
1:A:15:THR:O	1:A:15:THR:HG23	1.97	0.62
1:C:205:ALA:N	2:C:1226:3PP:HCB1	2.15	0.62
1:E:159:LYS:HE2	1:E:162:VAL:HG21	1.81	0.62
1:F:180:LEU:HA	1:F:199:THR:HG23	1.81	0.62
1:B:37:GLU:CD	1:B:219:TRP:HH2	1.97	0.62
1:H:180:LEU:HA	1:H:199:THR:HG23	1.80	0.62
1:H:159:LYS:HE2	1:H:162:VAL:HG21	1.81	0.62
1:E:185:ILE:HG21	1:E:202:VAL:HG11	1.82	0.62
1:E:144:GLU:OE2	1:E:182:GLY:HA3	1.99	0.62
1:E:163:ILE:O	1:E:167:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:THR:HG23	1:E:15:THR:O	1.98	0.62
1:H:111:ARG:NH2	1:H:136:LEU:O	2.27	0.62
1:D:15:THR:O	1:D:15:THR:HG23	1.99	0.62
1:B:34:VAL:HG13	1:B:219:TRP:CZ3	2.34	0.61
1:A:159:LYS:HE2	1:A:162:VAL:HG21	1.82	0.61
1:F:15:THR:O	1:F:15:THR:HG23	1.98	0.61
1:C:94:LEU:HB3	1:C:101:MET:CE	2.30	0.61
1:A:163:ILE:O	1:A:167:VAL:HG23	2.00	0.61
1:G:193:LYS:HD2	3:G:2043:HOH:O	1.98	0.61
1:C:159:LYS:HE2	1:C:162:VAL:HG21	1.81	0.61
1:C:15:THR:O	1:C:15:THR:HG23	1.99	0.61
1:D:180:LEU:HA	1:D:199:THR:HG23	1.81	0.61
1:G:159:LYS:HE2	1:G:162:VAL:HG21	1.82	0.61
1:B:159:LYS:HE2	1:B:162:VAL:HG21	1.82	0.60
1:E:58:VAL:HG13	1:E:60:ILE:HG12	1.83	0.60
1:A:58:VAL:HG13	1:A:60:ILE:HG12	1.83	0.60
1:D:111:ARG:NH2	1:D:136:LEU:O	2.29	0.60
1:G:15:THR:HG22	1:H:73:GLY:O	2.01	0.60
1:B:163:ILE:O	1:B:167:VAL:HG23	2.00	0.60
1:B:94:LEU:HB3	1:B:101:MET:CE	2.31	0.60
1:C:58:VAL:HG13	1:C:60:ILE:HG12	1.83	0.60
1:D:164:THR:HG22	3:D:2041:HOH:O	2.02	0.60
1:B:111:ARG:NH2	1:B:136:LEU:O	2.29	0.60
1:F:94:LEU:HB3	1:F:101:MET:CE	2.32	0.60
1:C:96:HIS:CE1	2:C:1226:3PP:OE1	2.48	0.60
1:A:144:GLU:OE2	1:A:182:GLY:HA3	2.01	0.59
1:F:159:LYS:HE2	1:F:162:VAL:HG21	1.83	0.59
1:H:163:ILE:O	1:H:167:VAL:HG23	2.03	0.59
1:G:182:GLY:O	1:G:183:ALA:HB3	2.03	0.59
1:A:111:ARG:NH2	1:A:136:LEU:O	2.26	0.59
1:G:15:THR:O	1:G:15:THR:HG23	2.02	0.59
1:D:94:LEU:HB3	1:D:101:MET:CE	2.33	0.59
1:C:185:ILE:HG21	1:C:202:VAL:HG11	1.84	0.59
1:E:94:LEU:HB3	1:E:101:MET:CE	2.33	0.59
1:G:58:VAL:HG13	1:G:60:ILE:HG12	1.84	0.59
1:D:159:LYS:HE2	1:D:162:VAL:HG21	1.83	0.59
1:A:94:LEU:HB3	1:A:101:MET:CE	2.33	0.59
1:B:185:ILE:HG21	1:B:202:VAL:HG11	1.84	0.59
1:D:144:GLU:OE2	1:D:182:GLY:HA3	2.02	0.59
1:H:94:LEU:HB3	1:H:101:MET:CE	2.33	0.59
1:A:185:ILE:HG21	1:A:202:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:ILE:O	1:F:167:VAL:HG23	2.02	0.58
1:A:204:LEU:HA	2:A:1226:3PP:HCB2	1.84	0.58
1:H:15:THR:O	1:H:15:THR:HG23	2.02	0.58
1:E:34:VAL:CG2	1:E:219:TRP:CZ2	2.80	0.58
1:B:34:VAL:HG22	1:B:219:TRP:NE1	2.15	0.58
1:G:34:VAL:O	1:G:38:THR:HB	2.03	0.58
1:F:111:ARG:NH2	1:F:136:LEU:O	2.30	0.58
1:F:199:THR:CG2	1:F:201:GLY:H	2.13	0.58
1:F:185:ILE:HG21	1:F:202:VAL:HG11	1.85	0.58
1:A:73:GLY:O	1:B:15:THR:HG22	2.03	0.58
1:B:34:VAL:CG2	1:B:219:TRP:CZ2	2.82	0.58
1:B:146:PRO:HA	1:B:149:ILE:CG1	2.33	0.58
1:C:146:PRO:HA	1:C:149:ILE:CG1	2.34	0.58
1:G:163:ILE:O	1:G:167:VAL:HG23	2.04	0.57
1:E:215:GLU:C	1:E:219:TRP:HD1	2.07	0.57
1:B:37:GLU:HG3	1:B:219:TRP:CZ3	2.38	0.57
1:G:146:PRO:HA	1:G:149:ILE:CG1	2.34	0.57
1:B:34:VAL:O	1:B:38:THR:HB	2.04	0.57
1:D:163:ILE:O	1:D:167:VAL:HG23	2.05	0.57
1:B:199:THR:CG2	1:B:201:GLY:H	2.14	0.57
1:A:182:GLY:O	1:A:183:ALA:HB3	2.04	0.57
1:F:144:GLU:OE2	1:F:182:GLY:HA3	2.04	0.57
1:E:37:GLU:HG3	1:E:219:TRP:CZ3	2.38	0.57
1:H:146:PRO:HA	1:H:149:ILE:CG1	2.33	0.57
1:F:146:PRO:HA	1:F:149:ILE:CG1	2.34	0.57
1:C:52:ARG:O	1:C:56:GLU:HG3	2.05	0.57
1:C:34:VAL:O	1:C:38:THR:HB	2.04	0.57
1:G:205:ALA:N	2:G:1226:3PP:HCB1	2.20	0.57
1:D:146:PRO:HA	1:D:149:ILE:CG1	2.34	0.57
1:H:182:GLY:O	1:H:183:ALA:HB3	2.04	0.57
1:H:185:ILE:HG21	1:H:202:VAL:HG11	1.87	0.57
1:C:182:GLY:O	1:C:183:ALA:HB3	2.05	0.57
1:G:204:LEU:HD21	1:G:221:LEU:HD13	1.87	0.57
1:E:146:PRO:HA	1:E:149:ILE:CG1	2.34	0.57
1:A:34:VAL:CG2	1:A:219:TRP:CZ2	2.82	0.56
1:D:155:VAL:HG13	1:D:183:ALA:O	2.05	0.56
1:B:15:THR:HG23	1:B:15:THR:O	2.04	0.56
1:B:148:LEU:HD12	1:B:155:VAL:HG12	1.87	0.56
2:C:1226:3PP:HCB2	3:C:2048:HOH:O	2.04	0.56
1:A:146:PRO:HA	1:A:149:ILE:CG1	2.34	0.56
1:C:144:GLU:OE2	1:C:182:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:VAL:O	1:E:38:THR:HB	2.05	0.56
1:E:205:ALA:CB	2:E:1226:3PP:HCB1	2.34	0.56
1:G:148:LEU:HD12	1:G:155:VAL:HG12	1.88	0.56
1:D:185:ILE:HG21	1:D:202:VAL:HG11	1.87	0.56
1:F:154:PRO:HB2	1:F:157:LYS:HG3	1.85	0.56
1:G:199:THR:CG2	1:G:201:GLY:H	2.15	0.56
1:F:34:VAL:O	1:F:38:THR:HB	2.06	0.56
1:A:34:VAL:O	1:A:38:THR:HB	2.05	0.56
1:H:58:VAL:HG11	1:H:60:ILE:HG12	1.88	0.56
1:F:199:THR:CG2	1:F:200:VAL:N	2.69	0.56
1:D:182:GLY:O	1:D:183:ALA:HB3	2.06	0.56
1:B:182:GLY:O	1:B:183:ALA:HB3	2.06	0.56
1:F:14:LYS:HE3	2:F:1226:3PP:HCG1	1.86	0.56
1:D:164:THR:HG23	3:D:2040:HOH:O	2.06	0.56
1:A:155:VAL:HG13	1:A:183:ALA:O	2.06	0.56
1:G:6:GLU:OE1	1:G:6:GLU:HA	2.04	0.56
1:E:155:VAL:HG13	1:E:183:ALA:O	2.06	0.56
1:G:111:ARG:NH2	1:G:136:LEU:O	2.28	0.56
1:B:144:GLU:OE2	1:B:182:GLY:HA3	2.05	0.56
1:G:185:ILE:HG21	1:G:202:VAL:HG11	1.88	0.55
1:A:204:LEU:HD21	1:A:221:LEU:HD13	1.89	0.55
1:H:155:VAL:HG13	1:H:183:ALA:O	2.06	0.55
1:A:215:GLU:C	1:A:219:TRP:HD1	2.09	0.55
1:H:148:LEU:HD12	1:H:155:VAL:HG12	1.88	0.55
1:F:52:ARG:O	1:F:56:GLU:HG3	2.06	0.55
1:A:205:ALA:HB3	2:A:1226:3PP:HCB1	1.88	0.55
1:B:215:GLU:C	1:B:219:TRP:HD1	2.09	0.55
1:D:34:VAL:O	1:D:38:THR:HB	2.06	0.55
1:G:204:LEU:HA	2:G:1226:3PP:HCB2	1.88	0.55
1:C:148:LEU:HD12	1:C:155:VAL:HG12	1.89	0.55
1:D:188:GLY:O	1:D:224:GLY:HA3	2.07	0.55
1:A:148:LEU:HD12	1:A:155:VAL:HG12	1.88	0.55
1:F:204:LEU:HD21	1:F:221:LEU:HD13	1.89	0.55
1:B:6:GLU:N	1:B:7:PRO:CD	2.70	0.55
1:E:111:ARG:NH2	1:E:136:LEU:O	2.29	0.55
1:G:144:GLU:OE2	1:G:182:GLY:HA3	2.07	0.55
1:H:204:LEU:HD21	1:H:221:LEU:HD13	1.89	0.54
1:C:111:ARG:NH2	1:C:136:LEU:O	2.28	0.54
1:B:155:VAL:HG13	1:B:183:ALA:O	2.07	0.54
1:G:52:ARG:O	1:G:56:GLU:HG3	2.07	0.54
1:E:204:LEU:HD21	1:E:221:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:VAL:O	1:H:38:THR:HB	2.07	0.54
1:B:32:GLU:HB2	1:B:58:VAL:HG13	1.90	0.54
1:D:204:LEU:HD21	1:D:221:LEU:HD13	1.90	0.54
1:G:145:PRO:HD2	1:G:155:VAL:HG11	1.88	0.54
1:C:145:PRO:HD2	1:C:155:VAL:HG11	1.88	0.54
1:G:200:VAL:CG1	1:G:200:VAL:O	2.56	0.54
1:D:46:PRO:CB	1:D:54:ILE:HD12	2.37	0.54
1:F:155:VAL:HG13	1:F:183:ALA:O	2.07	0.54
1:H:144:GLU:OE2	1:H:182:GLY:HA3	2.07	0.54
1:B:204:LEU:HD21	1:B:221:LEU:HD13	1.90	0.54
1:H:46:PRO:CB	1:H:54:ILE:HD12	2.37	0.54
1:F:94:LEU:HB3	1:F:101:MET:HE2	1.90	0.54
1:C:204:LEU:HD21	1:C:221:LEU:HD13	1.90	0.54
1:G:111:ARG:O	1:G:115:GLU:HG3	2.08	0.54
1:H:38:THR:CG2	1:H:40:VAL:HG23	2.38	0.54
1:B:215:GLU:CG	1:B:219:TRP:NE1	2.36	0.54
1:C:163:ILE:O	1:C:167:VAL:HG23	2.07	0.54
1:D:200:VAL:O	1:D:200:VAL:CG1	2.56	0.54
1:E:148:LEU:HD12	1:E:155:VAL:HG12	1.90	0.54
1:B:111:ARG:O	1:B:115:GLU:HG3	2.08	0.54
1:C:155:VAL:HG13	1:C:183:ALA:O	2.07	0.53
1:A:52:ARG:O	1:A:56:GLU:HG3	2.08	0.53
1:F:188:GLY:O	1:F:224:GLY:HA3	2.08	0.53
1:D:148:LEU:HD12	1:D:155:VAL:HG12	1.90	0.53
1:H:200:VAL:O	1:H:200:VAL:CG1	2.57	0.53
1:C:204:LEU:HA	2:C:1226:3PP:HCB2	1.89	0.53
1:B:46:PRO:CB	1:B:54:ILE:HD12	2.37	0.53
1:F:182:GLY:O	1:F:183:ALA:HB3	2.08	0.53
1:B:5:LYS:C	1:B:7:PRO:CD	2.77	0.53
1:B:129:VAL:HG23	1:D:107:GLU:HG2	1.91	0.53
1:D:107:GLU:HG3	3:D:2029:HOH:O	2.08	0.53
1:G:58:VAL:HG11	1:G:60:ILE:HG12	1.87	0.53
1:A:38:THR:CG2	1:A:40:VAL:HG23	2.38	0.53
1:D:199:THR:CG2	1:D:200:VAL:N	2.71	0.53
1:H:188:GLY:O	1:H:224:GLY:HA3	2.09	0.53
1:D:111:ARG:O	1:D:115:GLU:HG3	2.09	0.53
1:E:58:VAL:HG11	1:E:60:ILE:HG12	1.87	0.53
1:F:111:ARG:O	1:F:115:GLU:HG3	2.08	0.53
1:F:199:THR:HG22	1:F:200:VAL:N	2.22	0.53
1:G:94:LEU:HB3	1:G:101:MET:HE2	1.91	0.53
1:G:127:PRO:HD2	3:G:2038:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:PRO:CB	1:E:54:ILE:HD12	2.39	0.53
1:F:46:PRO:CB	1:F:54:ILE:HD12	2.38	0.53
1:E:182:GLY:O	1:E:183:ALA:HB3	2.09	0.53
1:E:199:THR:CG2	1:E:200:VAL:N	2.72	0.52
1:D:199:THR:CG2	1:D:201:GLY:H	2.14	0.52
1:D:38:THR:CG2	1:D:40:VAL:HG23	2.39	0.52
1:C:46:PRO:CB	1:C:54:ILE:HD12	2.39	0.52
1:B:34:VAL:HA	1:B:219:TRP:CZ3	2.37	0.52
1:F:38:THR:CG2	1:F:40:VAL:HG23	2.39	0.52
1:F:107:GLU:HG3	3:F:2028:HOH:O	2.09	0.52
1:G:107:GLU:O	1:G:111:ARG:HG2	2.09	0.52
1:G:155:VAL:HG13	1:G:183:ALA:O	2.09	0.52
1:F:148:LEU:HD12	1:F:155:VAL:HG12	1.92	0.52
1:E:52:ARG:O	1:E:56:GLU:HG3	2.10	0.52
1:B:188:GLY:O	1:B:224:GLY:HA3	2.09	0.52
1:B:38:THR:CG2	1:B:40:VAL:HG23	2.40	0.52
1:A:46:PRO:CB	1:A:54:ILE:HD12	2.39	0.52
1:B:199:THR:CG2	1:B:200:VAL:N	2.73	0.52
1:C:188:GLY:O	1:C:224:GLY:HA3	2.10	0.52
1:D:52:ARG:O	1:D:56:GLU:HG3	2.09	0.52
1:E:34:VAL:HG22	1:E:219:TRP:NE1	2.15	0.52
1:B:215:GLU:C	1:B:219:TRP:CD1	2.83	0.52
1:C:199:THR:CG2	1:C:200:VAL:N	2.72	0.52
1:C:111:ARG:O	1:C:115:GLU:HG3	2.10	0.52
1:B:107:GLU:O	1:B:111:ARG:HG2	2.10	0.52
1:A:215:GLU:CG	1:A:219:TRP:NE1	2.36	0.51
1:H:199:THR:CG2	1:H:200:VAL:N	2.73	0.51
1:G:46:PRO:CB	1:G:54:ILE:HD12	2.38	0.51
1:H:107:GLU:O	1:H:111:ARG:HG2	2.10	0.51
1:C:107:GLU:O	1:C:111:ARG:HG2	2.10	0.51
1:F:149:ILE:O	2:F:1226:3PP:O2	2.28	0.51
1:F:200:VAL:O	1:F:200:VAL:CG1	2.58	0.51
1:B:200:VAL:CG1	1:B:200:VAL:O	2.58	0.51
1:B:58:VAL:HG11	1:B:60:ILE:HG12	1.93	0.51
1:H:199:THR:HG22	1:H:200:VAL:N	2.25	0.51
1:H:111:ARG:O	1:H:115:GLU:HG3	2.11	0.51
1:C:58:VAL:HG11	1:C:60:ILE:HG12	1.89	0.51
1:G:188:GLY:O	1:G:224:GLY:HA3	2.11	0.51
1:D:199:THR:HG22	1:D:200:VAL:N	2.24	0.51
1:B:52:ARG:O	1:B:56:GLU:HG3	2.10	0.51
1:E:199:THR:CG2	1:E:201:GLY:H	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:GLU:C	1:E:219:TRP:CD1	2.81	0.51
1:A:199:THR:CG2	1:A:201:GLY:H	2.14	0.51
1:C:38:THR:CG2	1:C:40:VAL:HG23	2.41	0.51
1:A:107:GLU:O	1:A:111:ARG:HG2	2.11	0.51
1:F:107:GLU:O	1:F:111:ARG:HG2	2.11	0.51
1:A:34:VAL:HG22	1:A:219:TRP:NE1	2.16	0.51
1:E:111:ARG:O	1:E:115:GLU:HG3	2.10	0.51
1:D:107:GLU:O	1:D:111:ARG:HG2	2.10	0.51
1:A:58:VAL:HG11	1:A:60:ILE:HG12	1.90	0.51
1:A:94:LEU:HB3	1:A:101:MET:HE2	1.93	0.51
1:A:188:GLY:O	1:A:224:GLY:HA3	2.11	0.51
1:A:200:VAL:CG1	1:A:200:VAL:O	2.58	0.51
1:A:199:THR:CG2	1:A:200:VAL:N	2.74	0.51
1:G:199:THR:CG2	1:G:200:VAL:N	2.74	0.51
1:B:206:SER:HA	1:B:209:THR:HG22	1.93	0.51
1:G:16:TYR:CD2	1:G:209:THR:HG21	2.46	0.51
1:D:94:LEU:HB3	1:D:101:MET:HE2	1.91	0.51
1:E:34:VAL:HA	1:E:219:TRP:CZ3	2.40	0.51
1:H:199:THR:CG2	1:H:201:GLY:H	2.16	0.51
1:H:6:GLU:HA	1:H:6:GLU:OE1	2.11	0.51
1:A:206:SER:HA	1:A:209:THR:HG22	1.92	0.51
1:C:206:SER:HA	1:C:209:THR:HG22	1.93	0.51
1:F:145:PRO:HD2	1:F:155:VAL:HG11	1.91	0.51
1:E:199:THR:HG22	1:E:200:VAL:N	2.25	0.50
1:G:38:THR:CG2	1:G:40:VAL:HG23	2.41	0.50
1:E:188:GLY:O	1:E:224:GLY:HA3	2.11	0.50
1:A:111:ARG:O	1:A:115:GLU:HG3	2.11	0.50
1:F:16:TYR:CD2	1:F:209:THR:HG21	2.46	0.50
1:E:200:VAL:CG1	1:E:200:VAL:O	2.58	0.50
1:C:200:VAL:O	1:C:200:VAL:CG1	2.59	0.50
1:B:16:TYR:CD2	1:B:209:THR:HG21	2.46	0.50
1:G:206:SER:HA	1:G:209:THR:HG22	1.93	0.50
1:B:94:LEU:HB3	1:B:101:MET:HE2	1.92	0.50
1:D:145:PRO:HD2	1:D:155:VAL:HG11	1.93	0.50
1:B:6:GLU:N	1:B:7:PRO:HD3	2.27	0.50
1:D:206:SER:HA	1:D:209:THR:HG22	1.94	0.50
1:E:145:PRO:HD2	1:E:155:VAL:HG11	1.92	0.50
1:A:145:PRO:HD2	1:A:155:VAL:HG11	1.92	0.50
1:B:145:PRO:HD2	1:B:155:VAL:HG11	1.92	0.50
1:G:106:LEU:O	1:G:110:ILE:HG13	2.11	0.50
1:E:215:GLU:CG	1:E:219:TRP:NE1	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TYR:CD2	1:A:209:THR:HG21	2.47	0.50
1:C:94:LEU:HB3	1:C:101:MET:HE2	1.94	0.50
1:B:106:LEU:O	1:B:110:ILE:HG13	2.10	0.50
1:D:6:GLU:OE1	1:D:6:GLU:HA	2.12	0.50
1:B:5:LYS:C	1:B:7:PRO:HD2	2.32	0.49
1:E:206:SER:HA	1:E:209:THR:HG22	1.93	0.49
1:C:199:THR:HG22	1:C:200:VAL:N	2.26	0.49
1:A:34:VAL:HA	1:A:219:TRP:CZ3	2.41	0.49
1:F:206:SER:HA	1:F:209:THR:HG22	1.95	0.49
1:G:182:GLY:O	1:G:183:ALA:CB	2.59	0.49
1:B:199:THR:HG22	1:B:200:VAL:N	2.26	0.49
1:D:137:ASN:N	1:D:138:PRO:HD3	2.26	0.49
1:H:137:ASN:N	1:H:138:PRO:HD3	2.26	0.49
1:A:6:GLU:HB2	1:A:7:PRO:HD3	1.95	0.49
1:E:16:TYR:CD2	1:E:209:THR:HG21	2.48	0.49
1:H:145:PRO:HD2	1:H:155:VAL:HG11	1.94	0.49
1:A:34:VAL:CG2	1:A:219:TRP:CD2	2.88	0.49
1:F:129:VAL:HG23	1:H:107:GLU:HG2	1.95	0.49
1:F:58:VAL:HG11	1:F:60:ILE:HG12	1.94	0.49
1:B:199:THR:HG21	1:B:201:GLY:O	2.13	0.49
1:E:37:GLU:CD	1:E:219:TRP:HH2	1.99	0.49
1:D:6:GLU:HB2	1:D:7:PRO:HD3	1.95	0.49
1:H:159:LYS:N	1:H:160:PRO:CD	2.76	0.49
1:D:159:LYS:N	1:D:160:PRO:CD	2.76	0.49
1:F:137:ASN:N	1:F:138:PRO:HD3	2.26	0.49
1:D:16:TYR:CD2	1:D:209:THR:HG21	2.47	0.48
1:E:94:LEU:HB3	1:E:101:MET:HE2	1.95	0.48
1:C:16:TYR:CD2	1:C:209:THR:HG21	2.48	0.48
1:E:34:VAL:CG2	1:E:219:TRP:CD2	2.88	0.48
1:A:215:GLU:C	1:A:219:TRP:CD1	2.83	0.48
1:E:107:GLU:O	1:E:111:ARG:HG2	2.13	0.48
1:E:199:THR:HG21	1:E:201:GLY:O	2.12	0.48
1:G:75:HIS:CD2	1:H:15:THR:HG21	2.49	0.48
1:E:6:GLU:HA	1:E:6:GLU:OE1	2.13	0.48
1:A:6:GLU:OE1	1:A:6:GLU:HA	2.14	0.48
1:H:182:GLY:O	1:H:183:ALA:CB	2.61	0.48
1:B:182:GLY:O	1:B:183:ALA:CB	2.62	0.48
1:A:137:ASN:N	1:A:138:PRO:HD3	2.27	0.48
1:E:38:THR:CG2	1:E:40:VAL:HG23	2.43	0.48
1:E:96:HIS:HE1	2:E:1226:3PP:OE1	1.95	0.48
1:D:209:THR:CG2	1:D:210:LYS:HG2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:THR:HG22	1:G:200:VAL:N	2.27	0.48
1:G:199:THR:HG21	1:G:201:GLY:O	2.13	0.48
1:C:6:GLU:HB2	1:C:7:PRO:HD3	1.96	0.48
1:E:205:ALA:N	2:E:1226:3PP:CB	2.73	0.48
1:B:137:ASN:N	1:B:138:PRO:HD3	2.27	0.48
1:H:199:THR:HG21	1:H:201:GLY:O	2.14	0.48
1:H:206:SER:HA	1:H:209:THR:HG22	1.96	0.48
1:H:106:LEU:O	1:H:110:ILE:HG13	2.14	0.48
1:E:6:GLU:HB2	1:E:7:PRO:HD3	1.96	0.48
1:H:209:THR:CG2	1:H:210:LYS:HG2	2.43	0.48
1:B:94:LEU:HD22	1:B:101:MET:CE	2.44	0.48
1:C:199:THR:HG21	1:C:201:GLY:O	2.13	0.47
1:B:149:ILE:O	2:B:1226:3PP:O2	2.32	0.47
1:F:6:GLU:HB2	1:F:7:PRO:HD3	1.96	0.47
1:F:106:LEU:O	1:F:110:ILE:HG13	2.13	0.47
1:C:106:LEU:O	1:C:110:ILE:HG13	2.13	0.47
1:H:6:GLU:HB2	1:H:7:PRO:HD3	1.96	0.47
1:A:129:VAL:HG23	1:C:107:GLU:HG2	1.97	0.47
1:H:94:LEU:HD22	1:H:101:MET:CE	2.44	0.47
1:H:16:TYR:CD2	1:H:209:THR:HG21	2.48	0.47
1:G:168:GLU:HG3	1:G:169:LEU:N	2.29	0.47
1:F:150:GLY:N	3:F:2039:HOH:O	2.38	0.47
1:A:149:ILE:O	2:A:1226:3PP:O2	2.33	0.47
1:G:168:GLU:CG	1:G:169:LEU:N	2.78	0.47
1:C:182:GLY:O	1:C:183:ALA:CB	2.61	0.47
1:A:32:GLU:HG3	1:A:59:GLU:HG2	1.96	0.47
1:G:137:ASN:N	1:G:138:PRO:HD3	2.29	0.47
1:A:159:LYS:N	1:A:160:PRO:CD	2.75	0.47
1:C:6:GLU:OE1	1:C:6:GLU:HA	2.14	0.47
1:F:161:GLU:H	1:F:161:GLU:CD	2.18	0.47
1:A:182:GLY:O	1:A:183:ALA:CB	2.62	0.47
1:D:155:VAL:HG11	1:D:182:GLY:O	2.14	0.47
1:B:161:GLU:CD	1:B:161:GLU:H	2.18	0.47
1:F:6:GLU:HA	1:F:6:GLU:OE1	2.14	0.47
1:E:159:LYS:N	1:E:160:PRO:CD	2.75	0.47
1:E:137:ASN:N	1:E:138:PRO:HD3	2.28	0.47
1:A:199:THR:HG22	1:A:200:VAL:N	2.28	0.47
1:D:58:VAL:HG11	1:D:60:ILE:HG12	1.91	0.47
1:F:159:LYS:N	1:F:160:PRO:CD	2.75	0.47
1:G:161:GLU:CD	1:G:161:GLU:H	2.17	0.47
1:C:161:GLU:CD	1:C:161:GLU:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:N	1:B:160:PRO:CD	2.76	0.47
1:D:126:ASN:ND2	1:D:126:ASN:C	2.64	0.47
1:D:199:THR:HG21	1:D:201:GLY:O	2.14	0.47
1:E:12:ASN:HB3	2:E:1226:3PP:OE2	2.15	0.47
1:C:3:LYS:HE2	3:C:2047:HOH:O	2.15	0.47
1:C:137:ASN:N	1:C:138:PRO:HD3	2.30	0.46
1:H:52:ARG:O	1:H:56:GLU:HG3	2.15	0.46
1:G:96:HIS:CE1	2:G:1226:3PP:OE1	2.61	0.46
1:C:199:THR:CG2	1:C:201:GLY:H	2.14	0.46
1:G:38:THR:HG21	1:G:222:VAL:CG1	2.44	0.46
1:E:149:ILE:O	2:E:1226:3PP:O2	2.34	0.46
1:H:126:ASN:ND2	1:H:126:ASN:C	2.65	0.46
1:D:14:LYS:HE3	2:D:1226:3PP:HCG1	1.97	0.46
1:D:164:THR:O	1:D:168:GLU:HG3	2.16	0.46
1:F:157:LYS:HE3	1:F:190:ASP:OD1	2.15	0.46
1:E:36:LYS:HE2	3:E:2011:HOH:O	2.15	0.46
1:C:76:THR:O	1:C:78:HIS:HD2	1.99	0.46
1:A:199:THR:HG21	1:A:201:GLY:O	2.15	0.46
1:C:38:THR:HG21	1:C:222:VAL:CG1	2.43	0.46
1:D:161:GLU:CD	1:D:161:GLU:H	2.18	0.46
1:E:106:LEU:O	1:E:110:ILE:HG13	2.14	0.46
1:E:76:THR:O	1:E:78:HIS:HD2	1.98	0.46
1:A:76:THR:O	1:A:78:HIS:HD2	1.97	0.46
1:G:126:ASN:C	1:G:126:ASN:ND2	2.67	0.46
1:F:199:THR:HG21	1:F:201:GLY:O	2.16	0.46
1:C:126:ASN:C	1:C:126:ASN:ND2	2.66	0.46
1:H:161:GLU:H	1:H:161:GLU:CD	2.19	0.46
1:A:209:THR:CG2	1:A:210:LYS:HG2	2.44	0.46
1:H:94:LEU:HB3	1:H:101:MET:HE2	1.96	0.46
1:B:33:LYS:O	1:B:37:GLU:HG2	2.16	0.46
1:A:205:ALA:N	2:A:1226:3PP:CB	2.78	0.46
1:G:6:GLU:O	1:G:200:VAL:HG13	2.16	0.46
1:E:129:VAL:HG23	1:G:107:GLU:HG2	1.98	0.46
1:A:94:LEU:HD22	1:A:101:MET:CE	2.45	0.46
1:A:136:LEU:HD21	1:C:132:ALA:HB2	1.97	0.46
1:A:155:VAL:HG11	1:A:182:GLY:O	2.15	0.46
1:C:159:LYS:N	1:C:160:PRO:CD	2.78	0.45
1:E:94:LEU:HD22	1:E:101:MET:CE	2.46	0.45
1:D:182:GLY:O	1:D:183:ALA:CB	2.64	0.45
1:A:122:VAL:O	1:A:141:VAL:HA	2.16	0.45
1:F:122:VAL:O	1:F:141:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:HA	1:B:112:ARG:HH21	1.82	0.45
1:E:209:THR:CG2	1:E:210:LYS:HG2	2.45	0.45
1:G:159:LYS:N	1:G:160:PRO:CD	2.79	0.45
1:A:144:GLU:HG2	1:A:182:GLY:CA	2.47	0.45
1:E:126:ASN:ND2	1:E:126:ASN:C	2.65	0.45
1:C:45:ALA:HA	1:C:63:PHE:O	2.16	0.45
1:E:161:GLU:CD	1:E:161:GLU:H	2.19	0.45
1:F:155:VAL:HG11	1:F:182:GLY:O	2.17	0.45
1:H:33:LYS:HD3	1:H:215:GLU:CD	2.37	0.45
1:B:14:LYS:NZ	2:B:1226:3PP:HCG1	2.32	0.45
1:G:149:ILE:O	2:G:1226:3PP:O2	2.34	0.45
1:D:204:LEU:HA	2:D:1226:3PP:HCB1	1.99	0.45
1:H:155:VAL:CG1	1:H:183:ALA:HB3	2.47	0.45
1:E:122:VAL:O	1:E:141:VAL:HA	2.17	0.45
1:F:71:LYS:HA	1:F:112:ARG:HH21	1.82	0.45
1:E:164:THR:O	1:E:168:GLU:HG3	2.17	0.45
1:F:164:THR:O	1:F:168:GLU:HG3	2.16	0.45
1:C:33:LYS:O	1:C:37:GLU:HG2	2.16	0.45
1:E:107:GLU:HG2	1:G:129:VAL:CG2	2.44	0.45
1:H:164:THR:O	1:H:168:GLU:HG3	2.17	0.45
1:D:21:GLY:O	1:D:24:ALA:HB3	2.17	0.45
1:D:94:LEU:HD22	1:D:101:MET:CE	2.46	0.44
1:D:106:LEU:O	1:D:110:ILE:HG13	2.17	0.44
1:G:76:THR:O	1:G:78:HIS:HD2	2.00	0.44
1:G:33:LYS:O	1:G:37:GLU:HG2	2.17	0.44
1:H:205:ALA:H	2:H:1226:3PP:HCB1	1.78	0.44
1:B:126:ASN:ND2	1:B:126:ASN:C	2.64	0.44
1:G:155:VAL:CG1	1:G:183:ALA:HB3	2.46	0.44
1:B:215:GLU:CD	1:B:219:TRP:HE1	2.17	0.44
1:D:218:ILE:O	1:D:222:VAL:HG23	2.17	0.44
1:F:182:GLY:O	1:F:183:ALA:CB	2.65	0.44
1:G:122:VAL:O	1:G:141:VAL:HA	2.16	0.44
1:A:164:THR:O	1:A:168:GLU:HG3	2.17	0.44
1:B:8:ILE:HG13	1:B:8:ILE:H	1.42	0.44
1:G:199:THR:CG2	1:G:201:GLY:O	2.65	0.44
1:B:96:HIS:HE1	2:B:1226:3PP:OE2	2.00	0.44
1:D:155:VAL:CG1	1:D:183:ALA:HB3	2.47	0.44
1:C:94:LEU:HD22	1:C:101:MET:CE	2.47	0.44
1:H:155:VAL:HG11	1:H:182:GLY:O	2.17	0.44
1:E:33:LYS:O	1:E:37:GLU:HG2	2.18	0.44
1:B:33:LYS:HD3	1:B:215:GLU:CD	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:LEU:C	2:H:1226:3PP:HCB1	2.38	0.44
1:A:107:GLU:HG2	1:C:129:VAL:CG2	2.45	0.44
1:A:96:HIS:CE1	2:A:1226:3PP:OE1	2.59	0.44
1:D:159:LYS:HA	1:D:161:GLU:OE2	2.18	0.44
1:G:159:LYS:HA	1:G:161:GLU:OE2	2.18	0.44
3:G:2026:HOH:O	1:H:22:LYS:HD2	2.17	0.44
1:E:199:THR:CG2	1:E:201:GLY:O	2.66	0.44
1:H:40:VAL:HG21	1:H:222:VAL:HG13	2.00	0.44
1:A:126:ASN:C	1:A:126:ASN:ND2	2.66	0.44
1:E:182:GLY:O	1:E:183:ALA:CB	2.66	0.44
1:E:218:ILE:O	1:E:222:VAL:HG23	2.16	0.44
1:H:159:LYS:HA	1:H:161:GLU:OE2	2.18	0.44
1:G:165:ASN:HA	1:G:168:GLU:OE2	2.18	0.44
1:B:155:VAL:CG1	1:B:183:ALA:HB3	2.47	0.44
1:F:94:LEU:HD22	1:F:101:MET:CE	2.48	0.44
1:G:94:LEU:HD22	1:G:101:MET:CE	2.48	0.43
1:E:155:VAL:CG1	1:E:183:ALA:HB3	2.48	0.43
1:G:71:LYS:HA	1:G:112:ARG:HH21	1.82	0.43
1:E:45:ALA:HA	1:E:63:PHE:O	2.17	0.43
1:B:155:VAL:HG11	1:B:182:GLY:O	2.18	0.43
1:F:45:ALA:HA	1:F:63:PHE:O	2.18	0.43
1:A:33:LYS:HD3	1:A:215:GLU:CD	2.38	0.43
1:A:199:THR:CG2	1:A:201:GLY:O	2.67	0.43
1:E:71:LYS:HA	1:E:112:ARG:HH21	1.82	0.43
1:C:199:THR:CG2	1:C:201:GLY:O	2.66	0.43
1:F:33:LYS:HD3	1:F:215:GLU:CD	2.39	0.43
1:G:22:LYS:O	1:G:26:GLU:HG3	2.18	0.43
1:B:164:THR:O	1:B:168:GLU:HG3	2.18	0.43
1:E:33:LYS:HD3	1:E:215:GLU:CD	2.38	0.43
1:D:38:THR:HG21	1:D:222:VAL:CG1	2.46	0.43
1:C:155:VAL:CG1	1:C:183:ALA:HB3	2.47	0.43
1:D:33:LYS:HD3	1:D:215:GLU:CD	2.38	0.43
1:B:34:VAL:CA	1:B:219:TRP:CZ2	2.99	0.43
1:G:144:GLU:HG2	1:G:182:GLY:CA	2.49	0.43
1:G:33:LYS:HD3	1:G:215:GLU:CD	2.39	0.43
1:C:71:LYS:HA	1:C:112:ARG:HH21	1.83	0.43
1:B:199:THR:CG2	1:B:201:GLY:O	2.67	0.43
1:D:40:VAL:HG21	1:D:222:VAL:HG13	2.01	0.43
1:F:126:ASN:ND2	1:F:126:ASN:C	2.66	0.43
1:F:159:LYS:HA	1:F:161:GLU:OE2	2.18	0.43
1:F:95:ASN:H	1:F:101:MET:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:GLN:HA	3:E:2014:HOH:O	2.19	0.43
1:B:159:LYS:HA	1:B:161:GLU:OE2	2.18	0.43
1:B:180:LEU:HD22	1:B:201:GLY:CA	2.49	0.43
1:A:155:VAL:CG1	1:A:183:ALA:HB3	2.49	0.43
1:D:144:GLU:HG2	1:D:182:GLY:CA	2.48	0.43
1:B:76:THR:O	1:B:78:HIS:HD2	2.01	0.43
1:H:199:THR:CG2	1:H:201:GLY:O	2.67	0.43
1:G:180:LEU:HD22	1:G:201:GLY:CA	2.49	0.43
1:D:122:VAL:O	1:D:141:VAL:HA	2.19	0.43
1:G:45:ALA:HA	1:G:63:PHE:O	2.18	0.43
1:C:149:ILE:O	2:C:1226:3PP:O2	2.36	0.42
1:F:218:ILE:O	1:F:222:VAL:HG23	2.19	0.42
1:E:144:GLU:HG2	1:E:182:GLY:CA	2.49	0.42
1:E:155:VAL:HG11	1:E:182:GLY:O	2.19	0.42
1:H:33:LYS:O	1:H:37:GLU:HG2	2.18	0.42
1:H:45:ALA:HA	1:H:63:PHE:O	2.17	0.42
1:D:187:THR:CG2	1:D:189:GLU:H	2.09	0.42
1:E:136:LEU:HD21	1:G:132:ALA:HB2	2.00	0.42
1:E:159:LYS:HA	1:E:161:GLU:OE2	2.19	0.42
1:F:155:VAL:CG1	1:F:183:ALA:HB3	2.49	0.42
1:D:76:THR:O	1:D:78:HIS:HD2	2.01	0.42
1:C:122:VAL:O	1:C:141:VAL:HA	2.18	0.42
1:A:45:ALA:HA	1:A:63:PHE:O	2.19	0.42
1:D:126:ASN:HD21	1:D:129:VAL:HG23	1.84	0.42
1:G:75:HIS:HD2	1:H:15:THR:HG21	1.83	0.42
1:A:22:LYS:O	1:A:26:GLU:HG3	2.19	0.42
1:F:102:ILE:HA	1:H:102:ILE:HA	2.01	0.42
1:A:106:LEU:O	1:A:110:ILE:HG13	2.18	0.42
1:A:136:LEU:CD2	1:C:132:ALA:HB2	2.50	0.42
1:C:75:HIS:CD2	1:D:15:THR:HG21	2.54	0.42
1:F:144:GLU:HG2	1:F:182:GLY:CA	2.49	0.42
1:C:144:GLU:HG2	1:C:182:GLY:CA	2.49	0.42
1:C:164:THR:O	1:C:168:GLU:HG3	2.20	0.42
1:H:108:ALA:O	1:H:112:ARG:HB2	2.19	0.42
1:B:122:VAL:O	1:B:141:VAL:HA	2.19	0.42
1:H:38:THR:HG21	1:H:222:VAL:CG1	2.47	0.42
1:C:218:ILE:O	1:C:222:VAL:HG23	2.20	0.42
1:C:15:THR:HG21	1:D:75:HIS:HD2	1.84	0.42
1:D:95:ASN:H	1:D:101:MET:HE2	1.85	0.42
1:H:38:THR:HG22	1:H:40:VAL:N	2.21	0.42
1:B:218:ILE:O	1:B:222:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:THR:O	1:F:78:HIS:HD2	2.02	0.42
1:E:22:LYS:O	1:E:26:GLU:HG3	2.19	0.42
1:D:45:ALA:HA	1:D:63:PHE:O	2.18	0.42
1:C:15:THR:O	1:C:15:THR:CG2	2.68	0.42
1:H:141:VAL:O	1:H:141:VAL:HG13	2.20	0.42
1:G:157:LYS:HG3	3:G:2043:HOH:O	2.20	0.42
1:B:21:GLY:O	1:B:24:ALA:HB3	2.20	0.42
1:B:199:THR:HG22	1:B:201:GLY:N	2.17	0.41
1:C:159:LYS:HA	1:C:161:GLU:OE2	2.20	0.41
1:C:33:LYS:HD3	1:C:215:GLU:CD	2.40	0.41
1:G:205:ALA:CB	2:G:1226:3PP:HCB1	2.49	0.41
1:H:95:ASN:H	1:H:101:MET:HE2	1.85	0.41
1:B:144:GLU:HG2	1:B:182:GLY:CA	2.50	0.41
1:D:199:THR:CG2	1:D:201:GLY:O	2.68	0.41
1:C:6:GLU:HG2	3:C:2001:HOH:O	2.20	0.41
1:B:108:ALA:O	1:B:112:ARG:HB2	2.21	0.41
1:C:22:LYS:O	1:C:26:GLU:HG3	2.20	0.41
1:H:143:VAL:HG11	3:H:2038:HOH:O	2.19	0.41
1:D:33:LYS:O	1:D:37:GLU:HG2	2.20	0.41
1:D:100:ARG:HD2	3:D:2025:HOH:O	2.20	0.41
1:E:38:THR:HG22	1:E:40:VAL:N	2.21	0.41
1:G:165:ASN:C	1:G:168:GLU:HG2	2.39	0.41
1:D:205:ALA:H	2:D:1226:3PP:HCB1	1.84	0.41
1:D:204:LEU:HB2	3:D:2044:HOH:O	2.21	0.41
1:C:141:VAL:HG13	1:C:141:VAL:O	2.20	0.41
1:B:45:ALA:HA	1:B:63:PHE:O	2.21	0.41
1:G:149:ILE:O	1:G:149:ILE:CG2	2.68	0.41
1:G:111:ARG:HD3	1:G:111:ARG:HA	1.84	0.41
1:C:143:VAL:HG22	1:C:166:THR:HG21	2.02	0.41
1:G:155:VAL:HG11	1:G:182:GLY:O	2.20	0.41
1:E:101:MET:HE1	1:E:106:LEU:HD23	2.02	0.41
1:D:71:LYS:HA	1:D:112:ARG:HH21	1.85	0.41
1:A:71:LYS:HA	1:A:112:ARG:HH21	1.84	0.41
1:B:6:GLU:HA	1:B:6:GLU:OE1	2.20	0.41
1:B:14:LYS:HE3	2:B:1226:3PP:HCG1	2.03	0.41
1:G:149:ILE:HG22	1:G:149:ILE:O	2.20	0.41
1:H:31:ALA:HB1	1:H:42:ILE:HG21	2.03	0.41
1:A:215:GLU:CD	1:A:219:TRP:HE1	2.17	0.41
1:B:143:VAL:CG1	1:B:166:THR:HG21	2.46	0.41
1:G:165:ASN:HA	1:G:168:GLU:CD	2.41	0.41
1:C:155:VAL:HG11	1:C:182:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:VAL:HG13	1:D:141:VAL:O	2.20	0.41
1:C:31:ALA:HB1	1:C:42:ILE:HG21	2.03	0.41
1:F:40:VAL:HG21	1:F:222:VAL:HG13	2.02	0.41
1:F:33:LYS:O	1:F:37:GLU:HG2	2.21	0.41
1:G:21:GLY:O	1:G:24:ALA:HB3	2.21	0.41
1:E:34:VAL:CA	1:E:219:TRP:CZ2	2.98	0.40
1:D:111:ARG:HD3	1:D:111:ARG:HA	1.82	0.40
1:B:209:THR:CG2	1:B:210:LYS:HG2	2.43	0.40
1:H:21:GLY:O	1:H:24:ALA:HB3	2.21	0.40
1:H:218:ILE:O	1:H:222:VAL:HG23	2.21	0.40
1:G:209:THR:CG2	1:G:210:LYS:HG2	2.46	0.40
1:C:15:THR:HG21	1:D:75:HIS:CD2	2.57	0.40
1:F:141:VAL:O	1:F:141:VAL:HG13	2.21	0.40
1:G:218:ILE:O	1:G:222:VAL:HG23	2.22	0.40
1:C:40:VAL:HG21	1:C:222:VAL:HG13	2.02	0.40
1:A:6:GLU:CB	1:A:7:PRO:HD3	2.51	0.40
1:F:6:GLU:CB	1:F:7:PRO:HD3	2.51	0.40
1:H:162:VAL:CG1	3:H:2038:HOH:O	2.62	0.40
1:F:14:LYS:CE	2:F:1226:3PP:HCG1	2.49	0.40
1:C:155:VAL:O	1:C:158:ALA:O	2.39	0.40
1:A:102:ILE:HA	1:C:102:ILE:HA	2.03	0.40
1:H:14:LYS:HE3	2:H:1226:3PP:HCG1	2.02	0.40
1:B:155:VAL:O	1:B:158:ALA:O	2.39	0.40
1:C:112:ARG:HA	1:C:112:ARG:HD2	1.86	0.40
1:H:71:LYS:HA	1:H:112:ARG:HH21	1.86	0.40
1:B:31:ALA:HB1	1:B:42:ILE:HG21	2.02	0.40

All (4) 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:37:GLU:OE2	1:C:168:GLU:OE1[2_646]	1.73	0.47
1:E:37:GLU:CB	1:G:165:ASN:OD1[2_747]	1.92	0.28
1:F:137:ASN:OD1	1:G:212:LYS:NZ[2_647]	1.99	0.21
1:F:137:ASN:OD1	1:G:212:LYS:CE[2_647]	2.18	0.02

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	222/225 (99%)	205 (92%)	14 (6%)	3 (1%)	14	35
1	B	222/225 (99%)	206 (93%)	14 (6%)	2 (1%)	21	49
1	C	222/225 (99%)	206 (93%)	13 (6%)	3 (1%)	14	35
1	D	222/225 (99%)	204 (92%)	15 (7%)	3 (1%)	14	35
1	E	222/225 (99%)	206 (93%)	13 (6%)	3 (1%)	14	35
1	F	222/225 (99%)	206 (93%)	13 (6%)	3 (1%)	14	35
1	G	222/225 (99%)	207 (93%)	12 (5%)	3 (1%)	14	35
1	H	222/225 (99%)	206 (93%)	13 (6%)	3 (1%)	14	35
All	All	1776/1800 (99%)	1646 (93%)	107 (6%)	23 (1%)	15	37

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	C	6	GLU
1	D	6	GLU
1	E	6	GLU
1	F	6	GLU
1	H	6	GLU
1	A	149	ILE
1	B	149	ILE
1	C	149	ILE
1	D	149	ILE
1	E	149	ILE
1	F	149	ILE
1	G	149	ILE
1	H	149	ILE
1	A	183	ALA
1	B	183	ALA
1	C	183	ALA

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Mol	Chain	Res	Type
1	D	183	ALA
1	E	183	ALA
1	F	183	ALA
1	G	183	ALA
1	H	183	ALA
1	G	6	GLU

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	179/180 (99%)	172 (96%)	7 (4%)	39	70
1	B	179/180 (99%)	173 (97%)	6 (3%)	44	75
1	C	179/180 (99%)	172 (96%)	7 (4%)	39	70
1	D	179/180 (99%)	172 (96%)	7 (4%)	39	70
1	E	179/180 (99%)	172 (96%)	7 (4%)	39	70
1	F	179/180 (99%)	172 (96%)	7 (4%)	39	70
1	G	179/180 (99%)	171 (96%)	8 (4%)	34	65
1	H	179/180 (99%)	172 (96%)	7 (4%)	39	70
All	All	1432/1440 (99%)	1376 (96%)	56 (4%)	39	70

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	58	VAL
1	A	106	LEU
1	A	107	GLU
1	A	126	ASN
1	A	147	GLU
1	A	209	THR
1	B	15	THR
1	B	106	LEU

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Mol	Chain	Res	Type
1	B	107	GLU
1	B	126	ASN
1	B	147	GLU
1	B	209	THR
1	C	15	THR
1	C	58	VAL
1	C	106	LEU
1	C	107	GLU
1	C	126	ASN
1	C	147	GLU
1	C	209	THR
1	D	15	THR
1	D	58	VAL
1	D	106	LEU
1	D	107	GLU
1	D	126	ASN
1	D	147	GLU
1	D	209	THR
1	E	15	THR
1	E	58	VAL
1	E	106	LEU
1	E	107	GLU
1	E	126	ASN
1	E	147	GLU
1	E	209	THR
1	F	15	THR
1	F	58	VAL
1	F	106	LEU
1	F	107	GLU
1	F	126	ASN
1	F	147	GLU
1	F	209	THR
1	G	6	GLU
1	G	15	THR
1	G	58	VAL
1	G	106	LEU
1	G	107	GLU
1	G	126	ASN
1	G	147	GLU
1	G	209	THR
1	H	15	THR
1	H	58	VAL

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Mol	Chain	Res	Type
1	H	106	LEU
1	H	107	GLU
1	H	126	ASN
1	H	147	GLU
1	H	209	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	96	HIS
1	A	126	ASN
1	A	165	ASN
1	B	47	GLN
1	B	96	HIS
1	B	126	ASN
1	B	165	ASN
1	C	47	GLN
1	C	78	HIS
1	C	96	HIS
1	C	126	ASN
1	D	47	GLN
1	D	75	HIS
1	D	96	HIS
1	D	126	ASN
1	D	165	ASN
1	E	47	GLN
1	E	96	HIS
1	E	126	ASN
1	E	165	ASN
1	F	47	GLN
1	F	75	HIS
1	F	96	HIS
1	F	126	ASN
1	F	165	ASN
1	G	47	GLN
1	G	96	HIS
1	G	126	ASN
1	G	165	ASN
1	H	47	GLN
1	H	75	HIS
1	H	96	HIS

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Mol	Chain	Res	Type
1	H	126	ASN
1	H	165	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 carbohydrates 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	3PP	A	1226	-	5,8,8	2.49	2 (40%)	6,11,11	2.71	3 (50%)
2	3PP	B	1226	-	5,8,8	2.51	2 (40%)	6,11,11	2.52	4 (66%)
2	3PP	C	1226	-	5,8,8	2.23	3 (60%)	6,11,11	2.71	3 (50%)
2	3PP	D	1226	-	5,8,8	3.11	1 (20%)	6,11,11	2.56	3 (50%)
2	3PP	E	1226	-	5,8,8	2.50	3 (60%)	6,11,11	2.76	3 (50%)
2	3PP	F	1226	-	5,8,8	2.87	3 (60%)	6,11,11	2.62	3 (50%)
2	3PP	G	1226	-	5,8,8	2.29	3 (60%)	6,11,11	2.72	4 (66%)
2	3PP	H	1226	-	5,8,8	2.81	2 (40%)	6,11,11	2.57	3 (50%)

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	3PP	A	1226	-	-	0/4/6/6	0/0/0/0
2	3PP	B	1226	-	-	0/4/6/6	0/0/0/0
2	3PP	C	1226	-	-	0/4/6/6	0/0/0/0
2	3PP	D	1226	-	-	0/4/6/6	0/0/0/0
2	3PP	E	1226	-	-	0/4/6/6	0/0/0/0
2	3PP	F	1226	-	-	0/4/6/6	0/0/0/0
2	3PP	G	1226	-	-	0/4/6/6	0/0/0/0
2	3PP	H	1226	-	-	0/4/6/6	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1226	3PP	P-O3	-2.62	1.48	1.54
2	G	1226	3PP	P-O3	-2.56	1.48	1.54
2	C	1226	3PP	P-O1	-2.56	1.48	1.54
2	F	1226	3PP	P-O3	-2.43	1.49	1.54
2	G	1226	3PP	P-O1	-2.29	1.49	1.54
2	F	1226	3PP	P-O1	-2.28	1.49	1.54
2	E	1226	3PP	P-O3	-2.18	1.49	1.54
2	A	1226	3PP	P-O3	-2.18	1.49	1.54
2	H	1226	3PP	P-O1	-2.14	1.49	1.54
2	B	1226	3PP	P-O3	-2.12	1.49	1.54
2	E	1226	3PP	P-O1	-2.08	1.49	1.54
2	C	1226	3PP	P-CB	3.30	1.82	1.79
2	G	1226	3PP	P-CB	3.72	1.82	1.79
2	E	1226	3PP	P-CB	4.67	1.83	1.79
2	B	1226	3PP	P-CB	4.72	1.83	1.79
2	A	1226	3PP	P-CB	4.72	1.83	1.79
2	F	1226	3PP	P-CB	5.35	1.84	1.79
2	H	1226	3PP	P-CB	5.49	1.84	1.79
2	D	1226	3PP	P-CB	6.36	1.85	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1226	3PP	O2-P-CB	-4.77	100.56	111.22
2	A	1226	3PP	O2-P-CB	-4.69	100.74	111.22
2	F	1226	3PP	O2-P-CB	-4.46	101.27	111.22
2	H	1226	3PP	O2-P-CB	-4.42	101.35	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1226	3PP	O2-P-CB	-4.41	101.36	111.22
2	D	1226	3PP	O2-P-CB	-4.27	101.69	111.22
2	B	1226	3PP	O2-P-CB	-3.88	102.56	111.22
2	C	1226	3PP	O2-P-CB	-3.80	102.73	111.22
2	C	1226	3PP	O3-P-CB	-3.60	97.96	106.89
2	D	1226	3PP	O3-P-CB	-3.07	99.29	106.89
2	A	1226	3PP	O3-P-CB	-2.77	100.02	106.89
2	E	1226	3PP	O3-P-CB	-2.77	100.02	106.89
2	F	1226	3PP	O3-P-CB	-2.72	100.15	106.89
2	G	1226	3PP	O3-P-CB	-2.71	100.17	106.89
2	B	1226	3PP	O3-P-CB	-2.63	100.38	106.89
2	H	1226	3PP	O3-P-CB	-2.59	100.47	106.89
2	B	1226	3PP	O1-P-CB	-2.15	101.56	106.89
2	G	1226	3PP	O1-P-CB	-2.13	101.61	106.89
2	D	1226	3PP	O3-P-O1	2.57	115.67	108.13
2	H	1226	3PP	O3-P-O1	2.62	115.82	108.13
2	B	1226	3PP	O3-P-O1	2.67	115.94	108.13
2	F	1226	3PP	O3-P-O1	2.68	115.97	108.13
2	E	1226	3PP	O3-P-O1	2.74	116.17	108.13
2	A	1226	3PP	O3-P-O1	2.78	116.28	108.13
2	C	1226	3PP	O3-P-O1	2.82	116.39	108.13
2	G	1226	3PP	O3-P-O1	2.82	116.41	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1226	3PP	8	0
2	B	1226	3PP	5	0
2	C	1226	3PP	6	0
2	D	1226	3PP	4	0
2	E	1226	3PP	7	0
2	F	1226	3PP	4	0
2	G	1226	3PP	6	0
2	H	1226	3PP	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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