Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2021 – 02:14 PM GMT

PDB ID	:	6QU5
Title	:	Crystal Structure of Phosphofructokinase from Trypanosoma brucei in complex with an allosteric inhibitor ctcb12
Authors	:	McNae, I.W.; Dornan, J.; Walkinshaw, M.D.
Deposited on	:	2019-02-26
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

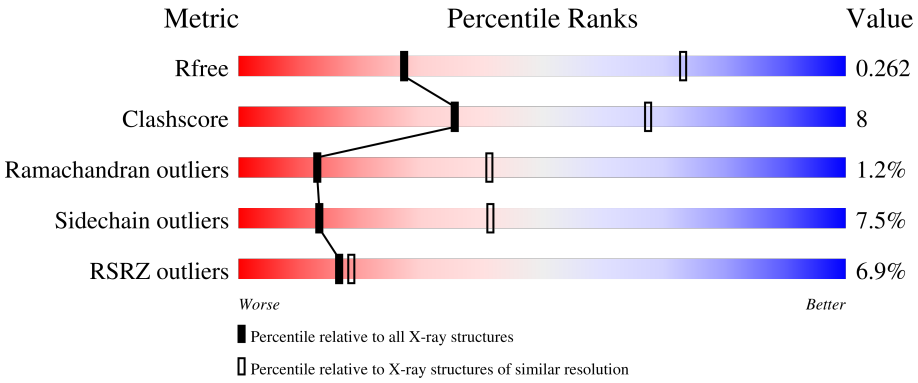
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1.dev1

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	507	% 71% 15% • 11%
1	B	507	4% 72% 16% • 9%
1	C	507	5% 71% 16% • 9%
1	D	507	6% 72% 16% • 11%
1	E	507	2% 70% 17% • 10%

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Mol	Chain	Length	Quality of chain
1	F	507	3% 72% 17% 10%
1	G	507	13% 68% 18% 10%
1	H	507	14% 71% 16% 11%

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
4	JJ8	B	503	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28255 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 ATP-dependent 6-phosphofructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3487	2187	639	644	17			
1	B	459	Total	C	N	O	S	0	0	0
			3539	2218	648	656	17			
1	C	461	Total	C	N	O	S	0	0	0
			3552	2226	651	658	17			
1	D	453	Total	C	N	O	S	0	0	0
			3493	2189	642	645	17			
1	E	456	Total	C	N	O	S	0	0	0
			3519	2205	648	649	17			
1	F	456	Total	C	N	O	S	0	0	0
			3514	2202	645	650	17			
1	G	455	Total	C	N	O	S	0	0	0
			3511	2201	646	647	17			
1	H	453	Total	C	N	O	S	0	0	0
			3496	2193	641	645	17			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O15648
A	-18	GLY	-	expression tag	UNP O15648
A	-17	SER	-	expression tag	UNP O15648
A	-16	SER	-	expression tag	UNP O15648
A	-15	HIS	-	expression tag	UNP O15648
A	-14	HIS	-	expression tag	UNP O15648
A	-13	HIS	-	expression tag	UNP O15648
A	-12	HIS	-	expression tag	UNP O15648
A	-11	HIS	-	expression tag	UNP O15648
A	-10	HIS	-	expression tag	UNP O15648
A	-9	SER	-	expression tag	UNP O15648
A	-8	SER	-	expression tag	UNP O15648
A	-7	GLY	-	expression tag	UNP O15648

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP O15648
A	-5	VAL	-	expression tag	UNP O15648
A	-4	PRO	-	expression tag	UNP O15648
A	-3	ARG	-	expression tag	UNP O15648
A	-2	GLY	-	expression tag	UNP O15648
A	-1	SER	-	expression tag	UNP O15648
A	0	HIS	-	expression tag	UNP O15648
B	-19	MET	-	initiating methionine	UNP O15648
B	-18	GLY	-	expression tag	UNP O15648
B	-17	SER	-	expression tag	UNP O15648
B	-16	SER	-	expression tag	UNP O15648
B	-15	HIS	-	expression tag	UNP O15648
B	-14	HIS	-	expression tag	UNP O15648
B	-13	HIS	-	expression tag	UNP O15648
B	-12	HIS	-	expression tag	UNP O15648
B	-11	HIS	-	expression tag	UNP O15648
B	-10	HIS	-	expression tag	UNP O15648
B	-9	SER	-	expression tag	UNP O15648
B	-8	SER	-	expression tag	UNP O15648
B	-7	GLY	-	expression tag	UNP O15648
B	-6	LEU	-	expression tag	UNP O15648
B	-5	VAL	-	expression tag	UNP O15648
B	-4	PRO	-	expression tag	UNP O15648
B	-3	ARG	-	expression tag	UNP O15648
B	-2	GLY	-	expression tag	UNP O15648
B	-1	SER	-	expression tag	UNP O15648
B	0	HIS	-	expression tag	UNP O15648
C	-19	MET	-	initiating methionine	UNP O15648
C	-18	GLY	-	expression tag	UNP O15648
C	-17	SER	-	expression tag	UNP O15648
C	-16	SER	-	expression tag	UNP O15648
C	-15	HIS	-	expression tag	UNP O15648
C	-14	HIS	-	expression tag	UNP O15648
C	-13	HIS	-	expression tag	UNP O15648
C	-12	HIS	-	expression tag	UNP O15648
C	-11	HIS	-	expression tag	UNP O15648
C	-10	HIS	-	expression tag	UNP O15648
C	-9	SER	-	expression tag	UNP O15648
C	-8	SER	-	expression tag	UNP O15648
C	-7	GLY	-	expression tag	UNP O15648
C	-6	LEU	-	expression tag	UNP O15648
C	-5	VAL	-	expression tag	UNP O15648

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP O15648
C	-3	ARG	-	expression tag	UNP O15648
C	-2	GLY	-	expression tag	UNP O15648
C	-1	SER	-	expression tag	UNP O15648
C	0	HIS	-	expression tag	UNP O15648
D	-19	MET	-	initiating methionine	UNP O15648
D	-18	GLY	-	expression tag	UNP O15648
D	-17	SER	-	expression tag	UNP O15648
D	-16	SER	-	expression tag	UNP O15648
D	-15	HIS	-	expression tag	UNP O15648
D	-14	HIS	-	expression tag	UNP O15648
D	-13	HIS	-	expression tag	UNP O15648
D	-12	HIS	-	expression tag	UNP O15648
D	-11	HIS	-	expression tag	UNP O15648
D	-10	HIS	-	expression tag	UNP O15648
D	-9	SER	-	expression tag	UNP O15648
D	-8	SER	-	expression tag	UNP O15648
D	-7	GLY	-	expression tag	UNP O15648
D	-6	LEU	-	expression tag	UNP O15648
D	-5	VAL	-	expression tag	UNP O15648
D	-4	PRO	-	expression tag	UNP O15648
D	-3	ARG	-	expression tag	UNP O15648
D	-2	GLY	-	expression tag	UNP O15648
D	-1	SER	-	expression tag	UNP O15648
D	0	HIS	-	expression tag	UNP O15648
E	-19	MET	-	initiating methionine	UNP O15648
E	-18	GLY	-	expression tag	UNP O15648
E	-17	SER	-	expression tag	UNP O15648
E	-16	SER	-	expression tag	UNP O15648
E	-15	HIS	-	expression tag	UNP O15648
E	-14	HIS	-	expression tag	UNP O15648
E	-13	HIS	-	expression tag	UNP O15648
E	-12	HIS	-	expression tag	UNP O15648
E	-11	HIS	-	expression tag	UNP O15648
E	-10	HIS	-	expression tag	UNP O15648
E	-9	SER	-	expression tag	UNP O15648
E	-8	SER	-	expression tag	UNP O15648
E	-7	GLY	-	expression tag	UNP O15648
E	-6	LEU	-	expression tag	UNP O15648
E	-5	VAL	-	expression tag	UNP O15648
E	-4	PRO	-	expression tag	UNP O15648
E	-3	ARG	-	expression tag	UNP O15648

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP O15648
E	-1	SER	-	expression tag	UNP O15648
E	0	HIS	-	expression tag	UNP O15648
F	-19	MET	-	initiating methionine	UNP O15648
F	-18	GLY	-	expression tag	UNP O15648
F	-17	SER	-	expression tag	UNP O15648
F	-16	SER	-	expression tag	UNP O15648
F	-15	HIS	-	expression tag	UNP O15648
F	-14	HIS	-	expression tag	UNP O15648
F	-13	HIS	-	expression tag	UNP O15648
F	-12	HIS	-	expression tag	UNP O15648
F	-11	HIS	-	expression tag	UNP O15648
F	-10	HIS	-	expression tag	UNP O15648
F	-9	SER	-	expression tag	UNP O15648
F	-8	SER	-	expression tag	UNP O15648
F	-7	GLY	-	expression tag	UNP O15648
F	-6	LEU	-	expression tag	UNP O15648
F	-5	VAL	-	expression tag	UNP O15648
F	-4	PRO	-	expression tag	UNP O15648
F	-3	ARG	-	expression tag	UNP O15648
F	-2	GLY	-	expression tag	UNP O15648
F	-1	SER	-	expression tag	UNP O15648
F	0	HIS	-	expression tag	UNP O15648
G	-19	MET	-	initiating methionine	UNP O15648
G	-18	GLY	-	expression tag	UNP O15648
G	-17	SER	-	expression tag	UNP O15648
G	-16	SER	-	expression tag	UNP O15648
G	-15	HIS	-	expression tag	UNP O15648
G	-14	HIS	-	expression tag	UNP O15648
G	-13	HIS	-	expression tag	UNP O15648
G	-12	HIS	-	expression tag	UNP O15648
G	-11	HIS	-	expression tag	UNP O15648
G	-10	HIS	-	expression tag	UNP O15648
G	-9	SER	-	expression tag	UNP O15648
G	-8	SER	-	expression tag	UNP O15648
G	-7	GLY	-	expression tag	UNP O15648
G	-6	LEU	-	expression tag	UNP O15648
G	-5	VAL	-	expression tag	UNP O15648
G	-4	PRO	-	expression tag	UNP O15648
G	-3	ARG	-	expression tag	UNP O15648
G	-2	GLY	-	expression tag	UNP O15648
G	-1	SER	-	expression tag	UNP O15648

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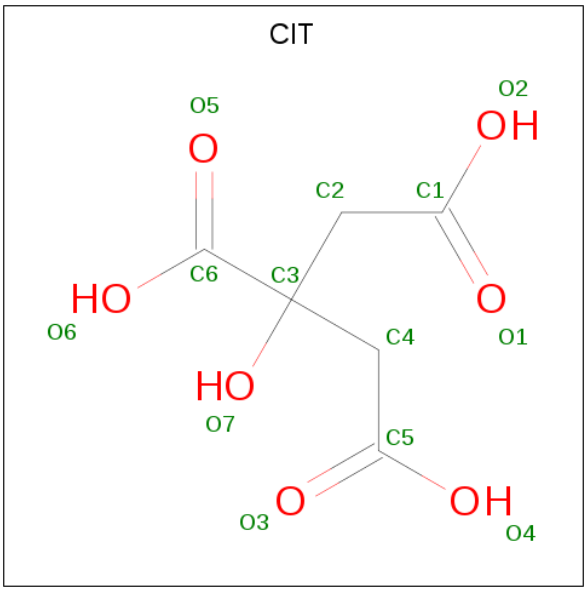
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP O15648
H	-19	MET	-	initiating methionine	UNP O15648
H	-18	GLY	-	expression tag	UNP O15648
H	-17	SER	-	expression tag	UNP O15648
H	-16	SER	-	expression tag	UNP O15648
H	-15	HIS	-	expression tag	UNP O15648
H	-14	HIS	-	expression tag	UNP O15648
H	-13	HIS	-	expression tag	UNP O15648
H	-12	HIS	-	expression tag	UNP O15648
H	-11	HIS	-	expression tag	UNP O15648
H	-10	HIS	-	expression tag	UNP O15648
H	-9	SER	-	expression tag	UNP O15648
H	-8	SER	-	expression tag	UNP O15648
H	-7	GLY	-	expression tag	UNP O15648
H	-6	LEU	-	expression tag	UNP O15648
H	-5	VAL	-	expression tag	UNP O15648
H	-4	PRO	-	expression tag	UNP O15648
H	-3	ARG	-	expression tag	UNP O15648
H	-2	GLY	-	expression tag	UNP O15648
H	-1	SER	-	expression tag	UNP O15648
H	0	HIS	-	expression tag	UNP O15648

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

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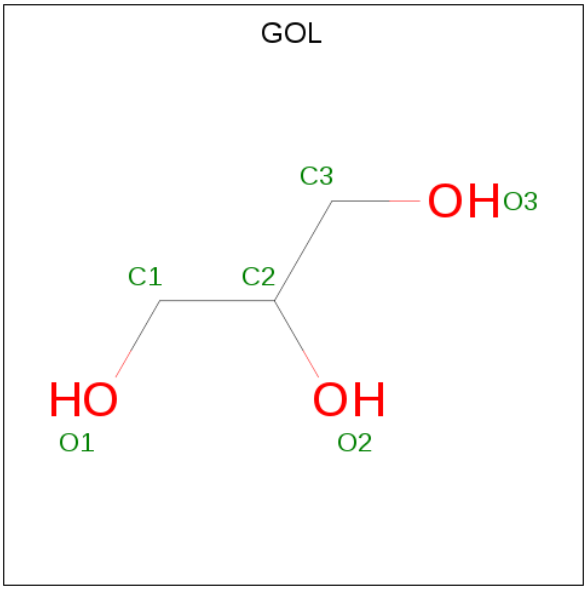
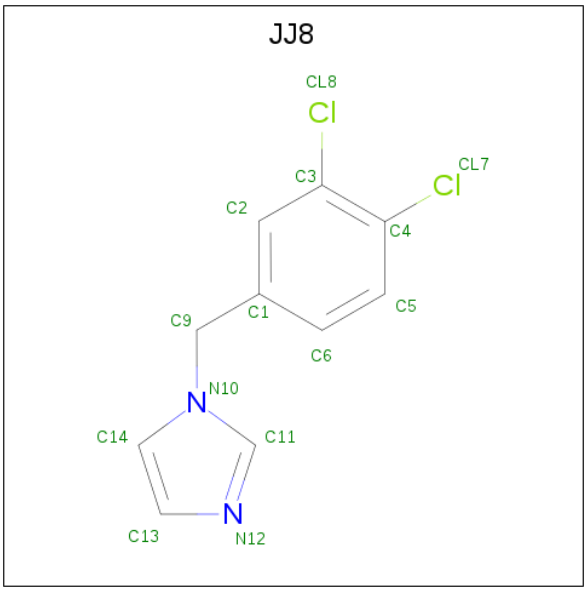
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is 1-[(3,4-dichlorophenyl)methyl]imidazole (three-letter code: JJ8) (formula: $C_{10}H_8Cl_2N_2$).



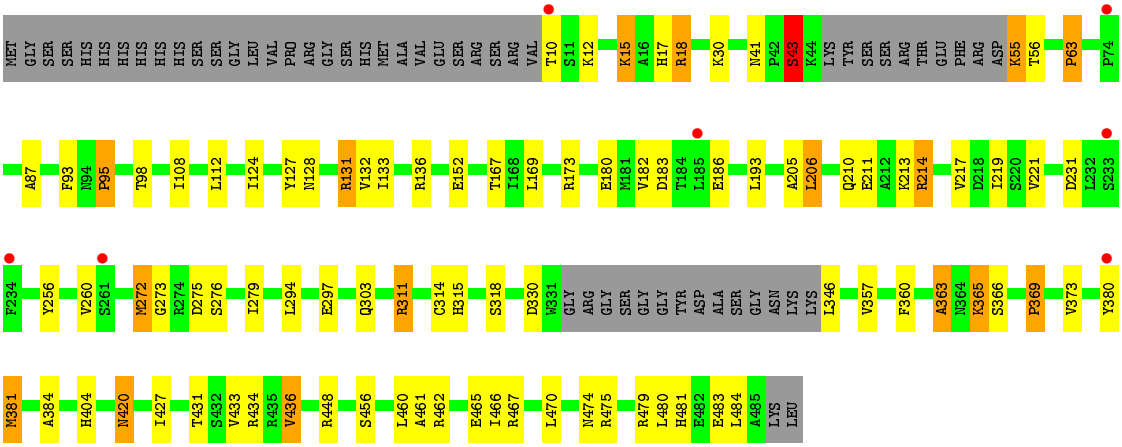
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			14	10	2	2		
4	B	1	Total	C	Cl	N	0	0
			14	10	2	2		

3 Residue-property plots (i)

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

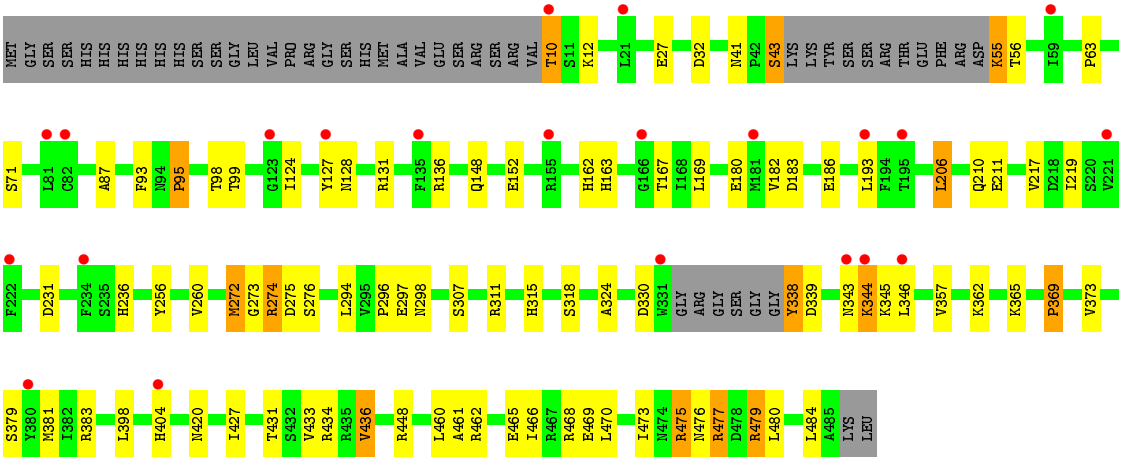
- Molecule 1: ATP-dependent 6-phosphofructokinase

Chain A:



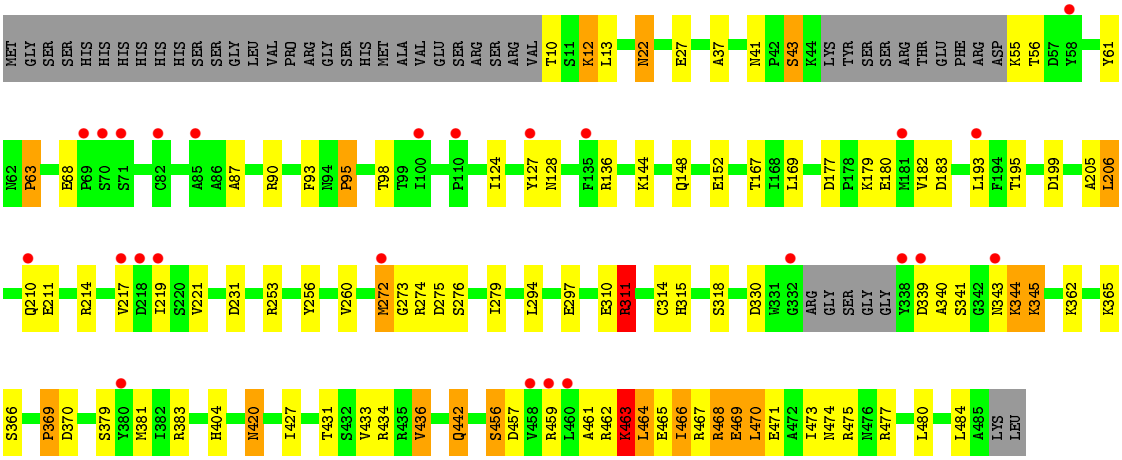
- Molecule 1: ATP-dependent 6-phosphofructokinase

Chain B:



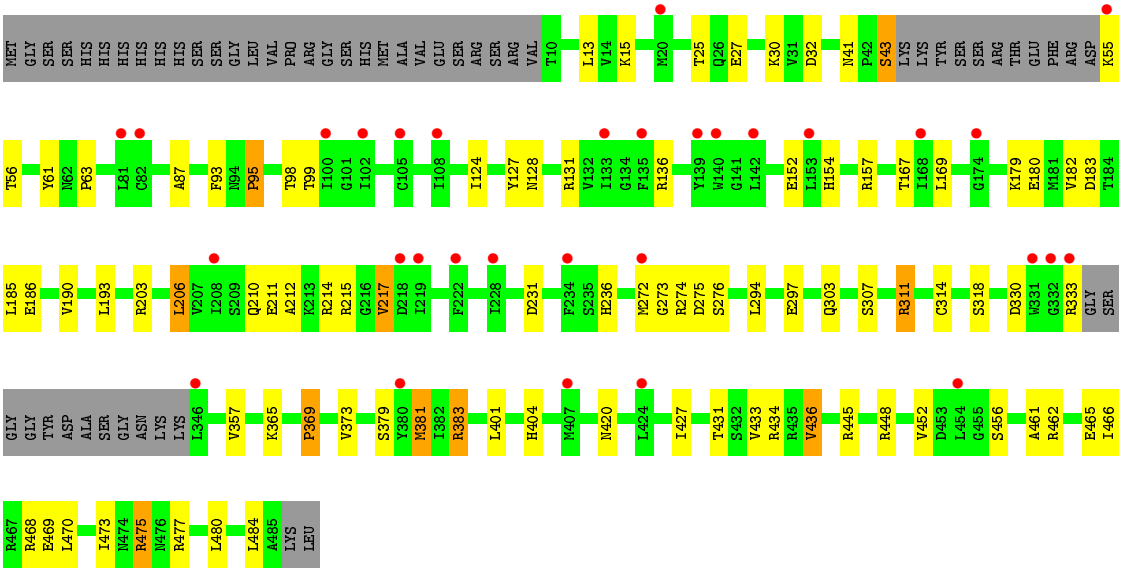
- Molecule 1: ATP-dependent 6-phosphofructokinase

Chain C:



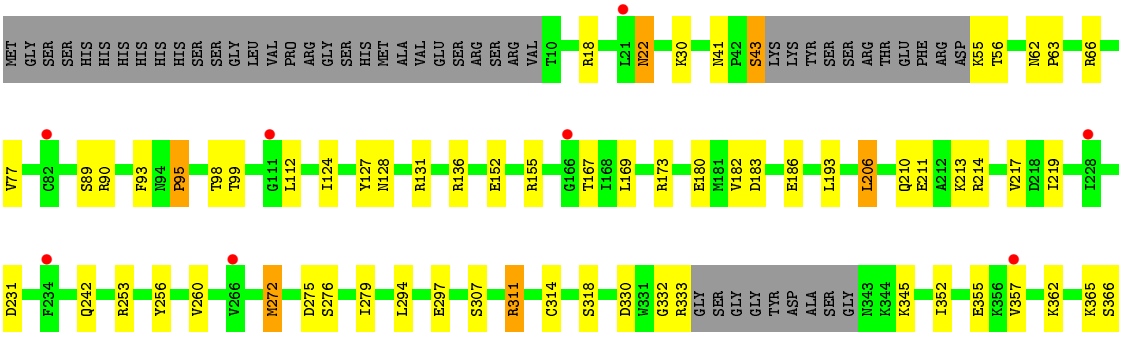
• Molecule 1: ATP-dependent 6-phosphofructokinase

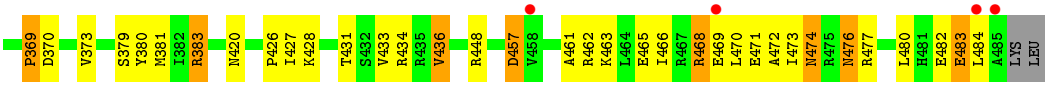
Chain D:



• Molecule 1: ATP-dependent 6-phosphofructokinase

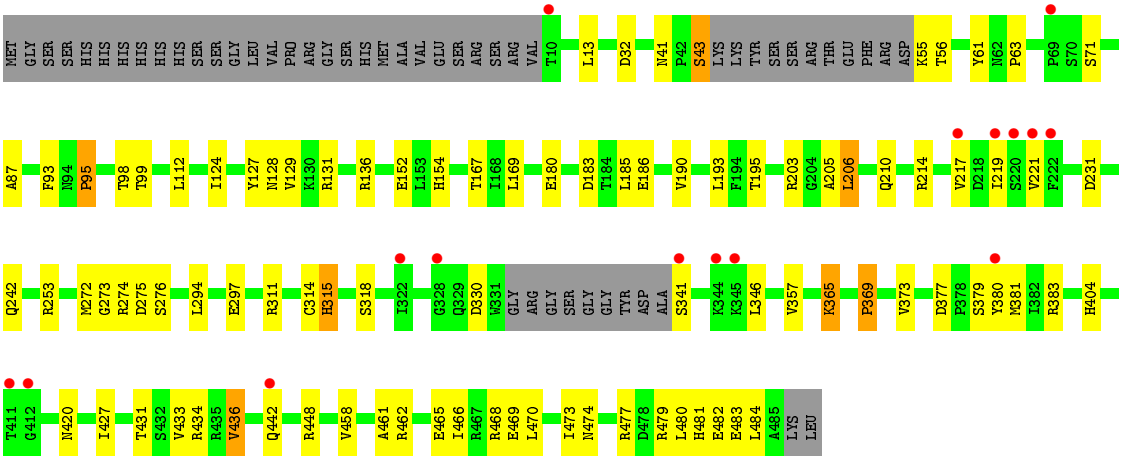
Chain E:





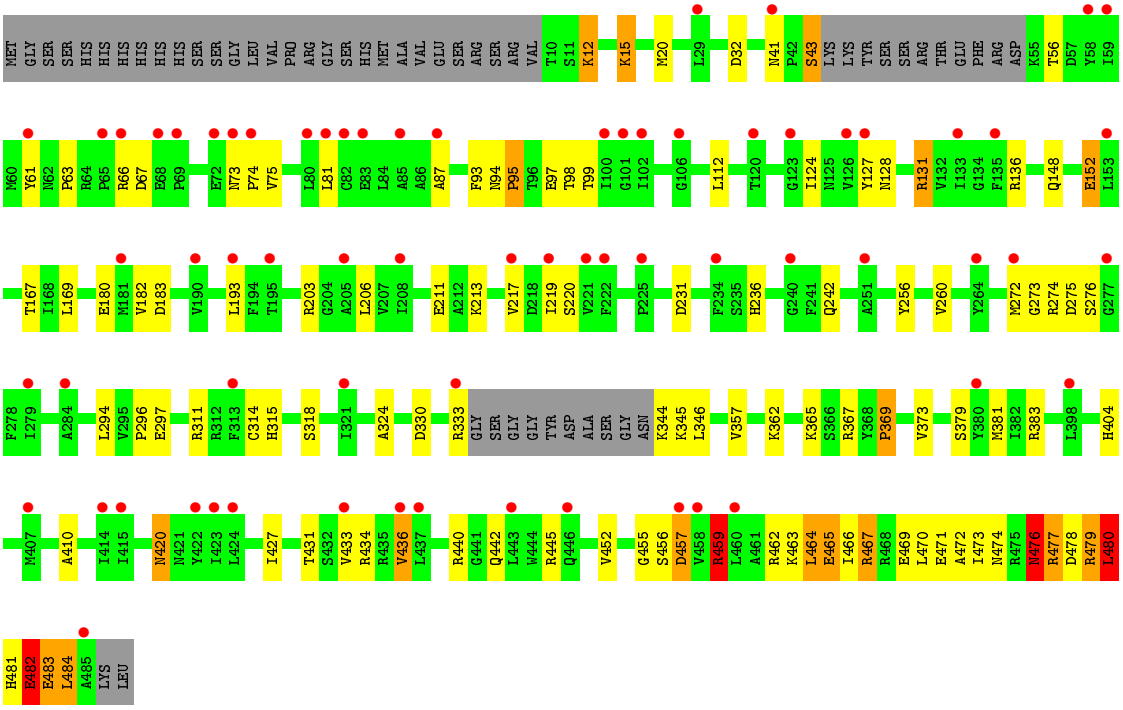
• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain F:



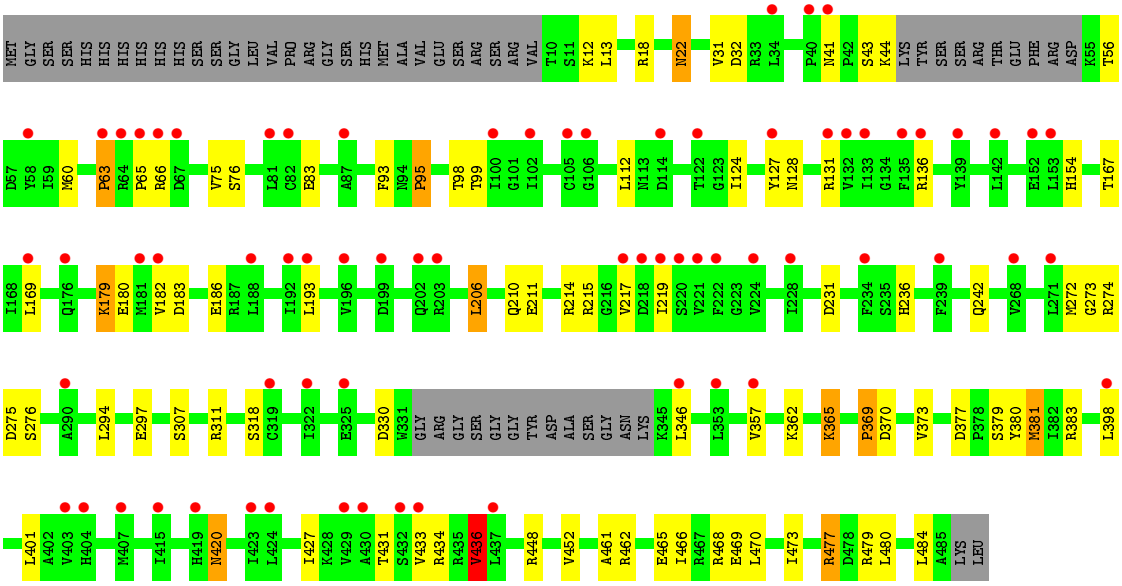
• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain G:



• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain H:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA VAL GLU SER ARG SER ARG VAL T10 S11 K12 L13 R18 N22 V31 D32 R33 L34 P40 N41 P42 S43 K44 LYS TYR SER SER ARG THR GLU PHE ARG ASP K55 T56
D57 Y58 I59 M60 P63 R64 P65 R66 D67 V75 S76 L81 C82 E83 A87 F93 N94 P95 T98 T99 I100 G101 I102 C105 G106 L112 N113 D114 T122 G123 I124 V127 N128 R131 V132 I133 G134 F135 R136 Y139 L142 E152 L153 H154 T167
I168 L169 Q176 K179 E180 M181 V182 D183 E186 R187 L188 I192 L193 V196 D199 Q202 R203 L206 Q210 E211 R214 R215 G216 V217 D218 I219 S220 V221 F222 G223 V224 I228 D231 P234 S235 H236 F239 Q242 V268 L271 M272 G273 R274
D275 S276 A290 L294 E297 S307 R311 S318 C319 I322 E325 D330 W331 GLY ARG GLY SER GLY GLY TYR ASP ALA SER GLY ASN LYS K345 L346 L353 V357 K362 K365 P369 D370 V373 D377 P378 S379 Y380 M381 I382 R383 L398
L401 A402 V403 H404 M407 Y415 H419 N420 I423 L424 I427 K428 V429 A430 T431 S432 V433 R434 R435 V436 L437 R448 V452 A461 R462 E465 I466 R467 R468 E469 L470 I473 R477 D478 R479 L480 L484 A485 LYS LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.25Å 132.51Å 282.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.67 – 3.40 96.67 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (96.67-3.40) 99.8 (96.67-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.8.0241	Depositor
R, R_{free}	0.250 , 0.267 0.245 , 0.262	Depositor DCC
R_{free} test set	2969 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	108.7	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28255	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, GOL, JJ8

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	0.72	0/3545	0.85	2/4798 (0.0%)
1	B	0.73	0/3598	0.83	2/4869 (0.0%)
1	C	0.74	0/3611	0.89	4/4885 (0.1%)
1	D	0.72	0/3551	0.81	0/4806
1	E	0.74	0/3577	0.85	0/4839
1	F	0.73	0/3572	0.84	1/4833 (0.0%)
1	G	0.73	0/3569	0.88	3/4828 (0.1%)
1	H	0.71	0/3554	0.81	0/4809
All	All	0.73	0/28577	0.85	12/38667 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	G	0	3
All	All	0	7

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	199	ASP	CB-CA-C	10.89	132.18	110.40
1	G	32	ASP	CB-CA-C	8.20	126.80	110.40
1	A	381	MET	CB-CG-SD	6.38	131.53	112.40
1	B	10	THR	CB-CA-C	6.15	128.21	111.60
1	G	476	ASN	CB-CA-C	5.96	122.32	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	315	HIS	CA-CB-CG	-5.83	103.68	113.60
1	F	315	HIS	CA-CB-CG	-5.75	103.83	113.60
1	A	363	ALA	N-CA-C	-5.61	95.84	111.00
1	C	311	ARG	CG-CD-NE	5.56	123.47	111.80
1	C	456	SER	CA-C-O	-5.30	108.96	120.10
1	C	469	GLU	CB-CA-C	5.15	120.69	110.40
1	G	465	GLU	CB-CA-C	5.10	120.59	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	LEU	Peptide
1	A	43	SER	Peptide
1	C	344	LYS	Peptide
1	C	456	SER	Mainchain
1	G	344	LYS	Peptide
1	G	455	GLY	Peptide
1	G	480	LEU	Peptide

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	3487	0	3549	54	0
1	B	3539	0	3594	55	0
1	C	3552	0	3610	76	0
1	D	3493	0	3552	65	0
1	E	3519	0	3584	57	0
1	F	3514	0	3576	59	0
1	G	3511	0	3578	91	0
1	H	3496	0	3560	63	0
2	A	13	0	5	1	0
2	B	13	0	5	1	0
2	C	13	0	5	0	0
2	D	13	0	5	1	0
2	E	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	13	0	5	1	0
2	G	13	0	5	0	0
2	H	13	0	5	0	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
4	A	14	0	0	1	0
4	B	14	0	0	1	0
All	All	28255	0	28659	463	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (463) 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:G:73:ASN:ND2	1:H:76:SER:O	1.64	1.31
1:F:380:TYR:CE2	1:F:381:MET:HG2	1.80	1.17
1:G:464:LEU:O	1:G:467:ARG:HG2	1.47	1.14
1:E:468:ARG:NH2	1:F:129:VAL:O	1.81	1.13
1:A:380:TYR:CE2	1:A:381:MET:HG3	1.91	1.05
1:G:464:LEU:O	1:G:467:ARG:CG	2.11	0.99
1:F:380:TYR:CZ	1:F:381:MET:HG2	1.98	0.98
1:A:480:LEU:HD23	1:C:470:LEU:HB3	1.46	0.97
1:G:75:VAL:HG22	1:H:75:VAL:HG12	1.49	0.94
1:G:479:ARG:HG3	1:G:480:LEU:H	1.32	0.94
1:E:472:ALA:HB1	1:F:154:HIS:CD2	2.05	0.92
1:C:457:ASP:HB2	1:C:461:ALA:HB3	1.55	0.88
1:A:360:PHE:O	1:A:363:ALA:O	1.92	0.86
1:C:315:HIS:HB3	1:C:462:ARG:HH21	1.42	0.84
1:C:37:ALA:O	1:C:90:ARG:HG3	1.78	0.84
1:E:62:ASN:ND2	1:E:77:VAL:CG2	2.41	0.83
1:H:12:LYS:HG3	1:H:13:LEU:HD22	1.60	0.81
1:C:340:ALA:HB2	1:C:345:LYS:HD2	1.63	0.80
1:E:62:ASN:ND2	1:E:77:VAL:HG21	1.97	0.80
1:B:477:ARG:HH12	1:D:477:ARG:CD	1.96	0.79
1:F:479:ARG:HA	1:F:482:GLU:HG3	1.65	0.78
1:C:37:ALA:O	1:C:90:ARG:CG	2.31	0.78
1:F:311:ARG:HD2	1:F:458:VAL:HG21	1.64	0.77
1:C:12:LYS:HG3	1:C:13:LEU:HD22	1.68	0.76
1:D:15:LYS:HD2	1:D:15:LYS:N	2.01	0.76
1:A:15:LYS:HD3	1:A:15:LYS:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:362:LYS:O	1:G:365:LYS:HG3	1.88	0.73
1:H:41:ASN:CG	1:H:43:SER:HG	1.92	0.73
1:E:471:GLU:O	1:E:474:ASN:OD1	2.08	0.72
1:A:475:ARG:HD3	1:B:152:GLU:HG3	1.71	0.72
1:C:471:GLU:O	1:C:474:ASN:OD1	2.07	0.72
1:C:206:LEU:HD22	1:C:210:GLN:HE21	1.54	0.72
1:F:474:ASN:OD1	1:H:477:ARG:NE	2.21	0.72
1:G:131:ARG:NH2	1:G:152:GLU:OE2	2.23	0.71
1:G:464:LEU:O	1:G:467:ARG:NH1	2.23	0.70
1:G:471:GLU:O	1:G:474:ASN:OD1	2.09	0.70
1:D:152:GLU:O	1:D:157:ARG:NH1	2.25	0.69
1:C:315:HIS:HB3	1:C:462:ARG:NH2	2.07	0.69
1:F:274:ARG:HD2	1:F:346:LEU:HD11	1.74	0.69
1:C:468:ARG:N	1:C:471:GLU:OE1	2.26	0.68
1:A:474:ASN:OD1	1:C:477:ARG:NH1	2.27	0.68
1:F:131:ARG:NH2	1:F:152:GLU:OE2	2.24	0.68
1:F:206:LEU:HD22	1:F:210:GLN:HE21	1.60	0.67
1:H:22:ASN:O	1:H:22:ASN:ND2	2.27	0.67
1:B:206:LEU:HD22	1:B:210:GLN:HE21	1.59	0.67
1:G:456:SER:HB2	1:G:459:ARG:HE	1.60	0.67
1:C:22:ASN:O	1:C:22:ASN:ND2	2.27	0.67
1:G:236:HIS:HB3	1:H:420:ASN:HD21	1.59	0.66
1:D:93:PHE:HB3	1:D:98:THR:HG21	1.78	0.66
1:H:179:LYS:HG2	1:H:215:ARG:HH21	1.59	0.66
1:C:231:ASP:HB3	1:C:276:SER:HB3	1.78	0.66
1:H:93:PHE:HB3	1:H:98:THR:HG21	1.77	0.66
1:F:380:TYR:CZ	1:F:381:MET:CG	2.75	0.66
1:D:231:ASP:HB3	1:D:276:SER:HB3	1.78	0.65
1:B:131:ARG:NH2	1:B:152:GLU:OE2	2.26	0.65
1:D:99:THR:HG23	1:D:131:ARG:HG3	1.78	0.65
1:E:470:LEU:O	1:E:473:ILE:HG12	1.98	0.64
1:F:93:PHE:HB3	1:F:98:THR:HG21	1.80	0.64
1:C:93:PHE:HB3	1:C:98:THR:HG21	1.78	0.64
1:E:231:ASP:HB3	1:E:276:SER:HB3	1.79	0.64
1:F:480:LEU:HD23	1:H:470:LEU:HG	1.79	0.64
1:A:231:ASP:HB3	1:A:276:SER:HB3	1.79	0.64
1:B:231:ASP:HB3	1:B:276:SER:HB3	1.78	0.64
1:E:99:THR:HG23	1:E:131:ARG:HG3	1.78	0.64
1:B:93:PHE:HB3	1:B:98:THR:HG21	1.81	0.63
1:E:93:PHE:HB3	1:E:98:THR:HG21	1.79	0.63
1:F:231:ASP:HB3	1:F:276:SER:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:231:ASP:HB3	1:G:276:SER:HB3	1.78	0.63
1:C:339:ASP:CG	1:C:344:LYS:HA	2.19	0.63
1:G:93:PHE:HB3	1:G:98:THR:HG21	1.79	0.63
1:A:93:PHE:HB3	1:A:98:THR:HG21	1.80	0.62
1:D:297:GLU:HG3	1:D:436:VAL:HG22	1.81	0.62
1:F:99:THR:HG23	1:F:131:ARG:HG3	1.82	0.62
1:H:99:THR:HG23	1:H:131:ARG:HG3	1.81	0.62
1:H:31:VAL:HG22	1:H:83:GLU:OE1	1.99	0.62
1:A:206:LEU:HD22	1:A:210:GLN:HE21	1.65	0.62
1:G:315:HIS:HB3	1:G:462:ARG:NH2	2.15	0.62
1:F:380:TYR:CE2	1:F:381:MET:CG	2.71	0.62
1:G:315:HIS:HB3	1:G:462:ARG:HH21	1.64	0.61
1:G:20:MET:CE	1:G:203:ARG:HG2	2.30	0.61
1:B:466:ILE:HD12	1:D:484:LEU:CD1	2.30	0.61
1:G:315:HIS:HB3	1:G:462:ARG:HE	1.65	0.61
1:C:463:LYS:H	1:C:465:GLU:CD	2.03	0.61
1:C:297:GLU:HG3	1:C:436:VAL:HG22	1.83	0.61
1:E:206:LEU:HD22	1:E:210:GLN:HE21	1.66	0.61
1:B:99:THR:HG23	1:B:131:ARG:HG3	1.83	0.60
1:B:477:ARG:HH12	1:D:477:ARG:HD3	1.66	0.60
1:C:63:PRO:HB3	1:D:63:PRO:HB3	1.84	0.60
1:F:93:PHE:HB3	1:F:98:THR:CG2	2.32	0.60
1:H:231:ASP:HB3	1:H:276:SER:HB3	1.82	0.60
1:F:297:GLU:HG3	1:F:436:VAL:HG22	1.82	0.60
1:D:206:LEU:HD22	1:D:210:GLN:HE21	1.65	0.60
1:H:274:ARG:HG2	1:H:346:LEU:HD11	1.84	0.60
1:C:465:GLU:HG2	1:C:466:ILE:H	1.67	0.60
1:D:25:THR:OG1	1:D:27:GLU:HG2	2.02	0.59
1:G:315:HIS:HB3	1:G:462:ARG:NE	2.18	0.59
1:A:480:LEU:HD23	1:C:470:LEU:CB	2.28	0.59
1:G:440:ARG:O	1:G:440:ARG:HG3	2.01	0.59
1:F:311:ARG:HD2	1:F:458:VAL:CG2	2.32	0.59
1:A:93:PHE:HB3	1:A:98:THR:CG2	2.33	0.59
1:B:93:PHE:HB3	1:B:98:THR:CG2	2.33	0.59
1:E:93:PHE:HB3	1:E:98:THR:CG2	2.32	0.59
1:D:93:PHE:HB3	1:D:98:THR:CG2	2.32	0.59
1:G:297:GLU:HG3	1:G:436:VAL:HG22	1.83	0.59
1:A:381:MET:CE	1:D:381:MET:HG2	2.32	0.59
1:H:214:ARG:O	1:H:214:ARG:NH1	2.33	0.59
1:E:426:PRO:HB3	1:E:428:LYS:HE2	1.85	0.59
1:C:93:PHE:HB3	1:C:98:THR:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:PHE:HB3	1:H:98:THR:CG2	2.33	0.58
1:G:63:PRO:HB3	1:H:63:PRO:HB3	1.85	0.58
1:D:215:ARG:HB2	1:D:217:VAL:HG22	1.84	0.58
1:G:93:PHE:HB3	1:G:98:THR:CG2	2.33	0.58
1:B:274:ARG:HG2	1:B:346:LEU:HD11	1.86	0.58
1:B:298:ASN:ND2	3:B:502:GOL:O3	2.36	0.58
1:G:242:GLN:HE22	1:H:242:GLN:HE22	1.50	0.58
1:B:297:GLU:HG3	1:B:436:VAL:HG22	1.85	0.57
1:A:173:ARG:NH2	2:A:501:CIT:O3	2.36	0.57
1:E:297:GLU:HG3	1:E:436:VAL:HG22	1.86	0.57
1:C:420:ASN:HD21	1:D:236:HIS:HB3	1.69	0.57
1:F:466:ILE:HD12	1:H:484:LEU:CD1	2.34	0.57
1:C:468:ARG:NH1	1:D:124:ILE:HG23	2.20	0.57
1:D:179:LYS:HE2	1:D:211:GLU:OE2	2.04	0.57
1:E:62:ASN:HD22	1:E:77:VAL:CG2	2.16	0.57
1:B:480:LEU:HD23	1:D:470:LEU:HG	1.87	0.57
1:E:55:LYS:HE2	1:E:89:SER:OG	2.04	0.57
1:G:464:LEU:C	1:G:467:ARG:HG2	2.23	0.57
1:C:464:LEU:O	1:C:467:ARG:HD2	2.05	0.56
1:F:297:GLU:CG	1:F:436:VAL:HG22	2.35	0.56
1:H:31:VAL:HG23	1:H:31:VAL:O	2.04	0.56
1:A:297:GLU:HG3	1:A:436:VAL:HG22	1.86	0.56
1:C:297:GLU:CG	1:C:436:VAL:HG22	2.36	0.56
1:G:297:GLU:CG	1:G:436:VAL:HG22	2.36	0.55
1:D:179:LYS:HD3	1:D:215:ARG:HH21	1.71	0.55
1:E:242:GLN:HE22	1:F:242:GLN:HE22	1.54	0.55
1:G:456:SER:HB2	1:G:459:ARG:NE	2.20	0.55
1:A:297:GLU:CG	1:A:436:VAL:HG22	2.36	0.55
1:A:55:LYS:O	1:A:55:LYS:HG3	2.07	0.55
1:D:297:GLU:CG	1:D:436:VAL:HG22	2.36	0.55
1:C:41:ASN:OD1	1:C:43:SER:HB2	2.06	0.55
1:B:297:GLU:CG	1:B:436:VAL:HG22	2.36	0.54
1:E:297:GLU:CG	1:E:436:VAL:HG22	2.37	0.54
1:D:15:LYS:HD2	1:D:15:LYS:H	1.73	0.54
1:H:206:LEU:HD22	1:H:210:GLN:HE21	1.72	0.54
1:G:463:LYS:O	1:G:466:ILE:HG12	2.08	0.54
1:B:41:ASN:OD1	1:B:43:SER:HB2	2.08	0.54
1:F:377:ASP:OD1	1:F:379:SER:OG	2.24	0.54
1:F:41:ASN:OD1	1:F:43:SER:HB2	2.08	0.54
1:C:457:ASP:HB2	1:C:461:ALA:CB	2.35	0.54
1:G:15:LYS:HD3	1:G:15:LYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:ARG:HB2	1:H:75:VAL:HG23	1.90	0.54
1:A:481:HIS:O	1:A:484:LEU:HD13	2.08	0.53
1:G:236:HIS:HB3	1:H:420:ASN:ND2	2.23	0.53
1:D:203:ARG:HE	1:D:431:THR:HB	1.73	0.53
1:E:55:LYS:HE2	1:E:89:SER:CB	2.38	0.53
1:G:66:ARG:HG3	1:G:67:ASP:OD1	2.08	0.53
1:H:362:LYS:O	1:H:365:LYS:HG3	2.08	0.53
1:H:297:GLU:HG3	1:H:436:VAL:HG22	1.89	0.53
1:A:41:ASN:OD1	1:A:43:SER:HB2	2.09	0.52
1:B:343:ASN:ND2	2:B:501:CIT:O6	2.43	0.52
1:E:41:ASN:OD1	1:E:43:SER:HB2	2.08	0.52
1:G:236:HIS:CB	1:H:420:ASN:ND2	2.72	0.52
1:G:479:ARG:HG3	1:G:480:LEU:N	2.15	0.52
1:E:482:GLU:OE1	1:E:482:GLU:N	2.36	0.52
1:G:20:MET:HE1	1:G:203:ARG:HG2	1.91	0.52
1:A:381:MET:HE3	1:D:381:MET:HG2	1.91	0.52
1:G:41:ASN:OD1	1:G:43:SER:HB2	2.10	0.52
1:D:41:ASN:OD1	1:D:43:SER:HB2	2.09	0.51
1:H:297:GLU:CG	1:H:436:VAL:HG22	2.40	0.51
1:C:463:LYS:N	1:C:465:GLU:CD	2.64	0.51
1:G:236:HIS:CG	1:H:420:ASN:ND2	2.78	0.51
1:F:466:ILE:HD12	1:H:484:LEU:HD12	1.93	0.51
1:E:473:ILE:HD12	1:G:477:ARG:HG2	1.91	0.51
1:G:480:LEU:O	1:G:482:GLU:N	2.44	0.51
1:B:55:LYS:O	1:B:55:LYS:HG2	2.11	0.51
1:G:74:PRO:HG2	1:H:60:MET:HG2	1.93	0.51
1:G:81:LEU:HD22	1:H:65:PRO:HG3	1.93	0.51
1:B:484:LEU:CD1	1:D:466:ILE:HD12	2.41	0.51
2:F:501:CIT:O3	2:F:501:CIT:O7	2.29	0.51
1:C:182:VAL:HG21	1:C:211:GLU:HG3	1.93	0.51
1:B:466:ILE:HD12	1:D:484:LEU:HD11	1.92	0.50
1:G:236:HIS:CB	1:H:420:ASN:HD21	2.24	0.50
1:C:420:ASN:ND2	1:D:236:HIS:CG	2.80	0.50
1:C:470:LEU:HG	1:C:471:GLU:OE1	2.11	0.50
1:C:217:VAL:HG12	1:C:219:ILE:HG13	1.94	0.50
1:G:75:VAL:HG22	1:H:75:VAL:CG1	2.30	0.50
1:G:379:SER:O	1:G:383:ARG:HG3	2.12	0.50
1:A:131:ARG:HG2	1:A:132:VAL:N	2.27	0.50
1:F:217:VAL:HG12	1:F:219:ILE:HG13	1.94	0.50
1:C:340:ALA:CB	1:C:345:LYS:HD2	2.39	0.50
1:F:379:SER:O	1:F:383:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ASN:HD21	1:D:236:HIS:CB	2.25	0.49
1:E:468:ARG:HD3	1:F:124:ILE:HD13	1.92	0.49
1:D:203:ARG:HG3	1:D:431:THR:HG21	1.93	0.49
1:E:379:SER:O	1:E:383:ARG:HG3	2.12	0.49
1:G:217:VAL:HG12	1:G:219:ILE:HG13	1.95	0.49
1:C:379:SER:O	1:C:383:ARG:HG3	2.12	0.49
1:C:464:LEU:O	1:C:467:ARG:HG3	2.13	0.49
1:G:367:ARG:HD2	1:G:367:ARG:O	2.12	0.49
1:G:442:GLN:HG3	1:H:401:LEU:HD21	1.93	0.49
1:B:338:TYR:HA	1:B:345:LYS:HB2	1.94	0.49
1:E:63:PRO:HB3	1:F:63:PRO:HB3	1.94	0.49
1:G:182:VAL:HG21	1:G:211:GLU:HG3	1.95	0.49
1:A:131:ARG:HG3	1:A:152:GLU:OE1	2.12	0.49
1:A:217:VAL:HG12	1:A:219:ILE:HG13	1.94	0.49
1:C:95:PRO:HB3	1:C:127:TYR:O	2.12	0.49
1:C:339:ASP:OD1	1:C:344:LYS:HA	2.12	0.49
1:E:95:PRO:HB3	1:E:127:TYR:O	2.13	0.49
1:E:217:VAL:HG12	1:E:219:ILE:HG13	1.93	0.49
1:G:203:ARG:HG3	1:G:431:THR:HG21	1.94	0.49
1:H:31:VAL:O	1:H:31:VAL:CG2	2.59	0.49
1:A:18:ARG:O	1:A:18:ARG:CG	2.61	0.49
1:A:275:ASP:OD2	4:A:503:JJ8:N12	2.45	0.49
1:C:177:ASP:OD1	1:C:179:LYS:HG2	2.12	0.49
1:G:459:ARG:HD2	1:G:462:ARG:HB3	1.94	0.49
1:B:162:HIS:NE2	1:B:163:HIS:CE1	2.81	0.49
1:H:217:VAL:HG12	1:H:219:ILE:HG13	1.94	0.49
1:D:379:SER:O	1:D:383:ARG:HG3	2.13	0.49
1:F:481:HIS:O	1:F:484:LEU:HD22	2.12	0.48
1:H:379:SER:O	1:H:383:ARG:HG3	2.13	0.48
1:A:95:PRO:HB3	1:A:127:TYR:O	2.13	0.48
1:A:470:LEU:HG	1:C:480:LEU:HD23	1.95	0.48
1:B:379:SER:O	1:B:383:ARG:HG3	2.13	0.48
1:G:95:PRO:HB3	1:G:127:TYR:O	2.13	0.48
1:G:315:HIS:HB3	1:G:462:ARG:CZ	2.43	0.48
1:F:95:PRO:HB3	1:F:127:TYR:O	2.14	0.48
1:D:186:GLU:CD	1:D:217:VAL:HG11	2.33	0.48
1:A:182:VAL:HG21	1:A:211:GLU:HG3	1.95	0.48
1:B:95:PRO:HB3	1:B:127:TYR:O	2.13	0.48
1:B:484:LEU:HD12	1:D:466:ILE:HD12	1.94	0.48
1:E:155:ARG:HH12	1:F:465:GLU:HA	1.78	0.48
1:C:462:ARG:HA	1:C:465:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:PRO:HB3	1:D:127:TYR:O	2.14	0.48
1:H:95:PRO:HB3	1:H:127:TYR:O	2.13	0.48
1:B:217:VAL:HG12	1:B:219:ILE:HG13	1.96	0.48
1:E:463:LYS:HD2	1:G:483:GLU:HG3	1.96	0.48
1:D:15:LYS:N	1:D:15:LYS:CD	2.75	0.48
1:C:27:GLU:OE1	1:C:27:GLU:HA	2.14	0.47
1:B:275:ASP:HB3	1:B:434:ARG:NH1	2.29	0.47
1:H:275:ASP:HB3	1:H:434:ARG:NH1	2.29	0.47
1:A:275:ASP:HB3	1:A:434:ARG:NH1	2.30	0.47
1:D:124:ILE:O	1:D:128:ASN:HA	2.15	0.47
1:D:182:VAL:HG21	1:D:211:GLU:HG3	1.95	0.47
1:E:474:ASN:O	1:E:476:ASN:OD1	2.32	0.47
1:G:99:THR:HG23	1:G:131:ARG:CD	2.44	0.47
1:G:464:LEU:O	1:G:467:ARG:CD	2.60	0.47
1:A:124:ILE:O	1:A:128:ASN:HA	2.15	0.47
1:E:275:ASP:HB3	1:E:434:ARG:NH1	2.29	0.47
1:F:124:ILE:O	1:F:128:ASN:HA	2.15	0.47
1:A:461:ALA:O	1:A:465:GLU:HG3	2.13	0.47
1:C:177:ASP:CG	1:C:179:LYS:HG2	2.34	0.47
1:G:476:ASN:O	1:G:478:ASP:O	2.32	0.47
1:B:182:VAL:HG21	1:B:211:GLU:HG3	1.96	0.47
1:D:275:ASP:HB3	1:D:434:ARG:NH1	2.30	0.47
1:E:352:ILE:O	1:E:355:GLU:HG2	2.14	0.47
1:F:203:ARG:HD3	1:F:431:THR:HB	1.96	0.47
1:G:124:ILE:O	1:G:128:ASN:HA	2.14	0.47
1:G:478:ASP:O	1:G:479:ARG:HB2	2.15	0.47
1:B:339:ASP:HA	1:B:344:LYS:HA	1.96	0.47
1:B:477:ARG:HH22	1:D:477:ARG:HE	1.60	0.47
1:C:10:THR:HG23	1:C:13:LEU:O	2.15	0.47
1:C:179:LYS:HG3	1:C:180:GLU:N	2.29	0.47
1:C:275:ASP:HB3	1:C:434:ARG:NH1	2.30	0.47
1:C:152:GLU:CD	1:D:475:ARG:HD3	2.35	0.47
1:H:461:ALA:O	1:H:465:GLU:HG3	2.15	0.47
1:C:124:ILE:O	1:C:128:ASN:HA	2.15	0.47
1:F:461:ALA:O	1:F:465:GLU:HG3	2.15	0.47
1:B:124:ILE:O	1:B:128:ASN:HA	2.15	0.46
1:E:124:ILE:O	1:E:128:ASN:HA	2.16	0.46
1:G:275:ASP:HB3	1:G:434:ARG:NH1	2.30	0.46
1:G:470:LEU:HA	1:G:473:ILE:HG12	1.97	0.46
1:F:427:ILE:O	1:F:431:THR:HG23	2.16	0.46
1:H:182:VAL:HG21	1:H:211:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ASP:OD1	1:B:330:ASP:N	2.49	0.46
1:C:152:GLU:HG3	1:D:475:ARG:CD	2.46	0.46
1:G:472:ALA:HB1	1:H:154:HIS:CG	2.50	0.46
1:H:112:LEU:HD12	1:H:112:LEU:HA	1.84	0.46
1:B:272:MET:SD	1:B:383:ARG:NH1	2.89	0.46
1:G:445:ARG:NH1	1:H:44:LYS:HG2	2.31	0.46
1:G:482:GLU:OE1	1:G:484:LEU:HD12	2.14	0.46
1:A:152:GLU:OE1	1:B:475:ARG:NH1	2.48	0.46
1:B:466:ILE:HD12	1:D:484:LEU:HD12	1.98	0.46
1:A:15:LYS:HD3	1:A:15:LYS:H	1.81	0.46
1:A:63:PRO:HB3	1:B:63:PRO:HB3	1.98	0.46
1:C:470:LEU:HD23	1:C:470:LEU:H	1.80	0.46
1:D:427:ILE:O	1:D:431:THR:HG23	2.16	0.46
1:E:182:VAL:HG21	1:E:211:GLU:HG3	1.97	0.46
1:G:20:MET:HE3	1:G:203:ARG:HG2	1.98	0.46
1:H:124:ILE:O	1:H:128:ASN:HA	2.15	0.46
1:D:461:ALA:O	1:D:465:GLU:HG3	2.16	0.45
1:E:66:ARG:HG3	1:E:77:VAL:HA	1.98	0.45
1:E:461:ALA:O	1:E:465:GLU:HG3	2.15	0.45
1:F:275:ASP:HB3	1:F:434:ARG:NH1	2.31	0.45
1:A:380:TYR:HE2	1:A:381:MET:HG3	1.70	0.45
1:A:427:ILE:O	1:A:431:THR:HG23	2.16	0.45
1:B:427:ILE:O	1:B:431:THR:HG23	2.16	0.45
1:B:461:ALA:O	1:B:465:GLU:HG3	2.16	0.45
1:E:469:GLU:O	1:E:473:ILE:HG23	2.17	0.45
1:D:470:LEU:HA	1:D:473:ILE:HG12	1.97	0.45
1:H:470:LEU:HA	1:H:473:ILE:HG12	1.98	0.45
1:A:18:ARG:O	1:A:18:ARG:HG3	2.17	0.45
1:B:476:ASN:HA	1:B:479:ARG:NH1	2.31	0.45
1:E:330:ASP:OD1	1:E:330:ASP:N	2.50	0.45
1:H:462:ARG:O	1:H:466:ILE:HG12	2.17	0.45
1:E:55:LYS:HE2	1:E:89:SER:HB3	1.97	0.45
1:A:131:ARG:HD2	1:A:133:ILE:HG13	1.99	0.45
1:C:462:ARG:CG	1:C:465:GLU:OE2	2.65	0.45
1:G:99:THR:HG23	1:G:131:ARG:HD3	1.98	0.45
1:H:365:LYS:O	1:H:369:PRO:HA	2.17	0.45
1:G:420:ASN:ND2	1:H:236:HIS:HB3	2.32	0.44
1:G:427:ILE:O	1:G:431:THR:HG23	2.18	0.44
1:H:31:VAL:CG2	1:H:83:GLU:OE1	2.66	0.44
1:C:420:ASN:ND2	1:D:236:HIS:CB	2.79	0.44
1:E:457:ASP:OD1	1:E:457:ASP:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:330:ASP:N	1:F:330:ASP:OD1	2.50	0.44
1:G:274:ARG:HG2	1:G:346:LEU:HD11	1.99	0.44
1:H:427:ILE:O	1:H:431:THR:HG23	2.18	0.44
1:A:330:ASP:N	1:A:330:ASP:OD1	2.50	0.44
1:D:15:LYS:H	1:D:15:LYS:CD	2.30	0.44
1:H:469:GLU:O	1:H:473:ILE:HG23	2.18	0.44
1:C:330:ASP:OD1	1:C:330:ASP:N	2.51	0.44
1:D:469:GLU:O	1:D:473:ILE:HG23	2.17	0.44
1:C:365:LYS:O	1:C:369:PRO:HA	2.18	0.44
1:D:480:LEU:O	1:D:484:LEU:HD13	2.17	0.44
1:E:186:GLU:OE2	1:E:217:VAL:HG21	2.18	0.44
1:E:462:ARG:O	1:E:466:ILE:HG12	2.17	0.44
1:B:462:ARG:O	1:B:466:ILE:HG13	2.17	0.44
1:D:365:LYS:O	1:D:369:PRO:HA	2.18	0.44
2:D:501:CIT:O1	2:D:501:CIT:C6	2.66	0.44
1:F:470:LEU:HA	1:F:473:ILE:HG12	1.99	0.44
1:G:330:ASP:OD1	1:G:330:ASP:N	2.50	0.44
1:E:365:LYS:O	1:E:369:PRO:HA	2.17	0.44
1:H:214:ARG:HD2	1:H:214:ARG:HA	1.73	0.44
1:A:420:ASN:HD21	1:B:236:HIS:HB3	1.83	0.43
1:C:462:ARG:HG3	1:C:465:GLU:OE2	2.18	0.43
1:F:365:LYS:O	1:F:369:PRO:HA	2.18	0.43
1:F:462:ARG:O	1:F:466:ILE:HG12	2.18	0.43
1:D:462:ARG:O	1:D:466:ILE:HG12	2.18	0.43
1:B:136:ARG:HA	1:B:169:LEU:O	2.18	0.43
1:D:136:ARG:HA	1:D:169:LEU:O	2.19	0.43
1:H:330:ASP:OD1	1:H:330:ASP:N	2.50	0.43
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.84	0.43
1:B:357:VAL:HG12	1:B:373:VAL:HG21	2.01	0.43
1:C:469:GLU:O	1:C:473:ILE:HG23	2.18	0.43
1:A:186:GLU:OE2	1:A:217:VAL:HG21	2.19	0.43
1:A:462:ARG:O	1:A:466:ILE:HG12	2.17	0.43
1:E:272:MET:HB2	1:E:279:ILE:HD12	2.00	0.43
1:F:470:LEU:HG	1:H:480:LEU:HD23	2.00	0.43
1:A:87:ALA:HA	1:A:404:HIS:HB3	2.00	0.43
1:C:87:ALA:HA	1:C:404:HIS:HB3	2.00	0.43
1:E:474:ASN:O	1:E:476:ASN:N	2.52	0.43
1:F:469:GLU:O	1:F:473:ILE:HG23	2.19	0.43
1:G:365:LYS:O	1:G:369:PRO:HA	2.19	0.43
1:G:463:LYS:HD3	1:G:463:LYS:N	2.33	0.43
1:C:214:ARG:CZ	1:C:214:ARG:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ASP:N	1:D:330:ASP:OD1	2.50	0.43
1:G:136:ARG:HA	1:G:169:LEU:O	2.19	0.43
1:B:365:LYS:O	1:B:369:PRO:HA	2.18	0.43
1:B:469:GLU:O	1:B:473:ILE:HG23	2.18	0.43
1:A:365:LYS:O	1:A:369:PRO:HA	2.18	0.42
1:C:442:GLN:HG3	1:D:401:LEU:HD21	2.01	0.42
1:F:136:ARG:HA	1:F:169:LEU:O	2.19	0.42
1:F:357:VAL:HG12	1:F:373:VAL:HG21	2.00	0.42
1:C:13:LEU:HD21	1:C:61:TYR:OH	2.19	0.42
1:G:12:LYS:HE3	1:G:61:TYR:OH	2.19	0.42
1:G:464:LEU:HD23	1:G:467:ARG:HB3	2.01	0.42
1:G:469:GLU:O	1:G:473:ILE:HG23	2.19	0.42
1:B:256:TYR:CE1	1:B:260:VAL:HG21	2.54	0.42
1:C:427:ILE:O	1:C:431:THR:HG23	2.19	0.42
1:F:112:LEU:HD12	1:F:112:LEU:HA	1.83	0.42
1:F:186:GLU:OE2	1:F:217:VAL:HG21	2.19	0.42
1:G:420:ASN:HD21	1:H:236:HIS:HB3	1.84	0.42
1:H:186:GLU:OE2	1:H:217:VAL:HG21	2.19	0.42
1:E:131:ARG:NH1	1:E:152:GLU:OE2	2.52	0.42
1:G:94:ASN:HB3	1:G:97:GLU:OE1	2.19	0.42
1:G:220:SER:OG	1:G:410:ALA:O	2.34	0.42
1:G:311:ARG:O	1:G:314:CYS:HB2	2.20	0.42
1:G:362:LYS:O	1:G:365:LYS:CG	2.63	0.42
1:A:180:GLU:O	1:A:183:ASP:HB2	2.19	0.42
1:B:186:GLU:OE2	1:B:217:VAL:HG21	2.19	0.42
1:E:426:PRO:CB	1:E:428:LYS:HE2	2.49	0.42
1:G:456:SER:CB	1:G:459:ARG:HE	2.29	0.42
1:A:272:MET:HB2	1:A:279:ILE:HD12	2.01	0.42
1:C:464:LEU:O	1:C:467:ARG:CD	2.67	0.42
1:C:274:ARG:NH2	1:C:343:ASN:HB3	2.34	0.42
1:E:136:ARG:HA	1:E:169:LEU:O	2.19	0.42
1:H:136:ARG:HA	1:H:169:LEU:O	2.19	0.42
1:A:136:ARG:HA	1:A:169:LEU:O	2.19	0.42
1:F:13:LEU:HD21	1:F:61:TYR:OH	2.20	0.42
1:G:464:LEU:O	1:G:467:ARG:CZ	2.67	0.42
1:H:398:LEU:HD23	1:H:398:LEU:HA	1.93	0.42
1:G:456:SER:O	1:G:457:ASP:O	2.38	0.42
1:G:476:ASN:HB3	1:G:479:ARG:NH1	2.35	0.42
1:D:212:ALA:O	1:D:217:VAL:HG23	2.20	0.42
1:E:357:VAL:HG12	1:E:373:VAL:HG21	2.02	0.42
1:H:377:ASP:OD1	1:H:379:SER:OG	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLU:O	1:B:183:ASP:HB2	2.20	0.41
1:C:272:MET:HB2	1:C:279:ILE:HD12	2.02	0.41
1:E:180:GLU:O	1:E:183:ASP:HB2	2.20	0.41
1:E:380:TYR:CG	1:E:381:MET:N	2.88	0.41
1:F:87:ALA:HA	1:F:404:HIS:HB3	2.02	0.41
1:B:339:ASP:H	1:B:345:LYS:H	1.68	0.41
1:C:136:ARG:HA	1:C:169:LEU:O	2.18	0.41
1:C:206:LEU:HD23	1:C:206:LEU:HA	1.92	0.41
1:E:311:ARG:O	1:E:314:CYS:HB2	2.20	0.41
1:F:203:ARG:HD3	1:F:431:THR:CB	2.50	0.41
1:F:479:ARG:CA	1:F:482:GLU:HG3	2.42	0.41
1:C:468:ARG:HH12	1:D:124:ILE:HG23	1.86	0.41
1:G:357:VAL:HG12	1:G:373:VAL:HG21	2.02	0.41
1:C:339:ASP:HA	1:C:344:LYS:O	2.19	0.41
1:F:311:ARG:HA	1:F:311:ARG:HD3	1.96	0.41
1:G:180:GLU:O	1:G:183:ASP:HB2	2.19	0.41
1:G:473:ILE:HA	1:G:476:ASN:OD1	2.20	0.41
1:A:108:ILE:HD12	1:A:384:ALA:HA	2.01	0.41
1:D:357:VAL:HG12	1:D:373:VAL:HG21	2.02	0.41
1:A:214:ARG:HA	1:A:214:ARG:HD3	1.88	0.41
1:C:205:ALA:HB1	1:C:221:VAL:CG1	2.51	0.41
1:C:475:ARG:HA	1:C:475:ARG:HD3	1.97	0.41
1:D:180:GLU:O	1:D:183:ASP:HB2	2.20	0.41
1:E:473:ILE:O	1:E:476:ASN:OD1	2.37	0.41
1:F:180:GLU:O	1:F:183:ASP:HB2	2.20	0.41
1:F:205:ALA:HB1	1:F:221:VAL:CG1	2.51	0.41
1:C:180:GLU:O	1:C:183:ASP:HB2	2.20	0.41
1:G:87:ALA:HA	1:G:404:HIS:HB3	2.02	0.41
1:H:357:VAL:HG12	1:H:373:VAL:HG21	2.01	0.41
1:D:87:ALA:HA	1:D:404:HIS:HB3	2.02	0.41
1:D:212:ALA:O	1:D:217:VAL:CG2	2.69	0.41
1:F:311:ARG:O	1:F:314:CYS:HB2	2.21	0.41
1:G:15:LYS:N	1:G:15:LYS:CD	2.84	0.41
1:A:311:ARG:O	1:A:314:CYS:HB2	2.20	0.41
1:B:470:LEU:HA	1:B:473:ILE:HG12	2.01	0.41
1:D:311:ARG:O	1:D:314:CYS:HB2	2.21	0.41
1:E:256:TYR:CE1	1:E:260:VAL:HG21	2.56	0.41
1:E:427:ILE:O	1:E:431:THR:HG23	2.20	0.41
1:G:99:THR:HG23	1:G:131:ARG:HG3	2.02	0.41
1:H:180:GLU:O	1:H:183:ASP:HB2	2.20	0.41
1:C:37:ALA:O	1:C:90:ARG:HG2	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:TYR:CG	1:A:381:MET:N	2.89	0.40
1:B:162:HIS:CE1	1:B:163:HIS:CE1	3.09	0.40
1:F:195:THR:HG21	1:F:205:ALA:HB2	2.03	0.40
1:H:380:TYR:CG	1:H:381:MET:N	2.88	0.40
1:B:398:LEU:HD23	1:B:398:LEU:HA	1.93	0.40
1:C:311:ARG:O	1:C:314:CYS:HB2	2.20	0.40
1:D:154:HIS:CE1	1:D:157:ARG:HB2	2.56	0.40
1:D:185:LEU:HD22	1:D:190:VAL:HG11	2.03	0.40
1:F:185:LEU:HD22	1:F:190:VAL:HG11	2.04	0.40
1:A:256:TYR:CE1	1:A:260:VAL:HG21	2.55	0.40
1:C:256:TYR:CE1	1:C:260:VAL:HG21	2.56	0.40
1:A:205:ALA:HB1	1:A:221:VAL:CG1	2.52	0.40
1:B:296:PRO:HD3	1:B:324:ALA:HB3	2.03	0.40
1:B:470:LEU:HG	1:D:480:LEU:HD23	2.02	0.40
1:E:112:LEU:HD12	1:E:112:LEU:HA	1.83	0.40
1:E:332:GLY:O	1:E:333:ARG:HB2	2.22	0.40
1:F:315:HIS:ND1	1:F:458:VAL:HG12	2.37	0.40
1:F:380:TYR:CG	1:F:381:MET:N	2.89	0.40
1:G:112:LEU:HD12	1:G:112:LEU:HA	1.84	0.40
1:G:296:PRO:HD3	1:G:324:ALA:HB3	2.03	0.40
1:A:357:VAL:HG12	1:A:373:VAL:HG21	2.04	0.40
1:B:87:ALA:HA	1:B:404:HIS:HB3	2.03	0.40
4:B:503:JJ8:C6	4:B:503:JJ8:C14	2.98	0.40
1:C:195:THR:HG21	1:C:205:ALA:HB2	2.03	0.40
1:D:13:LEU:HD21	1:D:61:TYR:OH	2.22	0.40
1:E:22:ASN:HD22	1:E:22:ASN:C	2.24	0.40
1:G:256:TYR:CE1	1:G:260:VAL:HG21	2.57	0.40

There are no symmetry-related clashes.

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	446/507 (88%)	404 (91%)	38 (8%)	4 (1%)	17 49
1	B	453/507 (89%)	412 (91%)	38 (8%)	3 (1%)	22 55
1	C	455/507 (90%)	402 (88%)	44 (10%)	9 (2%)	7 30
1	D	447/507 (88%)	408 (91%)	35 (8%)	4 (1%)	17 49
1	E	450/507 (89%)	407 (90%)	39 (9%)	4 (1%)	17 49
1	F	450/507 (89%)	411 (91%)	35 (8%)	4 (1%)	17 49
1	G	449/507 (89%)	403 (90%)	35 (8%)	11 (2%)	6 28
1	H	447/507 (88%)	407 (91%)	35 (8%)	5 (1%)	14 44
All	All	3597/4056 (89%)	3254 (90%)	299 (8%)	44 (1%)	13 41

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	PRO
1	B	369	PRO
1	C	345	LYS
1	C	369	PRO
1	C	484	LEU
1	D	369	PRO
1	E	369	PRO
1	E	483	GLU
1	F	369	PRO
1	G	369	PRO
1	G	457	ASP
1	G	484	LEU
1	H	369	PRO
1	A	483	GLU
1	C	463	LYS
1	C	466	ILE
1	E	474	ASN
1	G	12	LYS
1	G	459	ARG
1	G	481	HIS
1	C	459	ARG
1	C	468	ARG
1	G	479	ARG
1	F	483	GLU
1	G	482	GLU
1	B	95	PRO
1	D	452	VAL

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Mol	Chain	Res	Type
1	E	95	PRO
1	G	452	VAL
1	A	95	PRO
1	A	273	GLY
1	B	273	GLY
1	C	273	GLY
1	D	95	PRO
1	F	95	PRO
1	G	95	PRO
1	H	95	PRO
1	H	273	GLY
1	H	436	VAL
1	C	95	PRO
1	D	273	GLY
1	F	273	GLY
1	G	273	GLY
1	H	452	VAL

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	377/422 (89%)	345 (92%)	32 (8%)	10	35
1	B	382/422 (90%)	351 (92%)	31 (8%)	11	38
1	C	383/422 (91%)	353 (92%)	30 (8%)	12	39
1	D	377/422 (89%)	349 (93%)	28 (7%)	13	42
1	E	380/422 (90%)	346 (91%)	34 (9%)	9	33
1	F	380/422 (90%)	358 (94%)	22 (6%)	20	50
1	G	379/422 (90%)	351 (93%)	28 (7%)	13	42
1	H	378/422 (90%)	354 (94%)	24 (6%)	18	47
All	All	3036/3376 (90%)	2807 (92%)	229 (8%)	13	41

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	12	LYS
1	A	15	LYS
1	A	17	HIS
1	A	18	ARG
1	A	30	LYS
1	A	43	SER
1	A	55	LYS
1	A	56	THR
1	A	63	PRO
1	A	131	ARG
1	A	167	THR
1	A	193	LEU
1	A	206	LEU
1	A	213	LYS
1	A	214	ARG
1	A	272	MET
1	A	294	LEU
1	A	303	GLN
1	A	311	ARG
1	A	315	HIS
1	A	318	SER
1	A	365	LYS
1	A	366	SER
1	A	420	ASN
1	A	433	VAL
1	A	436	VAL
1	A	448	ARG
1	A	456	SER
1	A	460	LEU
1	A	467	ARG
1	A	479	ARG
1	B	10	THR
1	B	12	LYS
1	B	27	GLU
1	B	32	ASP
1	B	43	SER
1	B	55	LYS
1	B	56	THR
1	B	71	SER
1	B	148	GLN
1	B	167	THR
1	B	193	LEU

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Mol	Chain	Res	Type
1	B	206	LEU
1	B	272	MET
1	B	274	ARG
1	B	294	LEU
1	B	307	SER
1	B	311	ARG
1	B	318	SER
1	B	338	TYR
1	B	344	LYS
1	B	362	LYS
1	B	381	MET
1	B	420	ASN
1	B	433	VAL
1	B	436	VAL
1	B	448	ARG
1	B	460	LEU
1	B	468	ARG
1	B	475	ARG
1	B	477	ARG
1	B	479	ARG
1	C	12	LYS
1	C	22	ASN
1	C	43	SER
1	C	55	LYS
1	C	56	THR
1	C	63	PRO
1	C	68	GLU
1	C	144	LYS
1	C	148	GLN
1	C	167	THR
1	C	193	LEU
1	C	206	LEU
1	C	253	ARG
1	C	272	MET
1	C	294	LEU
1	C	310	GLU
1	C	311	ARG
1	C	318	SER
1	C	341	SER
1	C	362	LYS
1	C	366	SER
1	C	370	ASP

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Mol	Chain	Res	Type
1	C	381	MET
1	C	420	ASN
1	C	433	VAL
1	C	436	VAL
1	C	442	GLN
1	C	463	LYS
1	C	464	LEU
1	C	470	LEU
1	D	30	LYS
1	D	32	ASP
1	D	43	SER
1	D	55	LYS
1	D	56	THR
1	D	167	THR
1	D	193	LEU
1	D	206	LEU
1	D	214	ARG
1	D	217	VAL
1	D	272	MET
1	D	274	ARG
1	D	294	LEU
1	D	303	GLN
1	D	307	SER
1	D	311	ARG
1	D	318	SER
1	D	333	ARG
1	D	381	MET
1	D	383	ARG
1	D	420	ASN
1	D	433	VAL
1	D	436	VAL
1	D	445	ARG
1	D	448	ARG
1	D	456	SER
1	D	468	ARG
1	D	475	ARG
1	E	18	ARG
1	E	22	ASN
1	E	30	LYS
1	E	43	SER
1	E	56	THR
1	E	90	ARG

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Mol	Chain	Res	Type
1	E	167	THR
1	E	173	ARG
1	E	193	LEU
1	E	206	LEU
1	E	213	LYS
1	E	214	ARG
1	E	253	ARG
1	E	272	MET
1	E	294	LEU
1	E	307	SER
1	E	311	ARG
1	E	318	SER
1	E	345	LYS
1	E	362	LYS
1	E	366	SER
1	E	370	ASP
1	E	383	ARG
1	E	420	ASN
1	E	433	VAL
1	E	436	VAL
1	E	448	ARG
1	E	457	ASP
1	E	468	ARG
1	E	476	ASN
1	E	477	ARG
1	E	480	LEU
1	E	483	GLU
1	E	484	LEU
1	F	32	ASP
1	F	43	SER
1	F	55	LYS
1	F	56	THR
1	F	71	SER
1	F	167	THR
1	F	193	LEU
1	F	206	LEU
1	F	214	ARG
1	F	253	ARG
1	F	272	MET
1	F	294	LEU
1	F	318	SER
1	F	341	SER

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Mol	Chain	Res	Type
1	F	365	LYS
1	F	420	ASN
1	F	433	VAL
1	F	436	VAL
1	F	442	GLN
1	F	448	ARG
1	F	468	ARG
1	F	477	ARG
1	G	15	LYS
1	G	43	SER
1	G	56	THR
1	G	131	ARG
1	G	148	GLN
1	G	152	GLU
1	G	167	THR
1	G	193	LEU
1	G	206	LEU
1	G	213	LYS
1	G	272	MET
1	G	294	LEU
1	G	318	SER
1	G	333	ARG
1	G	345	LYS
1	G	381	MET
1	G	420	ASN
1	G	433	VAL
1	G	436	VAL
1	G	459	ARG
1	G	464	LEU
1	G	465	GLU
1	G	467	ARG
1	G	476	ASN
1	G	477	ARG
1	G	480	LEU
1	G	482	GLU
1	G	483	GLU
1	H	18	ARG
1	H	22	ASN
1	H	32	ASP
1	H	56	THR
1	H	63	PRO
1	H	167	THR

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Mol	Chain	Res	Type
1	H	179	LYS
1	H	193	LEU
1	H	206	LEU
1	H	272	MET
1	H	294	LEU
1	H	307	SER
1	H	311	ARG
1	H	318	SER
1	H	365	LYS
1	H	370	ASP
1	H	381	MET
1	H	420	ASN
1	H	433	VAL
1	H	436	VAL
1	H	448	ARG
1	H	468	ARG
1	H	477	ARG
1	H	479	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	420	ASN
1	B	94	ASN
1	B	160	ASN
1	B	163	HIS
1	B	210	GLN
1	B	298	ASN
1	B	343	ASN
1	C	148	GLN
1	C	160	ASN
1	C	210	GLN
1	C	420	ASN
1	C	481	HIS
1	D	160	ASN
1	D	210	GLN
1	D	298	ASN
1	E	17	HIS
1	E	22	ASN
1	E	210	GLN
1	E	242	GLN

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Mol	Chain	Res	Type
1	E	298	ASN
1	F	210	GLN
1	F	298	ASN
1	G	298	ASN
1	G	420	ASN
1	H	210	GLN
1	H	242	GLN
1	H	420	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 monosaccharides in this entry.

5.6 Ligand geometry

12 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	CIT	G	501	-	3,12,12	0.32	0	3,17,17	1.59	1 (33%)
2	CIT	B	501	-	3,12,12	0.62	0	3,17,17	0.81	0
3	GOL	A	502	-	5,5,5	0.09	0	5,5,5	0.27	0
4	JJ8	B	503	-	14,15,15	1.24	4 (28%)	18,20,20	0.96	0
2	CIT	D	501	-	3,12,12	0.58	0	3,17,17	1.18	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CIT	E	501	-	3,12,12	0.47	0	3,17,17	1.33	1 (33%)
3	GOL	B	502	-	5,5,5	0.11	0	5,5,5	0.31	0
2	CIT	A	501	-	3,12,12	0.73	0	3,17,17	1.37	1 (33%)
4	JJ8	A	503	-	14,15,15	1.23	3 (21%)	18,20,20	0.78	0
2	CIT	H	501	1	3,12,12	0.36	0	3,17,17	1.27	1 (33%)
2	CIT	F	501	-	3,12,12	0.46	0	3,17,17	1.50	1 (33%)
2	CIT	C	501	-	3,12,12	0.55	0	3,17,17	1.32	1 (33%)

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	CIT	G	501	-	-	6/6/16/16	-
2	CIT	B	501	-	-	2/6/16/16	-
3	GOL	A	502	-	-	0/4/4/4	-
4	JJ8	B	503	-	-	2/4/4/4	0/2/2/2
2	CIT	D	501	-	-	6/6/16/16	-
2	CIT	E	501	-	-	1/6/16/16	-
3	GOL	B	502	-	-	2/4/4/4	-
2	CIT	A	501	-	-	6/6/16/16	-
4	JJ8	A	503	-	-	2/4/4/4	0/2/2/2
2	CIT	H	501	1	-	6/6/16/16	-
2	CIT	F	501	-	-	6/6/16/16	-
2	CIT	C	501	-	-	1/6/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	JJ8	C3-CL8	2.70	1.80	1.73
4	B	503	JJ8	C9-N10	-2.37	1.44	1.49
4	B	503	JJ8	C14-N10	-2.27	1.33	1.37
4	B	503	JJ8	C4-CL7	2.26	1.79	1.73
4	A	503	JJ8	C4-CL7	2.18	1.78	1.73
4	A	503	JJ8	C14-N10	-2.17	1.33	1.37
4	B	503	JJ8	C3-CL8	2.09	1.78	1.73

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	CIT	C3-C2-C1	2.45	118.90	114.98
2	E	501	CIT	C3-C2-C1	2.31	118.68	114.98
2	C	501	CIT	C3-C2-C1	2.21	118.52	114.98
2	G	501	CIT	C3-C2-C1	2.17	118.46	114.98
2	A	501	CIT	C3-C2-C1	2.13	118.39	114.98
2	H	501	CIT	C3-C2-C1	2.11	118.37	114.98
2	D	501	CIT	C3-C2-C1	2.03	118.23	114.98

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CIT	C1-C2-C3-O7
2	A	501	CIT	C1-C2-C3-C6
2	A	501	CIT	C2-C3-C4-C5
2	A	501	CIT	C6-C3-C4-C5
2	D	501	CIT	C2-C3-C4-C5
2	D	501	CIT	C6-C3-C4-C5
2	F	501	CIT	C1-C2-C3-O7
2	F	501	CIT	C1-C2-C3-C6
2	F	501	CIT	C2-C3-C4-C5
2	F	501	CIT	C6-C3-C4-C5
2	G	501	CIT	C1-C2-C3-O7
2	G	501	CIT	C1-C2-C3-C4
2	G	501	CIT	C1-C2-C3-C6
2	G	501	CIT	C2-C3-C4-C5
2	G	501	CIT	O7-C3-C4-C5
2	G	501	CIT	C6-C3-C4-C5
2	H	501	CIT	C1-C2-C3-O7
2	H	501	CIT	C1-C2-C3-C4
2	H	501	CIT	C1-C2-C3-C6
2	A	501	CIT	C1-C2-C3-C4
2	F	501	CIT	C1-C2-C3-C4
2	D	501	CIT	O7-C3-C4-C5
2	F	501	CIT	O7-C3-C4-C5
3	B	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O2-C2-C3-O3
2	A	501	CIT	O7-C3-C4-C5
2	B	501	CIT	C1-C2-C3-O7
2	D	501	CIT	C1-C2-C3-O7
2	H	501	CIT	C2-C3-C4-C5
2	D	501	CIT	C1-C2-C3-C4
2	C	501	CIT	C1-C2-C3-O7

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Mol	Chain	Res	Type	Atoms
2	D	501	CIT	C1-C2-C3-C6
2	H	501	CIT	C6-C3-C4-C5
2	H	501	CIT	O7-C3-C4-C5
4	B	503	JJ8	C2-C1-C9-N10
4	B	503	JJ8	C6-C1-C9-N10
2	E	501	CIT	C1-C2-C3-O7
2	B	501	CIT	C1-C2-C3-C4
4	A	503	JJ8	C6-C1-C9-N10
4	A	503	JJ8	C2-C1-C9-N10

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	CIT	1	0
4	B	503	JJ8	1	0
2	D	501	CIT	1	0
3	B	502	GOL	1	0
2	A	501	CIT	1	0
4	A	503	JJ8	1	0
2	F	501	CIT	1	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

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	452/507 (89%)	0.35	7 (1%) 73 72	71, 100, 144, 171	0
1	B	459/507 (90%)	0.55	22 (4%) 30 31	77, 109, 137, 156	0
1	C	461/507 (90%)	0.56	25 (5%) 25 26	81, 114, 155, 187	0
1	D	453/507 (89%)	0.56	31 (6%) 17 19	82, 120, 156, 179	0
1	E	456/507 (89%)	0.36	12 (2%) 56 54	80, 109, 152, 204	0
1	F	456/507 (89%)	0.55	16 (3%) 44 43	75, 104, 135, 170	0
1	G	455/507 (89%)	0.86	68 (14%) 2 2	99, 137, 177, 229	0
1	H	453/507 (89%)	0.94	71 (15%) 2 2	116, 152, 188, 208	0
All	All	3645/4056 (89%)	0.59	252 (6%) 16 18	71, 117, 168, 229	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	460	LEU	8.0
1	H	219	ILE	7.2
1	G	82	CYS	7.0
1	G	72	GLU	6.3
1	E	485	ALA	5.9
1	G	81	LEU	5.6
1	H	181	MET	5.5
1	G	457	ASP	5.1
1	H	102	ILE	5.1
1	D	218	ASP	5.1
1	G	458	VAL	4.9
1	H	65	PRO	4.9
1	C	69	PRO	4.8
1	H	66	ARG	4.7
1	G	58	TYR	4.7
1	H	67	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	G	65	PRO	4.6
1	H	224	VAL	4.6
1	C	343	ASN	4.5
1	G	219	ILE	4.5
1	F	341	SER	4.4
1	H	153	LEU	4.4
1	H	217	VAL	4.4
1	C	459	ARG	4.3
1	G	422	TYR	4.3
1	G	225	PRO	4.3
1	H	132	VAL	4.2
1	G	127	TYR	4.2
1	G	153	LEU	4.1
1	H	234	PHE	4.1
1	H	152	GLU	4.1
1	G	100	ILE	4.0
1	G	414	ILE	4.0
1	H	40	PRO	3.9
1	G	221	VAL	3.9
1	H	139	TYR	3.8
1	H	100	ILE	3.8
1	G	234	PHE	3.8
1	C	71	SER	3.8
1	C	458	VAL	3.8
1	B	221	VAL	3.7
1	C	219	ILE	3.7
1	D	219	ILE	3.7
1	D	135	PHE	3.6
1	G	193	LEU	3.6
1	D	102	ILE	3.6
1	F	219	ILE	3.5
1	B	344	LYS	3.5
1	H	199	ASP	3.5
1	F	380	TYR	3.5
1	D	331	TRP	3.4
1	C	339	ASP	3.4
1	B	21	LEU	3.4
1	H	63	PRO	3.4
1	H	64	ARG	3.4
1	G	423	ILE	3.4
1	H	133	ILE	3.4
1	H	176	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	3.3
1	G	73	ASN	3.3
1	F	412	GLY	3.3
1	G	101	GLY	3.3
1	H	218	ASP	3.3
1	G	135	PHE	3.3
1	C	127	TYR	3.3
1	G	41	ASN	3.3
1	G	68	GLU	3.3
1	G	133	ILE	3.3
1	G	272	MET	3.3
1	H	419	HIS	3.3
1	D	332	GLY	3.2
1	H	407	MET	3.2
1	G	83	GLU	3.2
1	G	61	TYR	3.2
1	B	234	PHE	3.2
1	H	192	ILE	3.2
1	C	82	CYS	3.2
1	H	222	PHE	3.2
1	H	346	LEU	3.1
1	C	135	PHE	3.1
1	G	424	LEU	3.1
1	H	169	LEU	3.1
1	H	82	CYS	3.1
1	G	85	ALA	3.1
1	G	284	ALA	3.1
1	D	234	PHE	3.0
1	G	313	PHE	3.0
1	A	261	SER	3.0
1	B	222	PHE	3.0
1	H	114	ASP	3.0
1	H	81	LEU	3.0
1	B	135	PHE	3.0
1	H	403	VAL	3.0
1	H	221	VAL	2.9
1	C	70	SER	2.9
1	C	85	ALA	2.9
1	G	217	VAL	2.9
1	H	135	PHE	2.9
1	H	404	HIS	2.9
1	D	454	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	29	LEU	2.9
1	H	136	ARG	2.9
1	G	222	PHE	2.9
1	G	251	ALA	2.9
1	D	133	ILE	2.9
1	D	139	TYR	2.9
1	H	58	TYR	2.8
1	B	195	THR	2.8
1	H	357	VAL	2.8
1	G	181	MET	2.8
1	G	69	PRO	2.8
1	A	234	PHE	2.8
1	G	74	PRO	2.8
1	H	105	CYS	2.8
1	H	87	ALA	2.8
1	H	182	VAL	2.8
1	H	432	SER	2.8
1	H	268	VAL	2.8
1	G	87	ALA	2.7
1	D	228	ILE	2.7
1	E	484	LEU	2.7
1	D	174	GLY	2.7
1	G	415	ILE	2.7
1	E	111	GLY	2.7
1	B	343	ASN	2.7
1	G	120	THR	2.7
1	G	485	ALA	2.7
1	C	218	ASP	2.6
1	H	353	LEU	2.6
1	D	82	CYS	2.6
1	H	271	LEU	2.6
1	F	328	GLY	2.6
1	G	277	GLY	2.6
1	H	106	GLY	2.6
1	B	380	TYR	2.6
1	E	166	GLY	2.6
1	B	331	TRP	2.6
1	F	442	GLN	2.6
1	H	127	TYR	2.6
1	E	458	VAL	2.6
1	B	155	ARG	2.6
1	H	41	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	59	ILE	2.6
1	D	105	CYS	2.5
1	B	123	GLY	2.5
1	F	221	VAL	2.5
1	E	21	LEU	2.5
1	D	81	LEU	2.5
1	C	210	GLN	2.5
1	G	264	TYR	2.5
1	G	123	GLY	2.5
1	D	153	LEU	2.5
1	H	193	LEU	2.5
1	H	424	LEU	2.5
1	F	411	THR	2.5
1	G	433	VAL	2.5
1	G	80	LEU	2.5
1	B	10	THR	2.5
1	F	69	PRO	2.5
1	H	415	ILE	2.5
1	H	34	LEU	2.5
1	H	398	LEU	2.5
1	F	10	THR	2.5
1	A	10	THR	2.4
1	H	433	VAL	2.4
1	H	239	PHE	2.4
1	G	205	ALA	2.4
1	E	82	CYS	2.4
1	C	193	LEU	2.4
1	D	222	PHE	2.4
1	F	222	PHE	2.4
1	B	181	MET	2.4
1	D	142	LEU	2.4
1	D	333	ARG	2.4
1	D	424	LEU	2.4
1	H	437	LEU	2.4
1	G	279	ILE	2.4
1	G	106	GLY	2.4
1	C	338	TYR	2.4
1	C	272	MET	2.4
1	H	131	ARG	2.4
1	H	220	SER	2.3
1	H	203	ARG	2.3
1	G	380	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	290	ALA	2.3
1	H	423	ILE	2.3
1	B	59	ILE	2.3
1	D	346	LEU	2.3
1	G	195	THR	2.3
1	G	66	ARG	2.3
1	A	233	SER	2.3
1	H	429	VAL	2.3
1	G	321	ILE	2.3
1	C	181	MET	2.2
1	B	127	TYR	2.2
1	G	126	VAL	2.2
1	G	437	LEU	2.2
1	D	168	ILE	2.2
1	G	208	ILE	2.2
1	G	190	VAL	2.2
1	F	345	LYS	2.2
1	C	58	TYR	2.2
1	B	82	CYS	2.2
1	H	430	ALA	2.2
1	D	100	ILE	2.2
1	D	208	ILE	2.2
1	H	228	ILE	2.2
1	B	193	LEU	2.2
1	D	407	MET	2.2
1	F	344	LYS	2.2
1	D	20	MET	2.2
1	G	333	ARG	2.2
1	G	240	GLY	2.2
1	G	446	GLN	2.2
1	H	202	GLN	2.2
1	H	142	LEU	2.2
1	E	357	VAL	2.2
1	H	196	VAL	2.2
1	D	140	TRP	2.2
1	G	102	ILE	2.2
1	A	380	TYR	2.1
1	F	220	SER	2.1
1	B	166	GLY	2.1
1	D	380	TYR	2.1
1	D	272	MET	2.1
1	G	407	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	443	LEU	2.1
1	F	322	ILE	2.1
1	C	100	ILE	2.1
1	H	122	THR	2.1
1	C	110	PRO	2.1
1	E	234	PHE	2.1
1	F	217	VAL	2.1
1	C	332	GLY	2.1
1	A	185	LEU	2.1
1	G	398	LEU	2.1
1	G	460	LEU	2.1
1	E	469	GLU	2.1
1	H	325	GLU	2.1
1	C	380	TYR	2.1
1	C	217	VAL	2.1
1	B	346	LEU	2.1
1	D	108	ILE	2.1
1	H	322	ILE	2.1
1	H	319	CYS	2.0
1	B	404	HIS	2.0
1	H	188	LEU	2.0
1	G	436	VAL	2.0
1	A	74	PRO	2.0
1	E	266	VAL	2.0
1	E	228	ILE	2.0
1	D	55	LYS	2.0

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	G	501	13/13	0.73	0.25	155,155,155,155	0
2	CIT	A	501	13/13	0.76	0.23	155,155,155,155	0
2	CIT	D	501	13/13	0.77	0.24	155,155,155,155	0
2	CIT	H	501	13/13	0.78	0.27	155,155,155,155	0
2	CIT	E	501	13/13	0.79	0.18	155,155,155,155	0
2	CIT	F	501	13/13	0.79	0.36	155,155,155,155	0
4	JJ8	B	503	14/14	0.79	0.52	155,155,155,155	0
3	GOL	A	502	6/6	0.83	0.51	155,155,155,155	0
3	GOL	B	502	6/6	0.84	0.46	155,155,155,155	0
2	CIT	B	501	13/13	0.84	0.31	155,155,155,155	0
4	JJ8	A	503	14/14	0.87	0.55	155,155,155,155	0
2	CIT	C	501	13/13	0.87	0.23	155,155,155,155	0

6.5 Other polymers (i)

There are no such residues in this entry.