



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:45 AM UTC

PDB ID : 6QU5 / pdb_00006qu5
Title : Crystal Structure of Phosphofructokinase from Trypanosoma brucei in complex with an allosteric inhibitor etcb12
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

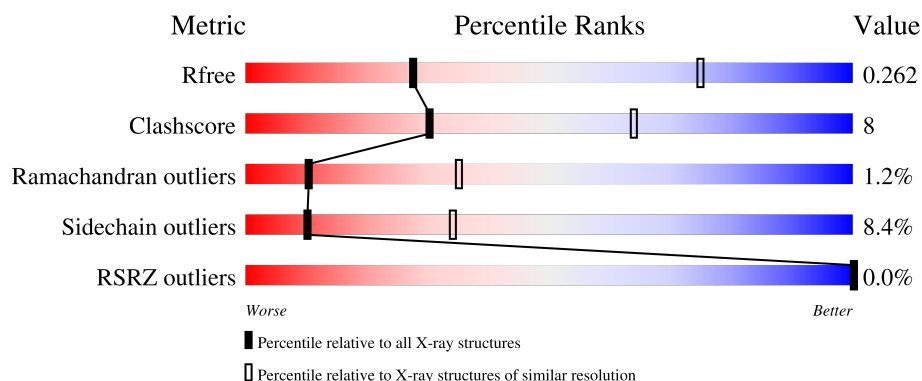
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	507	 69% 17% • 11%
1	B	507	 71% 17% • 9%
1	C	507	 69% 17% • • 9%
1	D	507	 70% 16% • 11%
1	E	507	 69% 18% • 10%

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Mol	Chain	Length	Quality of chain
1	F	507	71%17%10%
1	G	507	67%18%10%
1	H	507	70%17%11%

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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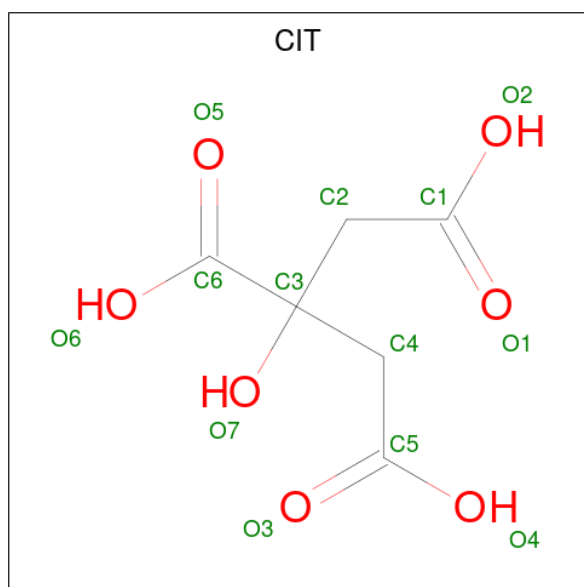
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP O15648
E	-1	SER	-	expression tag	UNP O15648
E	0	HIS	-	expression tag	UNP O15648
F	-19	MET	-	initiating methionine	UNP O15648
F	-18	GLY	-	expression tag	UNP O15648
F	-17	SER	-	expression tag	UNP O15648
F	-16	SER	-	expression 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 (CCD ID: CIT) (formula: $C_6H_8O_7$).



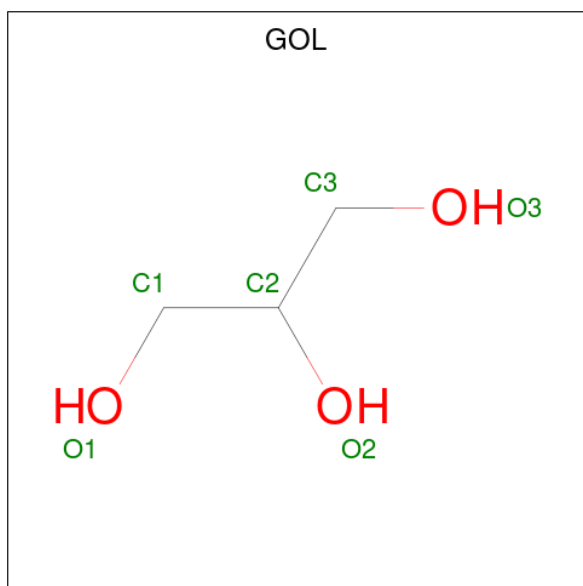
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

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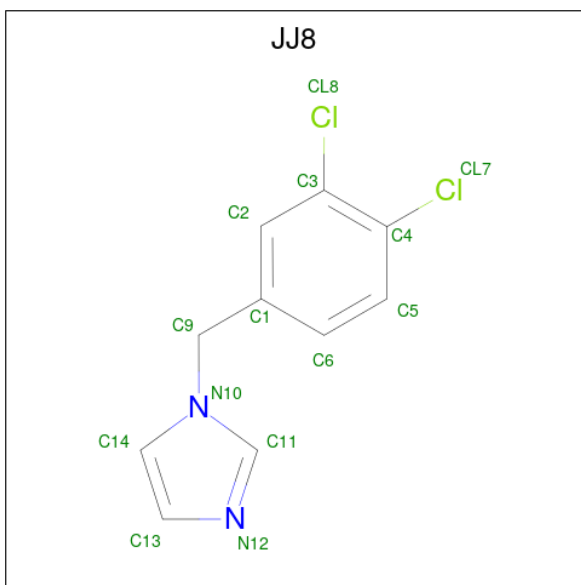
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

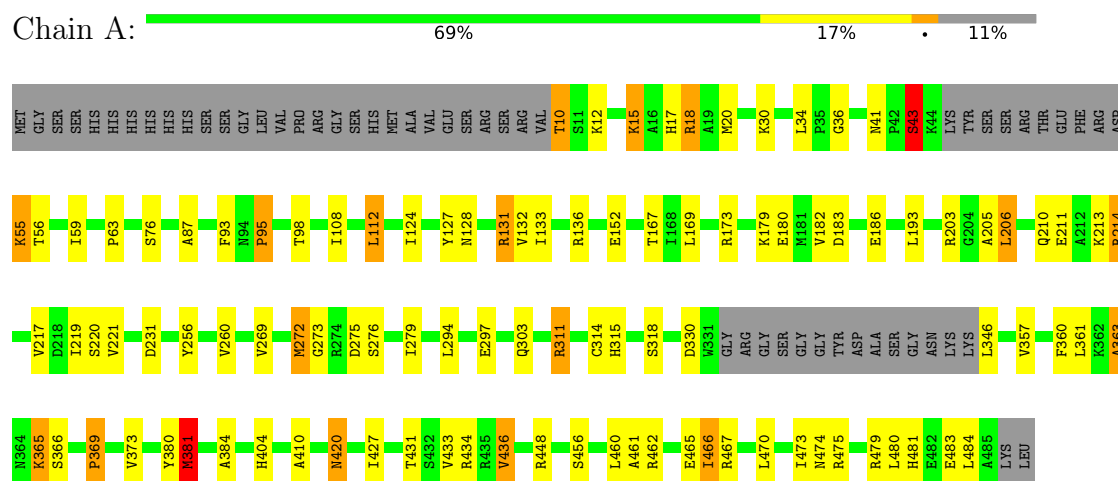


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			14	10	2	2		
4	B	1	Total	C	Cl	N	0	0
			14	10	2	2		

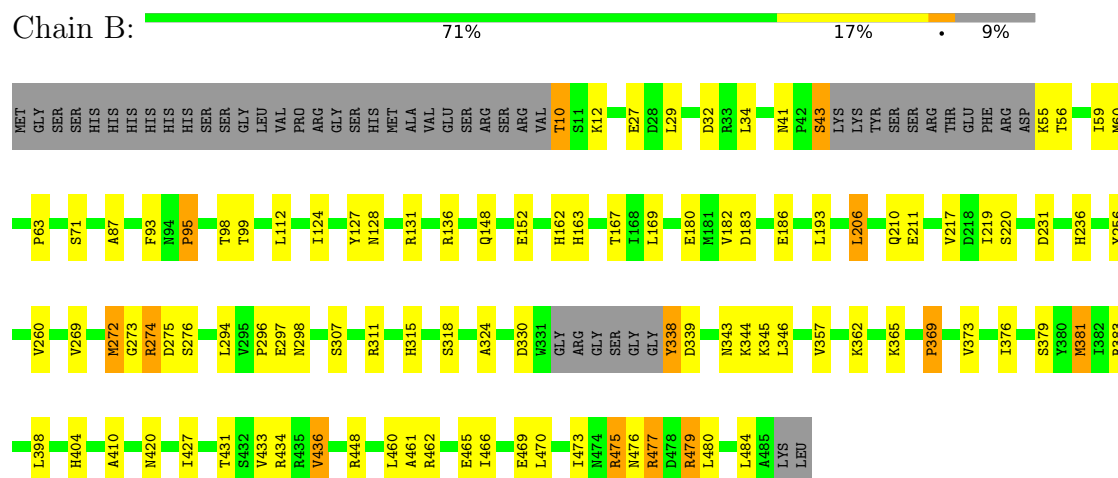
3 Residue-property plots [i](#)

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

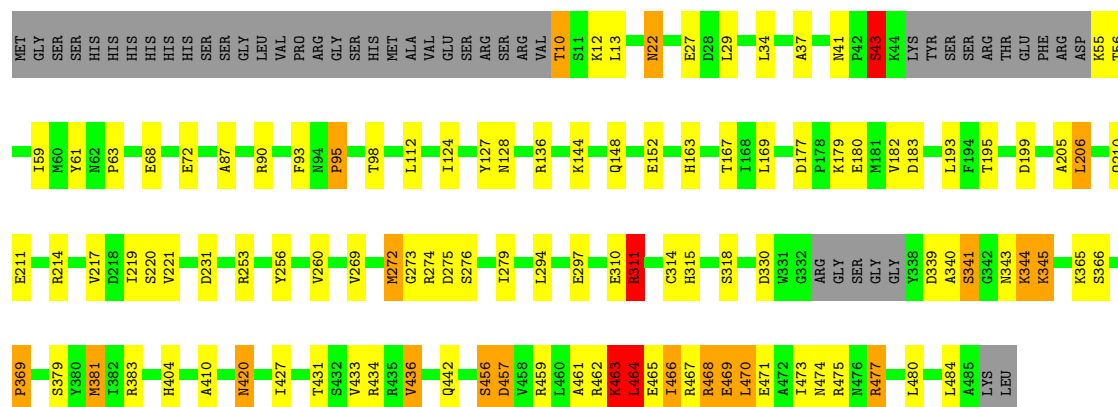


- Molecule 1: ATP-dependent 6-phosphofructokinase



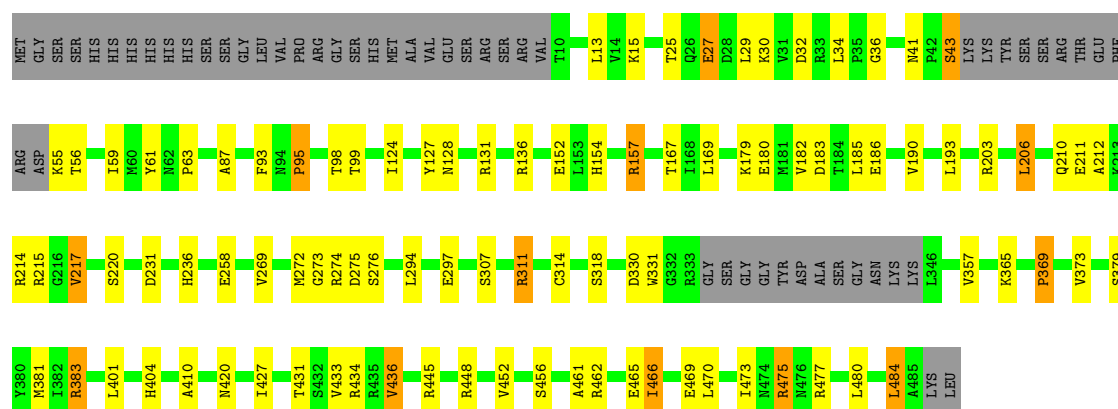
- Molecule 1: ATP-dependent 6-phosphofructokinase





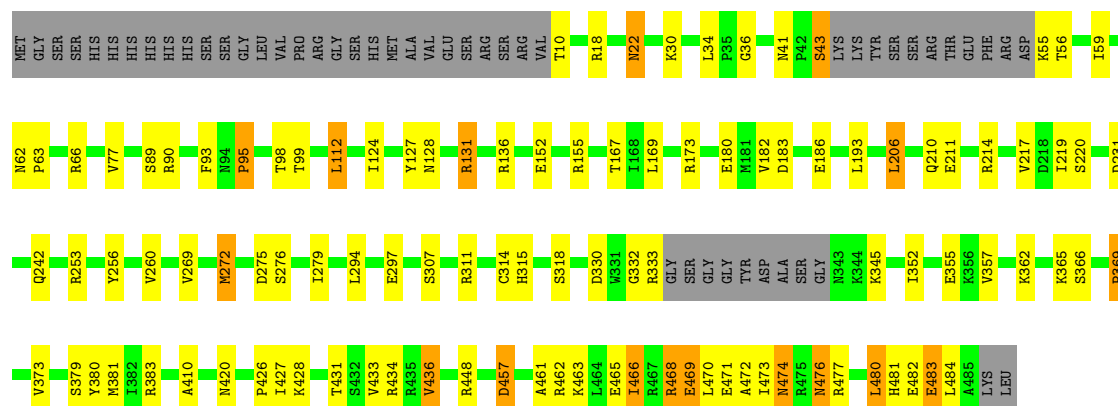
- Molecule 1: ATP-dependent 6-phosphofructokinase

Chain D: 70% 16% 11%



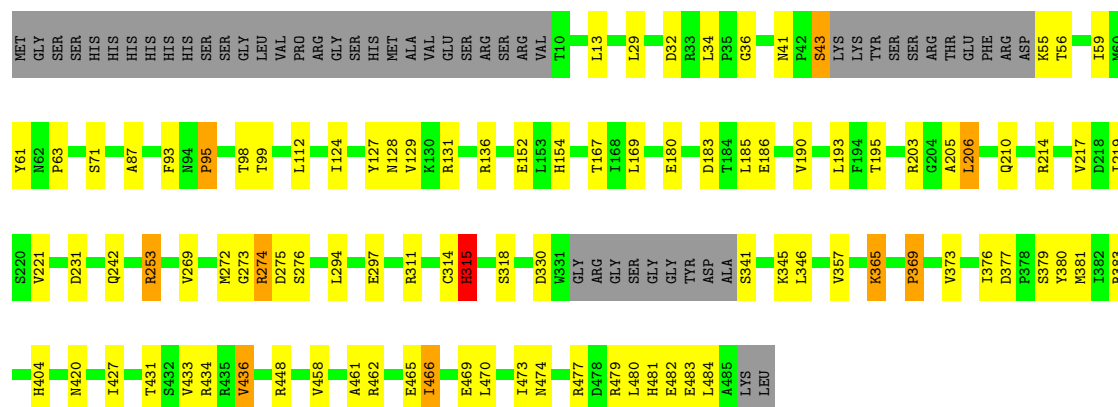
- Molecule 1: ATP-dependent 6-phosphofructokinase

Chain E: 69% 18% 10%



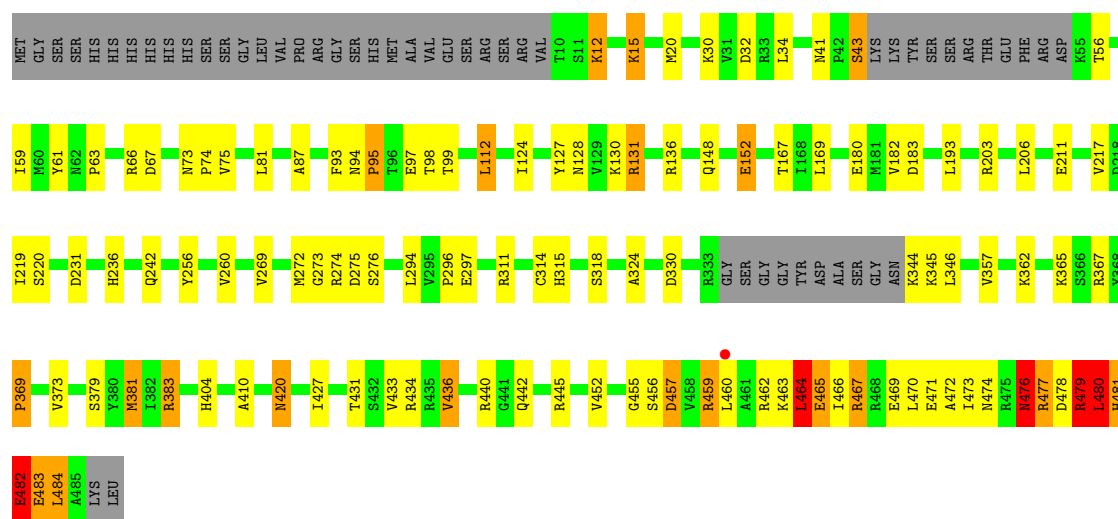
- Molecule 1: ATP-dependent 6-phosphofructokinase

Chain F: 71% 17% 10%



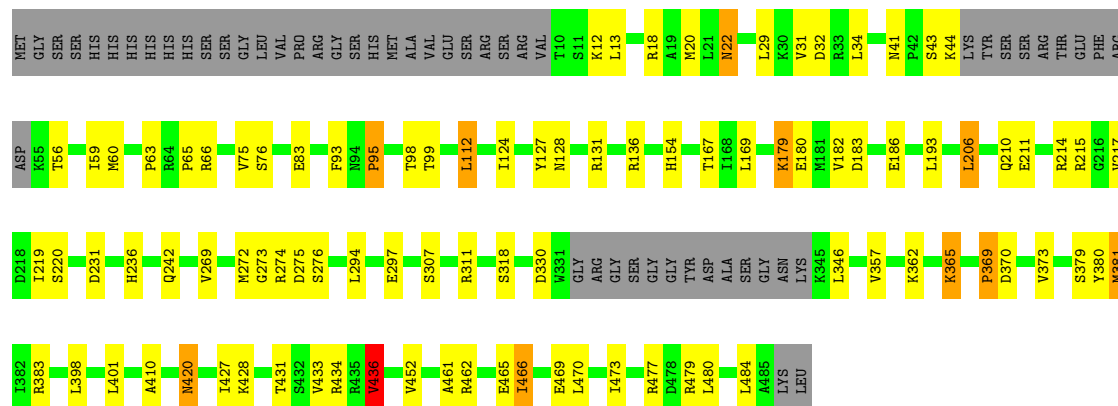
• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain G: 67% 18% 10%



• Molecule 1: ATP-dependent 6-phosphofructokinase

Chain H: 70% 17% 11%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (4.92%)	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)	0.33 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.07	0/3545	1.48	6/4798 (0.1%)
1	B	1.07	0/3598	1.47	2/4869 (0.0%)
1	C	1.10	3/3611 (0.1%)	1.51	10/4885 (0.2%)
1	D	1.06	0/3551	1.46	4/4806 (0.1%)
1	E	1.09	1/3577 (0.0%)	1.49	7/4839 (0.1%)
1	F	1.08	0/3572	1.48	5/4833 (0.1%)
1	G	1.10	0/3569	1.50	11/4828 (0.2%)
1	H	1.05	0/3554	1.45	0/4809
All	All	1.08	4/28577 (0.0%)	1.48	45/38667 (0.1%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	480	LEU	C-O	6.35	1.31	1.23
1	C	341	SER	C-O	5.36	1.28	1.23
1	C	163	HIS	CE1-NE2	5.07	1.37	1.32
1	C	457	ASP	C-O	5.03	1.29	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ASP	CB-CA-C	12.88	132.18	110.79
1	C	456	SER	CA-C-O	-10.80	108.96	121.16
1	G	32	ASP	CB-CA-C	10.57	126.80	109.89
1	B	315	HIS	CA-CB-CG	-10.12	103.68	113.80
1	F	315	HIS	CA-CB-CG	-9.97	103.83	113.80
1	G	32	ASP	CA-CB-CG	9.13	121.73	112.60
1	A	363	ALA	N-CA-C	-9.09	95.84	110.20
1	B	10	THR	CB-CA-C	8.69	128.21	109.10
1	C	199	ASP	CA-C-O	-8.22	111.83	120.55
1	G	479	ARG	CA-C-N	6.88	130.19	120.28
1	G	479	ARG	C-N-CA	6.88	130.19	120.28
1	A	473	ILE	CB-CA-C	-6.84	102.91	112.14
1	D	331	TRP	CA-C-N	6.83	126.83	120.34
1	D	331	TRP	C-N-CA	6.83	126.83	120.34
1	G	476	ASN	CB-CA-C	6.75	122.32	110.85
1	G	476	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	381	MET	CB-CG-SD	6.28	131.53	112.70
1	E	481	HIS	CA-CB-CG	6.26	120.06	113.80
1	G	476	ASN	N-CA-CB	6.21	119.35	110.16
1	C	10	THR	CA-CB-OG1	-6.08	100.49	109.60
1	C	469	GLU	CB-CA-C	5.97	120.69	110.79
1	A	10	THR	CB-CA-C	5.84	121.95	109.10
1	G	465	GLU	CB-CA-C	5.73	120.59	110.85
1	A	36	GLY	CA-C-O	-5.65	117.47	121.88
1	D	36	GLY	CA-C-O	-5.55	117.55	121.88
1	F	345	LYS	CA-C-N	5.45	128.51	120.82
1	F	345	LYS	C-N-CA	5.45	128.51	120.82
1	E	131	ARG	CB-CG-CD	-5.40	98.89	111.30
1	E	315	HIS	CA-CB-CG	-5.37	108.43	113.80
1	D	157	ARG	CB-CG-CD	5.35	123.61	111.30
1	F	253	ARG	CB-CG-CD	5.31	123.51	111.30
1	F	36	GLY	CA-C-O	-5.28	117.76	121.88
1	C	311	ARG	CG-CD-NE	5.21	123.47	112.00
1	G	32	ASP	N-CA-CB	5.19	117.58	109.85
1	E	469	GLU	CB-CA-C	5.17	119.37	110.79
1	C	464	LEU	CA-C-N	5.16	127.46	120.65
1	C	464	LEU	C-N-CA	5.16	127.46	120.65
1	E	10	THR	CA-C-N	5.10	128.47	121.33
1	E	10	THR	C-N-CA	5.10	128.47	121.33
1	C	43	SER	CB-CA-C	5.10	116.99	109.29
1	E	36	GLY	CA-C-O	-5.09	117.91	121.88
1	G	460	LEU	N-CA-C	-5.08	105.98	113.61
1	C	311	ARG	CB-CG-CD	5.08	122.98	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	THR	CA-CB-OG1	5.07	117.21	109.60
1	G	464	LEU	N-CA-C	-5.07	107.38	113.21

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

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	59	0
1	B	3539	0	3594	59	0
1	C	3552	0	3610	78	0
1	D	3493	0	3552	66	0
1	E	3519	0	3584	58	0
1	F	3514	0	3576	61	0
1	G	3511	0	3578	93	0
1	H	3496	0	3560	65	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	0	1	0
4	B	14	0	0	1	0
All	All	28255	0	28659	479	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 (479) 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:H:41:ASN:CG	1:H:43:SER:HG	1.92	0.77
1:F:311:ARG:HD2	1:F:458:VAL:HG21	1.64	0.77
1:A:380:TYR:OH	1:A:381:MET:HE2	1.85	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
1:G:362:LYS:O	1:G:365:LYS:HG3	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:339:ASP:CG	1:C:344:LYS:HA	2.19	0.67
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:C:463:LYS:H	1:C:465:GLU:CD	2.03	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
1:G:231:ASP:HB3	1:G:276:SER:HB3	1.78	0.63
1:G:93:PHE:HB3	1:G:98:THR:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:464:LEU:C	1:G:467:ARG:HG2	2.23	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:20:MET:HE2	1:H:428:LYS:HE3	1.85	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:C:464:LEU:O	1:C:467:ARG:HD2	2.05	0.56
1:C:463:LYS:N	1:C:465:GLU:CD	2.64	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:G:20:MET:HE3	1:G:203:ARG:HG2	1.89	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:F:380:TYR:OH	1:F:381:MET:HE2	2.07	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:D:186:GLU:CD	1:D:217:VAL:HG11	2.33	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:C:177:ASP:CG	1:C:179:LYS:HG2	2.34	0.52
1:E:482:GLU:OE1	1:E:482:GLU:N	2.36	0.52
1:C:152:GLU:CD	1:D:475:ARG:HD3	2.35	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:G:236:HIS:CG	1:H:420:ASN:ND2	2.78	0.51
1:B:376:ILE:HG23	1:C:381:MET:HE1	1.92	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
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: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
1:D:95:PRO:HB3	1:D:127:TYR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:G:478:ASP:O	1:G:479:ARG:HB2	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:381:MET:HE3	1:D:381:MET:HG2	1.98	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:H:462:ARG:O	1:H:466:ILE:HG12	2.17	0.45
1:E:22:ASN:C	1:E:22:ASN:HD22	2.24	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:F:376:ILE:HG23	1:G:381:MET:HE1	1.99	0.44
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:427:ILE:O	1:H:431:THR:HG23	2.18	0.44
1:A:361:LEU:C	1:A:363:ALA:O	2.61	0.44
1:C:220:SER:OG	1:C:410:ALA:O	2.34	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:E:330:ASP:OD1	1:E:330:ASP:N	2.50	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:220:SER:OG	1:E:410:ALA:O	2.35	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:D:220:SER:OG	1:D:410:ALA:O	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:220:SER:OG	1:G:410:ALA:O	2.34	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:H:20:MET:HE2	1:H:428:LYS:CE	2.47	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:B:220:SER:OG	1:B:410:ALA:O	2.34	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: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:H:220:SER:OG	1:H:410:ALA:O	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:398:LEU:HD23	1:H:398:LEU:HA	1.93	0.42
1:A:220:SER:OG	1:A:410:ALA:O	2.34	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: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:G:381:MET:HE3	1:G:381:MET:N	2.35	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:20:MET:HE3	1:A:203:ARG:HD2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:SER:HA	1:B:60:MET:HE1	2.03	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
2:F:501:CIT:O3	2:F:501:CIT:O7	2.29	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
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:381:MET:HE3	1:B:381:MET:N	2.37	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:A:380:TYR:CG	1:A:381:MET:N	2.89	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:G:256:TYR:CE1	1:G:260:VAL:HG21	2.57	0.40
1:G:480:LEU:O	1:G:481:HIS:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/507 (88%)	404 (91%)	38 (8%)	4 (1%)	14	42
1	B	453/507 (89%)	412 (91%)	38 (8%)	3 (1%)	18	47
1	C	455/507 (90%)	402 (88%)	44 (10%)	9 (2%)	6	25
1	D	447/507 (88%)	408 (91%)	35 (8%)	4 (1%)	14	42
1	E	450/507 (89%)	407 (90%)	39 (9%)	4 (1%)	14	42
1	F	450/507 (89%)	411 (91%)	35 (8%)	4 (1%)	14	42
1	G	449/507 (89%)	403 (90%)	35 (8%)	11 (2%)	4	22
1	H	447/507 (88%)	407 (91%)	35 (8%)	5 (1%)	11	38
All	All	3597/4056 (89%)	3254 (90%)	299 (8%)	44 (1%)	10	35

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	339 (90%)	38 (10%)	7	25
1	B	382/422 (90%)	349 (91%)	33 (9%)	10	33
1	C	383/422 (91%)	351 (92%)	32 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	377/422 (89%)	345 (92%)	32 (8%)	10	33
1	E	380/422 (90%)	345 (91%)	35 (9%)	8	29
1	F	380/422 (90%)	353 (93%)	27 (7%)	13	39
1	G	379/422 (90%)	347 (92%)	32 (8%)	10	34
1	H	378/422 (90%)	352 (93%)	26 (7%)	14	40
All	All	3036/3376 (90%)	2781 (92%)	255 (8%)	10	34

All (255) 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	34	LEU
1	A	43	SER
1	A	55	LYS
1	A	56	THR
1	A	59	ILE
1	A	112	LEU
1	A	131	ARG
1	A	167	THR
1	A	179	LYS
1	A	193	LEU
1	A	206	LEU
1	A	213	LYS
1	A	214	ARG
1	A	269	VAL
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	381	MET
1	A	420	ASN

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Mol	Chain	Res	Type
1	A	433	VAL
1	A	436	VAL
1	A	448	ARG
1	A	456	SER
1	A	460	LEU
1	A	466	ILE
1	A	467	ARG
1	A	479	ARG
1	B	10	THR
1	B	12	LYS
1	B	27	GLU
1	B	29	LEU
1	B	32	ASP
1	B	34	LEU
1	B	43	SER
1	B	56	THR
1	B	59	ILE
1	B	71	SER
1	B	112	LEU
1	B	148	GLN
1	B	167	THR
1	B	193	LEU
1	B	206	LEU
1	B	269	VAL
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	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	475	ARG
1	B	477	ARG
1	B	479	ARG
1	C	22	ASN

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Mol	Chain	Res	Type
1	C	29	LEU
1	C	34	LEU
1	C	43	SER
1	C	55	LYS
1	C	56	THR
1	C	59	ILE
1	C	68	GLU
1	C	72	GLU
1	C	112	LEU
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	269	VAL
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	366	SER
1	C	381	MET
1	C	420	ASN
1	C	433	VAL
1	C	436	VAL
1	C	463	LYS
1	C	464	LEU
1	C	470	LEU
1	C	477	ARG
1	D	27	GLU
1	D	29	LEU
1	D	30	LYS
1	D	32	ASP
1	D	34	LEU
1	D	43	SER
1	D	55	LYS
1	D	56	THR
1	D	59	ILE
1	D	167	THR
1	D	193	LEU

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Mol	Chain	Res	Type
1	D	206	LEU
1	D	214	ARG
1	D	217	VAL
1	D	258	GLU
1	D	269	VAL
1	D	272	MET
1	D	274	ARG
1	D	294	LEU
1	D	307	SER
1	D	311	ARG
1	D	318	SER
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	466	ILE
1	D	475	ARG
1	D	484	LEU
1	E	18	ARG
1	E	22	ASN
1	E	30	LYS
1	E	34	LEU
1	E	43	SER
1	E	56	THR
1	E	59	ILE
1	E	90	ARG
1	E	112	LEU
1	E	167	THR
1	E	173	ARG
1	E	193	LEU
1	E	206	LEU
1	E	214	ARG
1	E	253	ARG
1	E	269	VAL
1	E	272	MET
1	E	294	LEU
1	E	307	SER
1	E	318	SER
1	E	345	LYS

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Mol	Chain	Res	Type
1	E	362	LYS
1	E	366	SER
1	E	420	ASN
1	E	433	VAL
1	E	436	VAL
1	E	448	ARG
1	E	457	ASP
1	E	466	ILE
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	29	LEU
1	F	32	ASP
1	F	34	LEU
1	F	43	SER
1	F	55	LYS
1	F	56	THR
1	F	59	ILE
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	269	VAL
1	F	272	MET
1	F	274	ARG
1	F	294	LEU
1	F	315	HIS
1	F	318	SER
1	F	341	SER
1	F	365	LYS
1	F	420	ASN
1	F	433	VAL
1	F	436	VAL
1	F	448	ARG
1	F	466	ILE
1	F	477	ARG
1	G	15	LYS

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Mol	Chain	Res	Type
1	G	30	LYS
1	G	34	LEU
1	G	43	SER
1	G	56	THR
1	G	59	ILE
1	G	112	LEU
1	G	130	LYS
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	269	VAL
1	G	272	MET
1	G	294	LEU
1	G	318	SER
1	G	345	LYS
1	G	381	MET
1	G	383	ARG
1	G	420	ASN
1	G	433	VAL
1	G	436	VAL
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	29	LEU
1	H	32	ASP
1	H	34	LEU
1	H	56	THR
1	H	59	ILE
1	H	112	LEU
1	H	167	THR
1	H	179	LYS
1	H	193	LEU

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Mol	Chain	Res	Type
1	H	206	LEU
1	H	269	VAL
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	466	ILE
1	H	479	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	242	GLN
1	A	250	GLN
1	A	315	HIS
1	A	420	ASN
1	A	442	GLN
1	A	446	GLN
1	B	94	ASN
1	B	160	ASN
1	B	163	HIS
1	B	210	GLN
1	B	242	GLN
1	B	250	GLN
1	B	298	ASN
1	B	343	ASN
1	B	420	ASN
1	B	442	GLN
1	B	446	GLN
1	C	148	GLN
1	C	160	ASN
1	C	210	GLN
1	C	242	GLN
1	C	250	GLN

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Mol	Chain	Res	Type
1	C	343	ASN
1	C	420	ASN
1	C	442	GLN
1	C	446	GLN
1	C	481	HIS
1	D	160	ASN
1	D	210	GLN
1	D	242	GLN
1	D	298	ASN
1	D	421	ASN
1	D	446	GLN
1	E	17	HIS
1	E	22	ASN
1	E	210	GLN
1	E	298	ASN
1	E	421	ASN
1	E	446	GLN
1	F	17	HIS
1	F	210	GLN
1	F	242	GLN
1	F	250	GLN
1	F	298	ASN
1	F	343	ASN
1	F	420	ASN
1	F	442	GLN
1	F	446	GLN
1	G	242	GLN
1	G	250	GLN
1	G	298	ASN
1	G	364	ASN
1	G	420	ASN
1	G	421	ASN
1	G	442	GLN
1	G	446	GLN
1	H	210	GLN
1	H	250	GLN
1	H	420	ASN
1	H	442	GLN
1	H	446	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C	501	-	12,12,12	1.15	0	17,17,17	1.09	1 (5%)
2	CIT	E	501	-	12,12,12	1.24	1 (8%)	17,17,17	1.21	2 (11%)
2	CIT	H	501	-	12,12,12	1.25	1 (8%)	17,17,17	0.99	0
2	CIT	B	501	-	12,12,12	1.18	1 (8%)	17,17,17	1.20	2 (11%)
2	CIT	G	501	-	12,12,12	1.17	1 (8%)	17,17,17	1.22	2 (11%)
3	GOL	A	502	-	5,5,5	0.09	0	5,5,5	0.26	0
4	JJ8	B	503	-	15,15,15	1.08	2 (13%)	20,20,20	1.25	2 (10%)
2	CIT	F	501	-	12,12,12	1.22	1 (8%)	17,17,17	1.25	2 (11%)
2	CIT	A	501	-	12,12,12	1.13	0	17,17,17	1.18	1 (5%)
3	GOL	B	502	-	5,5,5	0.10	0	5,5,5	0.31	0
4	JJ8	A	503	-	15,15,15	1.10	2 (13%)	20,20,20	1.12	2 (10%)
2	CIT	D	501	-	12,12,12	1.17	1 (8%)	17,17,17	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	C	501	-	-	5/16/16/16	-
2	CIT	E	501	-	-	7/16/16/16	-
2	CIT	H	501	-	-	10/16/16/16	-
2	CIT	B	501	-	-	6/16/16/16	-
2	CIT	G	501	-	-	6/16/16/16	-
3	GOL	A	502	-	-	0/4/4/4	-
4	JJ8	B	503	-	-	0/4/4/4	0/2/2/2
2	CIT	F	501	-	-	10/16/16/16	-
2	CIT	A	501	-	-	10/16/16/16	-
3	GOL	B	502	-	-	2/4/4/4	-
4	JJ8	A	503	-	-	0/4/4/4	0/2/2/2
2	CIT	D	501	-	-	11/16/16/16	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	JJ8	C3-CL8	2.72	1.80	1.73
2	E	501	CIT	C3-C6	2.60	1.56	1.53
2	F	501	CIT	C3-C6	2.43	1.56	1.53
2	H	501	CIT	C3-C6	2.34	1.55	1.53
4	B	503	JJ8	C4-CL7	2.28	1.79	1.73
4	A	503	JJ8	C4-CL7	2.20	1.78	1.73
2	B	501	CIT	C3-C6	2.13	1.55	1.53
2	D	501	CIT	C3-C6	2.12	1.55	1.53
4	B	503	JJ8	C3-CL8	2.11	1.78	1.73
2	G	501	CIT	C3-C6	2.08	1.55	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	JJ8	C1-C9-N10	-2.90	106.83	112.39
4	A	503	JJ8	C1-C9-N10	-2.77	107.06	112.39
2	G	501	CIT	O5-C6-C3	-2.74	116.79	122.09
2	B	501	CIT	O6-C6-C3	2.72	118.36	113.14
4	B	503	JJ8	C14-N10-C11	2.70	110.08	106.71
2	B	501	CIT	O5-C6-C3	-2.65	116.95	122.09
2	F	501	CIT	O5-C6-C3	-2.58	117.09	122.09
2	E	501	CIT	O6-C6-C3	2.55	118.03	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	CIT	O6-C6-C3	2.54	118.01	113.14
2	G	501	CIT	O6-C6-C3	2.51	117.95	113.14
2	E	501	CIT	O5-C6-C3	-2.41	117.41	122.09
2	A	501	CIT	O5-C6-C3	-2.26	117.72	122.09
2	C	501	CIT	O5-C6-C3	-2.13	117.96	122.09
4	A	503	JJ8	C14-N10-C11	2.06	109.27	106.71

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CIT	C1-C2-C3-O7
2	A	501	CIT	C2-C3-C4-C5
2	A	501	CIT	C6-C3-C4-C5
2	A	501	CIT	O7-C3-C6-O5
2	A	501	CIT	O7-C3-C6-O6
2	A	501	CIT	C4-C3-C6-O5
2	A	501	CIT	C4-C3-C6-O6
2	B	501	CIT	O7-C3-C6-O5
2	B	501	CIT	O7-C3-C6-O6
2	B	501	CIT	C4-C3-C6-O5
2	B	501	CIT	C4-C3-C6-O6
2	C	501	CIT	O7-C3-C6-O5
2	C	501	CIT	O7-C3-C6-O6
2	C	501	CIT	C4-C3-C6-O5
2	C	501	CIT	C4-C3-C6-O6
2	D	501	CIT	C2-C3-C4-C5
2	D	501	CIT	C6-C3-C4-C5
2	D	501	CIT	O7-C3-C6-O5
2	D	501	CIT	O7-C3-C6-O6
2	D	501	CIT	C4-C3-C6-O5
2	D	501	CIT	C4-C3-C6-O6
2	E	501	CIT	O7-C3-C6-O5
2	E	501	CIT	O7-C3-C6-O6
2	E	501	CIT	C4-C3-C6-O5
2	E	501	CIT	C4-C3-C6-O6
2	F	501	CIT	C1-C2-C3-O7
2	F	501	CIT	C2-C3-C4-C5
2	F	501	CIT	C6-C3-C4-C5
2	F	501	CIT	O7-C3-C6-O5
2	F	501	CIT	O7-C3-C6-O6
2	F	501	CIT	C4-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
2	F	501	CIT	C4-C3-C6-O6
2	G	501	CIT	C1-C2-C3-O7
2	G	501	CIT	C1-C2-C3-C4
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	O7-C3-C6-O5
2	H	501	CIT	O7-C3-C6-O6
2	H	501	CIT	C4-C3-C6-O5
2	H	501	CIT	C4-C3-C6-O6
2	A	501	CIT	C1-C2-C3-C4
2	F	501	CIT	C1-C2-C3-C4
2	G	501	CIT	C1-C2-C3-C6
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	H	501	CIT	C1-C2-C3-C6
2	H	501	CIT	C6-C3-C4-C5
2	A	501	CIT	C1-C2-C3-C6
2	F	501	CIT	C1-C2-C3-C6
2	H	501	CIT	C2-C3-C4-C5
2	D	501	CIT	C1-C2-C3-C4
2	B	501	CIT	C1-C2-C3-O7
2	C	501	CIT	C1-C2-C3-O7
2	D	501	CIT	C1-C2-C3-O7
2	E	501	CIT	C2-C3-C6-O5
2	E	501	CIT	C2-C3-C6-O6
2	H	501	CIT	O7-C3-C4-C5
2	D	501	CIT	C3-C4-C5-O4
2	D	501	CIT	C3-C4-C5-O3
2	E	501	CIT	C1-C2-C3-O7
2	B	501	CIT	C1-C2-C3-C4

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

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	452/507 (89%)	-0.63	0 100 100	71, 100, 144, 171	0
1	B	459/507 (90%)	-0.53	0 100 100	77, 109, 137, 156	0
1	C	461/507 (90%)	-0.53	0 100 100	81, 114, 155, 187	0
1	D	453/507 (89%)	-0.60	0 100 100	82, 120, 156, 179	0
1	E	456/507 (89%)	-0.62	0 100 100	80, 109, 152, 204	0
1	F	456/507 (89%)	-0.61	0 100 100	75, 104, 135, 170	0
1	G	455/507 (89%)	-0.46	1 (0%) 91 87	99, 137, 177, 229	0
1	H	453/507 (89%)	-0.46	0 100 100	116, 152, 188, 208	0
All	All	3645/4056 (89%)	-0.56	1 (0%) 100 100	71, 117, 168, 229	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	460	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CIT	H	501	13/13	0.57	0.07	155,155,155,155	0
2	CIT	G	501	13/13	0.70	0.08	155,155,155,155	0
2	CIT	A	501	13/13	0.70	0.08	155,155,155,155	0
2	CIT	C	501	13/13	0.73	0.07	155,155,155,155	0
2	CIT	E	501	13/13	0.73	0.08	155,155,155,155	0
2	CIT	D	501	13/13	0.76	0.09	155,155,155,155	0
2	CIT	F	501	13/13	0.76	0.09	155,155,155,155	0
2	CIT	B	501	13/13	0.85	0.08	155,155,155,155	0
4	JJ8	B	503	14/14	0.88	0.15	155,155,155,155	0
4	JJ8	A	503	14/14	0.92	0.14	155,155,155,155	0
3	GOL	A	502	6/6	0.92	0.17	155,155,155,155	0
3	GOL	B	502	6/6	0.93	0.17	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.