Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 05:49 PM EDT

PDB ID	:	3E0V
Title	:	Crystal structure of pyruvate kinase from Leishmania mexicana in complex with sulphate ions
Authors	:	Tulloch, L.B.; Gillmore, L.A.; Walkinshaw, M.D.
Deposited on	:	2008-08-01
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

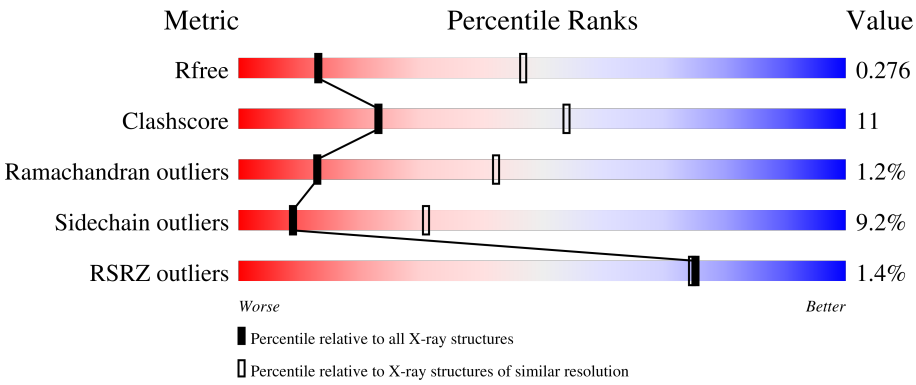
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	539	.% 65% 24% • 8%
1	B	539	2% 65% 24% • 8%
1	C	539	63% 25% • 8%
1	D	539	2% 69% 21% • 8%
1	E	539	.% 66% 23% • 8%

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Mol	Chain	Length	Quality of chain
1	F	539	2% 66% 24% 8%

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
3	GOL	E	508	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23331 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	494	3793	2368	666	732	27	0	2	0
1	B	497	3800	2369	668	736	27	0	1	0
1	C	494	3812	2379	673	733	27	0	4	0
1	D	495	3783	2357	667	732	27	0	1	0
1	E	495	3804	2372	670	735	27	0	3	0
1	F	496	3802	2371	667	737	27	0	3	0

There are 270 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	expression tag	UNP Q27686
A	-39	GLY	-	expression tag	UNP Q27686
A	-38	SER	-	expression tag	UNP Q27686
A	-37	SER	-	expression tag	UNP Q27686
A	-36	HIS	-	expression tag	UNP Q27686
A	-35	HIS	-	expression tag	UNP Q27686
A	-34	HIS	-	expression tag	UNP Q27686
A	-33	HIS	-	expression tag	UNP Q27686
A	-32	HIS	-	expression tag	UNP Q27686
A	-31	HIS	-	expression tag	UNP Q27686
A	-30	SER	-	expression tag	UNP Q27686
A	-29	SER	-	expression tag	UNP Q27686
A	-28	GLY	-	expression tag	UNP Q27686
A	-27	LEU	-	expression tag	UNP Q27686
A	-26	VAL	-	expression tag	UNP Q27686
A	-25	PRO	-	expression tag	UNP Q27686
A	-24	ARG	-	expression tag	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	GLY	-	expression tag	UNP Q27686
A	-22	SER	-	expression tag	UNP Q27686
A	-21	HIS	-	expression tag	UNP Q27686
A	-20	MET	-	expression tag	UNP Q27686
A	-19	GLY	-	expression tag	UNP Q27686
A	-18	SER	-	expression tag	UNP Q27686
A	-17	SER	-	expression tag	UNP Q27686
A	-16	HIS	-	expression tag	UNP Q27686
A	-15	HIS	-	expression tag	UNP Q27686
A	-14	HIS	-	expression tag	UNP Q27686
A	-13	HIS	-	expression tag	UNP Q27686
A	-12	HIS	-	expression tag	UNP Q27686
A	-11	HIS	-	expression tag	UNP Q27686
A	-10	SER	-	expression tag	UNP Q27686
A	-9	SER	-	expression tag	UNP Q27686
A	-8	GLY	-	expression tag	UNP Q27686
A	-7	LEU	-	expression tag	UNP Q27686
A	-6	VAL	-	expression tag	UNP Q27686
A	-5	PRO	-	expression tag	UNP Q27686
A	-4	ARG	-	expression tag	UNP Q27686
A	-3	GLY	-	expression tag	UNP Q27686
A	-2	SER	-	expression tag	UNP Q27686
A	-1	HIS	-	expression tag	UNP Q27686
A	382	SER	GLY	conflict	UNP Q27686
A	389	TYR	SER	conflict	UNP Q27686
A	404	ARG	ALA	conflict	UNP Q27686
A	405	SER	GLY	conflict	UNP Q27686
A	451	TRP	GLU	engineered mutation	UNP Q27686
B	-40	MET	-	expression tag	UNP Q27686
B	-39	GLY	-	expression tag	UNP Q27686
B	-38	SER	-	expression tag	UNP Q27686
B	-37	SER	-	expression tag	UNP Q27686
B	-36	HIS	-	expression tag	UNP Q27686
B	-35	HIS	-	expression tag	UNP Q27686
B	-34	HIS	-	expression tag	UNP Q27686
B	-33	HIS	-	expression tag	UNP Q27686
B	-32	HIS	-	expression tag	UNP Q27686
B	-31	HIS	-	expression tag	UNP Q27686
B	-30	SER	-	expression tag	UNP Q27686
B	-29	SER	-	expression tag	UNP Q27686
B	-28	GLY	-	expression tag	UNP Q27686
B	-27	LEU	-	expression tag	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-26	VAL	-	expression tag	UNP Q27686
B	-25	PRO	-	expression tag	UNP Q27686
B	-24	ARG	-	expression tag	UNP Q27686
B	-23	GLY	-	expression tag	UNP Q27686
B	-22	SER	-	expression tag	UNP Q27686
B	-21	HIS	-	expression tag	UNP Q27686
B	-20	MET	-	expression tag	UNP Q27686
B	-19	GLY	-	expression tag	UNP Q27686
B	-18	SER	-	expression tag	UNP Q27686
B	-17	SER	-	expression tag	UNP Q27686
B	-16	HIS	-	expression tag	UNP Q27686
B	-15	HIS	-	expression tag	UNP Q27686
B	-14	HIS	-	expression tag	UNP Q27686
B	-13	HIS	-	expression tag	UNP Q27686
B	-12	HIS	-	expression tag	UNP Q27686
B	-11	HIS	-	expression tag	UNP Q27686
B	-10	SER	-	expression tag	UNP Q27686
B	-9	SER	-	expression tag	UNP Q27686
B	-8	GLY	-	expression tag	UNP Q27686
B	-7	LEU	-	expression tag	UNP Q27686
B	-6	VAL	-	expression tag	UNP Q27686
B	-5	PRO	-	expression tag	UNP Q27686
B	-4	ARG	-	expression tag	UNP Q27686
B	-3	GLY	-	expression tag	UNP Q27686
B	-2	SER	-	expression tag	UNP Q27686
B	-1	HIS	-	expression tag	UNP Q27686
B	382	SER	GLY	conflict	UNP Q27686
B	389	TYR	SER	conflict	UNP Q27686
B	404	ARG	ALA	conflict	UNP Q27686
B	405	SER	GLY	conflict	UNP Q27686
B	451	TRP	GLU	engineered mutation	UNP Q27686
C	-40	MET	-	expression tag	UNP Q27686
C	-39	GLY	-	expression tag	UNP Q27686
C	-38	SER	-	expression tag	UNP Q27686
C	-37	SER	-	expression tag	UNP Q27686
C	-36	HIS	-	expression tag	UNP Q27686
C	-35	HIS	-	expression tag	UNP Q27686
C	-34	HIS	-	expression tag	UNP Q27686
C	-33	HIS	-	expression tag	UNP Q27686
C	-32	HIS	-	expression tag	UNP Q27686
C	-31	HIS	-	expression tag	UNP Q27686
C	-30	SER	-	expression tag	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-29	SER	-	expression tag	UNP Q27686
C	-28	GLY	-	expression tag	UNP Q27686
C	-27	LEU	-	expression tag	UNP Q27686
C	-26	VAL	-	expression tag	UNP Q27686
C	-25	PRO	-	expression tag	UNP Q27686
C	-24	ARG	-	expression tag	UNP Q27686
C	-23	GLY	-	expression tag	UNP Q27686
C	-22	SER	-	expression tag	UNP Q27686
C	-21	HIS	-	expression tag	UNP Q27686
C	-20	MET	-	expression tag	UNP Q27686
C	-19	GLY	-	expression tag	UNP Q27686
C	-18	SER	-	expression tag	UNP Q27686
C	-17	SER	-	expression tag	UNP Q27686
C	-16	HIS	-	expression tag	UNP Q27686
C	-15	HIS	-	expression tag	UNP Q27686
C	-14	HIS	-	expression tag	UNP Q27686
C	-13	HIS	-	expression tag	UNP Q27686
C	-12	HIS	-	expression tag	UNP Q27686
C	-11	HIS	-	expression tag	UNP Q27686
C	-10	SER	-	expression tag	UNP Q27686
C	-9	SER	-	expression tag	UNP Q27686
C	-8	GLY	-	expression tag	UNP Q27686
C	-7	LEU	-	expression tag	UNP Q27686
C	-6	VAL	-	expression tag	UNP Q27686
C	-5	PRO	-	expression tag	UNP Q27686
C	-4	ARG	-	expression tag	UNP Q27686
C	-3	GLY	-	expression tag	UNP Q27686
C	-2	SER	-	expression tag	UNP Q27686
C	-1	HIS	-	expression tag	UNP Q27686
C	382	SER	GLY	conflict	UNP Q27686
C	389	TYR	SER	conflict	UNP Q27686
C	404	ARG	ALA	conflict	UNP Q27686
C	405	SER	GLY	conflict	UNP Q27686
C	451	TRP	GLU	engineered mutation	UNP Q27686
D	-40	MET	-	expression tag	UNP Q27686
D	-39	GLY	-	expression tag	UNP Q27686
D	-38	SER	-	expression tag	UNP Q27686
D	-37	SER	-	expression tag	UNP Q27686
D	-36	HIS	-	expression tag	UNP Q27686
D	-35	HIS	-	expression tag	UNP Q27686
D	-34	HIS	-	expression tag	UNP Q27686
D	-33	HIS	-	expression tag	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-32	HIS	-	expression tag	UNP Q27686
D	-31	HIS	-	expression tag	UNP Q27686
D	-30	SER	-	expression tag	UNP Q27686
D	-29	SER	-	expression tag	UNP Q27686
D	-28	GLY	-	expression tag	UNP Q27686
D	-27	LEU	-	expression tag	UNP Q27686
D	-26	VAL	-	expression tag	UNP Q27686
D	-25	PRO	-	expression tag	UNP Q27686
D	-24	ARG	-	expression tag	UNP Q27686
D	-23	GLY	-	expression tag	UNP Q27686
D	-22	SER	-	expression tag	UNP Q27686
D	-21	HIS	-	expression tag	UNP Q27686
D	-20	MET	-	expression tag	UNP Q27686
D	-19	GLY	-	expression tag	UNP Q27686
D	-18	SER	-	expression tag	UNP Q27686
D	-17	SER	-	expression tag	UNP Q27686
D	-16	HIS	-	expression tag	UNP Q27686
D	-15	HIS	-	expression tag	UNP Q27686
D	-14	HIS	-	expression tag	UNP Q27686
D	-13	HIS	-	expression tag	UNP Q27686
D	-12	HIS	-	expression tag	UNP Q27686
D	-11	HIS	-	expression tag	UNP Q27686
D	-10	SER	-	expression tag	UNP Q27686
D	-9	SER	-	expression tag	UNP Q27686
D	-8	GLY	-	expression tag	UNP Q27686
D	-7	LEU	-	expression tag	UNP Q27686
D	-6	VAL	-	expression tag	UNP Q27686
D	-5	PRO	-	expression tag	UNP Q27686
D	-4	ARG	-	expression tag	UNP Q27686
D	-3	GLY	-	expression tag	UNP Q27686
D	-2	SER	-	expression tag	UNP Q27686
D	-1	HIS	-	expression tag	UNP Q27686
D	382	SER	GLY	conflict	UNP Q27686
D	389	TYR	SER	conflict	UNP Q27686
D	404	ARG	ALA	conflict	UNP Q27686
D	405	SER	GLY	conflict	UNP Q27686
D	451	TRP	GLU	engineered mutation	UNP Q27686
E	-40	MET	-	expression tag	UNP Q27686
E	-39	GLY	-	expression tag	UNP Q27686
E	-38	SER	-	expression tag	UNP Q27686
E	-37	SER	-	expression tag	UNP Q27686
E	-36	HIS	-	expression tag	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-35	HIS	-	expression tag	UNP Q27686
E	-34	HIS	-	expression tag	UNP Q27686
E	-33	HIS	-	expression tag	UNP Q27686
E	-32	HIS	-	expression tag	UNP Q27686
E	-31	HIS	-	expression tag	UNP Q27686
E	-30	SER	-	expression tag	UNP Q27686
E	-29	SER	-	expression tag	UNP Q27686
E	-28	GLY	-	expression tag	UNP Q27686
E	-27	LEU	-	expression tag	UNP Q27686
E	-26	VAL	-	expression tag	UNP Q27686
E	-25	PRO	-	expression tag	UNP Q27686
E	-24	ARG	-	expression tag	UNP Q27686
E	-23	GLY	-	expression tag	UNP Q27686
E	-22	SER	-	expression tag	UNP Q27686
E	-21	HIS	-	expression tag	UNP Q27686
E	-20	MET	-	expression tag	UNP Q27686
E	-19	GLY	-	expression tag	UNP Q27686
E	-18	SER	-	expression tag	UNP Q27686
E	-17	SER	-	expression tag	UNP Q27686
E	-16	HIS	-	expression tag	UNP Q27686
E	-15	HIS	-	expression tag	UNP Q27686
E	-14	HIS	-	expression tag	UNP Q27686
E	-13	HIS	-	expression tag	UNP Q27686
E	-12	HIS	-	expression tag	UNP Q27686
E	-11	HIS	-	expression tag	UNP Q27686
E	-10	SER	-	expression tag	UNP Q27686
E	-9	SER	-	expression tag	UNP Q27686
E	-8	GLY	-	expression tag	UNP Q27686
E	-7	LEU	-	expression tag	UNP Q27686
E	-6	VAL	-	expression tag	UNP Q27686
E	-5	PRO	-	expression tag	UNP Q27686
E	-4	ARG	-	expression tag	UNP Q27686
E	-3	GLY	-	expression tag	UNP Q27686
E	-2	SER	-	expression tag	UNP Q27686
E	-1	HIS	-	expression tag	UNP Q27686
E	382	SER	GLY	conflict	UNP Q27686
E	389	TYR	SER	conflict	UNP Q27686
E	404	ARG	ALA	conflict	UNP Q27686
E	405	SER	GLY	conflict	UNP Q27686
E	451	TRP	GLU	engineered mutation	UNP Q27686
F	-40	MET	-	expression tag	UNP Q27686
F	-39	GLY	-	expression tag	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-38	SER	-	expression tag	UNP Q27686
F	-37	SER	-	expression tag	UNP Q27686
F	-36	HIS	-	expression tag	UNP Q27686
F	-35	HIS	-	expression tag	UNP Q27686
F	-34	HIS	-	expression tag	UNP Q27686
F	-33	HIS	-	expression tag	UNP Q27686
F	-32	HIS	-	expression tag	UNP Q27686
F	-31	HIS	-	expression tag	UNP Q27686
F	-30	SER	-	expression tag	UNP Q27686
F	-29	SER	-	expression tag	UNP Q27686
F	-28	GLY	-	expression tag	UNP Q27686
F	-27	LEU	-	expression tag	UNP Q27686
F	-26	VAL	-	expression tag	UNP Q27686
F	-25	PRO	-	expression tag	UNP Q27686
F	-24	ARG	-	expression tag	UNP Q27686
F	-23	GLY	-	expression tag	UNP Q27686
F	-22	SER	-	expression tag	UNP Q27686
F	-21	HIS	-	expression tag	UNP Q27686
F	-20	MET	-	expression tag	UNP Q27686
F	-19	GLY	-	expression tag	UNP Q27686
F	-18	SER	-	expression tag	UNP Q27686
F	-17	SER	-	expression tag	UNP Q27686
F	-16	HIS	-	expression tag	UNP Q27686
F	-15	HIS	-	expression tag	UNP Q27686
F	-14	HIS	-	expression tag	UNP Q27686
F	-13	HIS	-	expression tag	UNP Q27686
F	-12	HIS	-	expression tag	UNP Q27686
F	-11	HIS	-	expression tag	UNP Q27686
F	-10	SER	-	expression tag	UNP Q27686
F	-9	SER	-	expression tag	UNP Q27686
F	-8	GLY	-	expression tag	UNP Q27686
F	-7	LEU	-	expression tag	UNP Q27686
F	-6	VAL	-	expression tag	UNP Q27686
F	-5	PRO	-	expression tag	UNP Q27686
F	-4	ARG	-	expression tag	UNP Q27686
F	-3	GLY	-	expression tag	UNP Q27686
F	-2	SER	-	expression tag	UNP Q27686
F	-1	HIS	-	expression tag	UNP Q27686
F	382	SER	GLY	conflict	UNP Q27686
F	389	TYR	SER	conflict	UNP Q27686
F	404	ARG	ALA	conflict	UNP Q27686
F	405	SER	GLY	conflict	UNP Q27686

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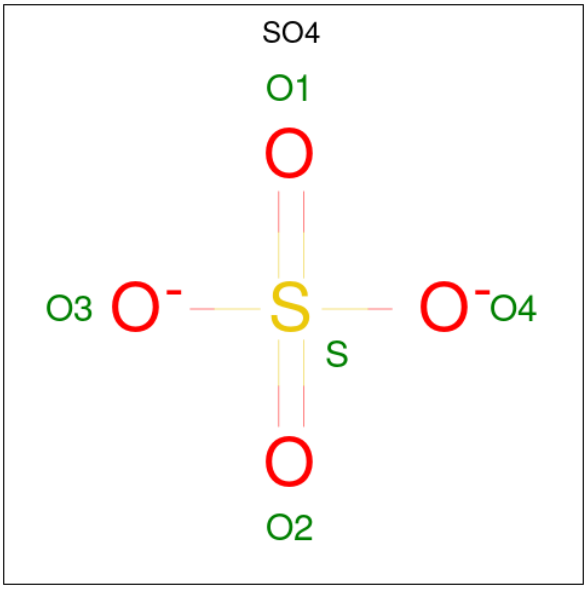
Chain	Residue	Modelled	Actual	Comment	Reference
F	451	TRP	GLU	engineered mutation	UNP Q27686

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	B	1	5	4	1		0	0
2	B	1	5	4	1		0	0
2	B	1	5	4	1		0	0
2	B	1	5	4	1		0	0
2	B	1	5	4	1		0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	10	8	2	0	1
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	E	1	5	4	1	0	0
			Total	O	S		
2	E	1	5	4	1	0	0
			Total	O	S		
2	E	1	5	4	1	0	0
			Total	O	S		
2	E	1	5	4	1	0	0

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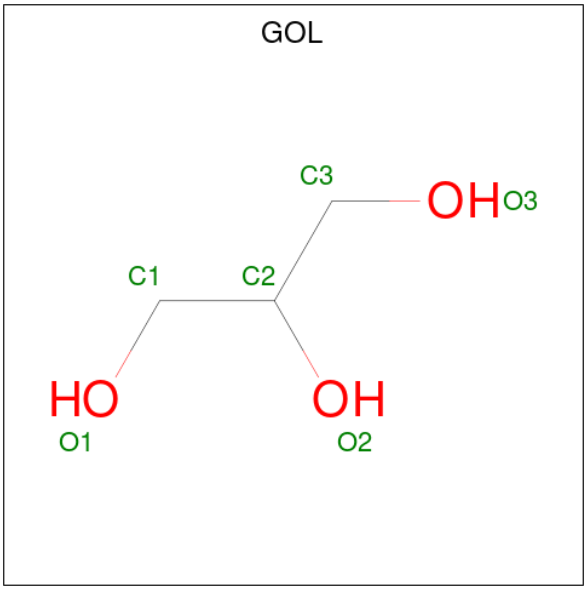
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- 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	A	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

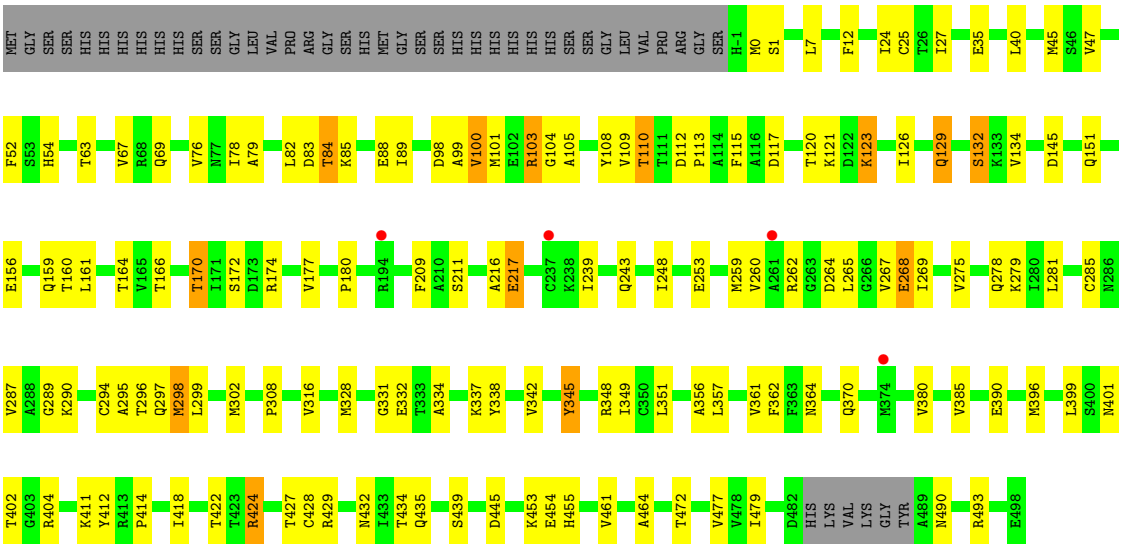
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	46	46	46	0	0
			Total	O		
4	B	59	59	59	0	0
			Total	O		
4	C	49	49	49	0	0
			Total	O		
4	D	51	51	51	0	0
			Total	O		
4	E	53	53	53	0	0
			Total	O		
4	F	56	56	56	0	0

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.

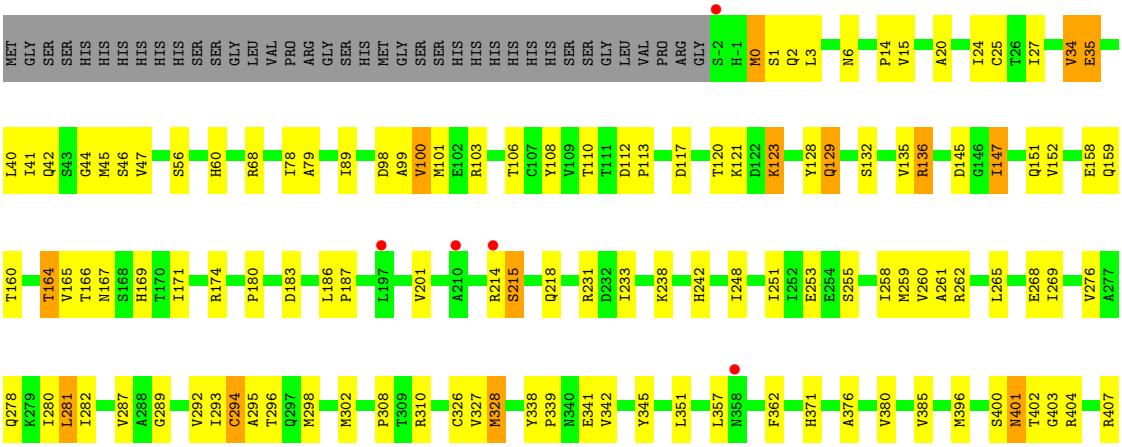
• Molecule 1: Pyruvate kinase

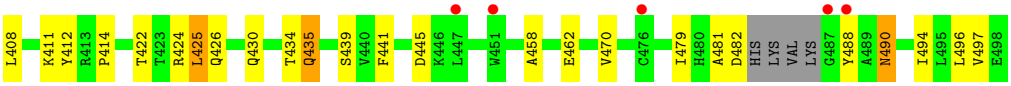
Chain A:



• Molecule 1: Pyruvate kinase

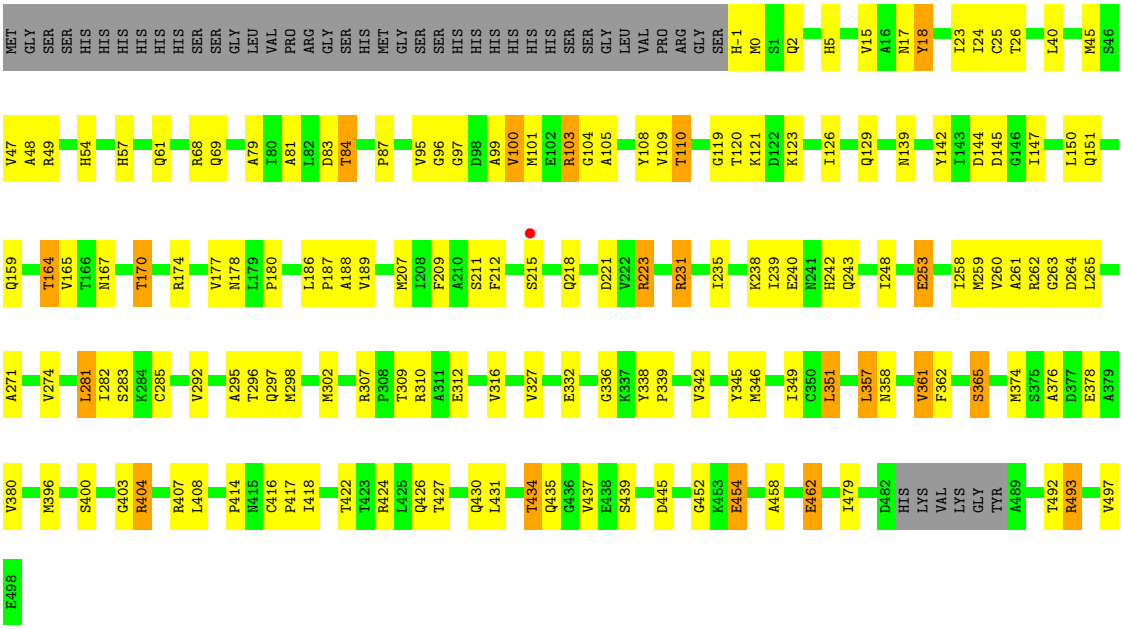
Chain B:





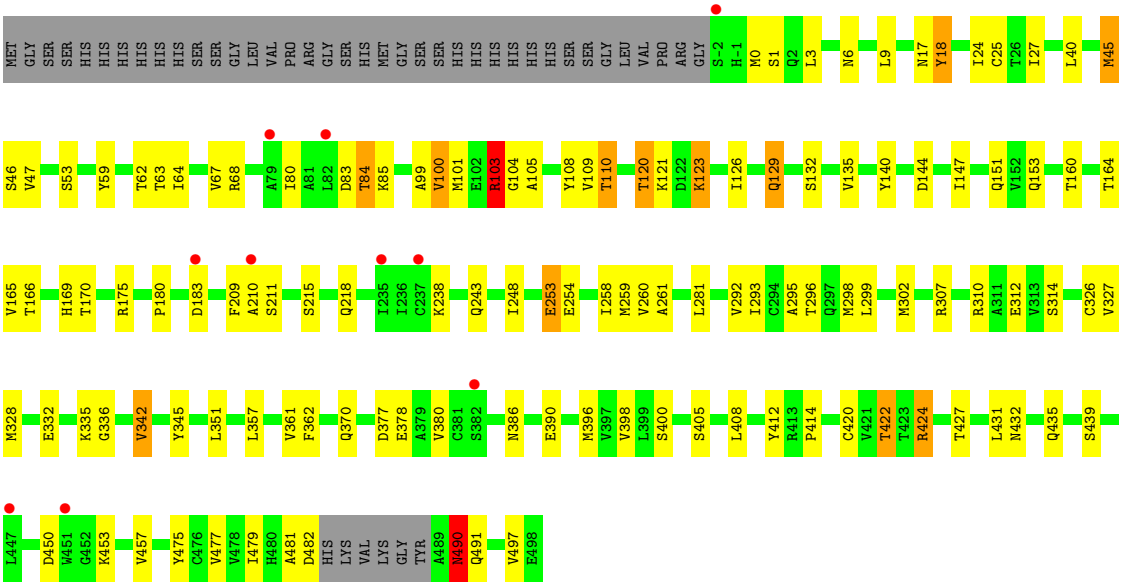
• Molecule 1: Pyruvate kinase

Chain C:



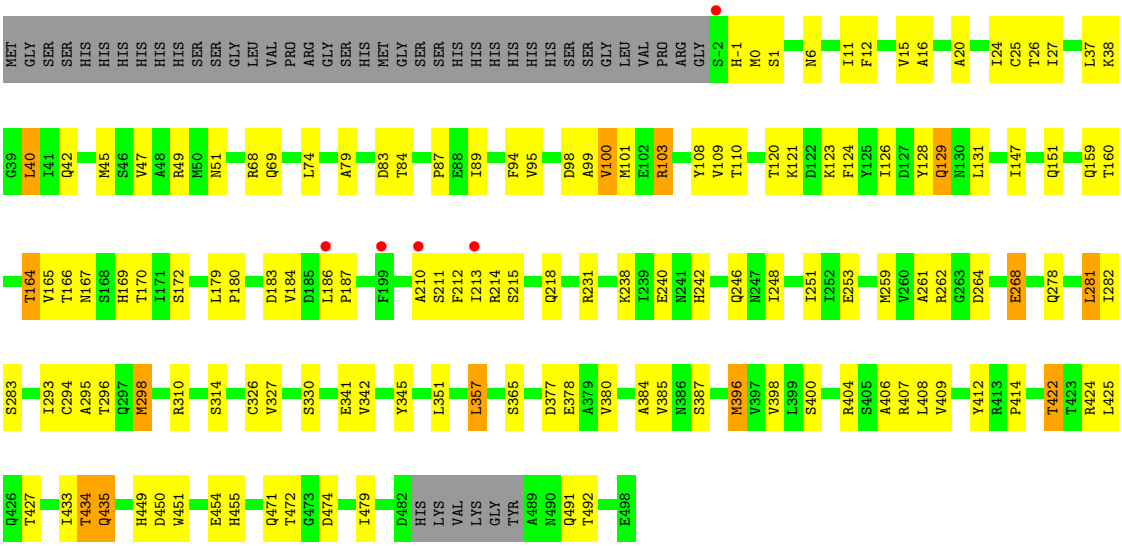
• Molecule 1: Pyruvate kinase

Chain D:



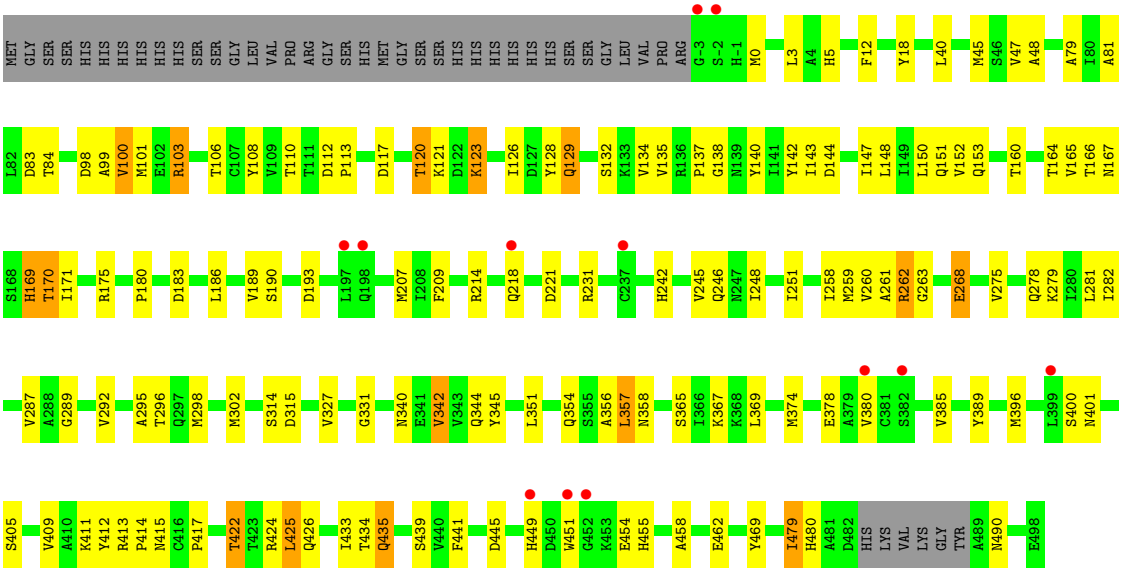
• Molecule 1: Pyruvate kinase

Chain E:



- Molecule 1: Pyruvate kinase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	261.95Å 261.95Å 185.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.06 – 3.30 99.06 – 3.30	Depositor EDS
% Data completeness (in resolution range)	87.2 (99.06-3.30) 87.4 (99.06-3.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.227 , 0.290 0.220 , 0.276	Depositor DCC
R_{free} test set	4284 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	86.0	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 104.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23331	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2039e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.46	0/3855	0.62	1/5219 (0.0%)
1	B	0.48	0/3861	0.63	1/5226 (0.0%)
1	C	0.47	0/3877	0.63	1/5247 (0.0%)
1	D	0.48	0/3843	0.62	0/5202
1	E	0.45	0/3868	0.61	1/5235 (0.0%)
1	F	0.46	0/3869	0.61	1/5237 (0.0%)
All	All	0.47	0/23173	0.62	5/31366 (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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	357	LEU	CA-CB-CG	6.27	129.72	115.30
1	E	357	LEU	CA-CB-CG	5.98	129.06	115.30
1	F	357	LEU	CA-CB-CG	5.19	127.25	115.30
1	B	408	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	357	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	294	CYS	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	3793	0	3784	90	0
1	B	3800	0	3790	88	0
1	C	3812	0	3809	105	0
1	D	3783	0	3778	83	0
1	E	3804	0	3799	85	0
1	F	3802	0	3794	93	0
2	A	30	0	0	1	0
2	B	45	0	0	0	0
2	C	35	0	0	2	0
2	D	35	0	0	0	0
2	E	30	0	0	0	0
2	F	30	0	0	0	0
3	A	12	0	16	0	0
3	E	6	0	8	1	0
4	A	46	0	0	3	0
4	B	59	0	0	8	0
4	C	49	0	0	2	0
4	D	51	0	0	5	0
4	E	53	0	0	4	0
4	F	56	0	0	4	0
All	All	23331	0	22778	522	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 11.

All (522) 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:C:338:TYR:O	1:C:342:VAL:HG23	1.47	1.12
1:A:338:TYR:O	1:A:342:VAL:HG23	1.58	1.03
1:C:396:MET:HE1	1:C:414:PRO:HG3	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:CYS:HB2	1:A:45:MET:HE3	1.41	1.00
1:E:84:THR:CG2	1:E:211:SER:H	1.76	0.99
1:B:99:ALA:O	1:B:100:VAL:HG22	1.64	0.96
1:A:25:CYS:HB2	1:A:45:MET:CE	1.96	0.93
1:C:223[A]:ARG:HH11	1:C:223[A]:ARG:HG3	1.30	0.93
1:C:396:MET:CE	1:C:414:PRO:HG3	1.98	0.93
1:A:302:MET:HE3	1:A:342:VAL:HA	1.51	0.92
1:F:84:THR:HG21	4:F:3011:HOH:O	1.67	0.92
1:F:110:THR:HG22	1:F:160:THR:HG23	1.51	0.91
1:D:396:MET:HE1	1:D:414:PRO:HG3	1.53	0.91
1:B:261:ALA:HA	1:B:295:ALA:CB	2.02	0.90
1:D:99:ALA:O	1:D:100:VAL:HG22	1.71	0.89
1:A:294:CYS:HB3	1:A:298:MET:HE1	1.56	0.85
1:A:129:GLN:HE21	1:A:129:GLN:HA	1.41	0.85
1:F:396:MET:CE	1:F:414:PRO:HG3	2.09	0.82
1:B:248:ILE:HG12	1:B:281:LEU:HD22	1.59	0.81
1:A:103:ARG:O	1:A:105:ALA:N	2.14	0.81
1:A:396:MET:CE	1:A:414:PRO:HG3	2.11	0.81
1:B:396:MET:CE	1:B:414:PRO:HG3	2.11	0.80
1:D:25:CYS:HB2	1:D:45:MET:HE3	1.61	0.80
1:A:422:THR:HG22	1:A:424:ARG:H	1.47	0.80
1:D:25:CYS:HB2	1:D:45:MET:CE	2.11	0.80
1:B:422:THR:HG22	1:B:424:ARG:H	1.47	0.79
1:C:422:THR:HG22	1:C:424:ARG:H	1.48	0.79
1:C:302:MET:CE	1:C:342:VAL:HA	2.13	0.78
1:D:396:MET:CE	1:D:414:PRO:HG3	2.14	0.78
1:D:261:ALA:HA	1:D:295:ALA:HB3	1.66	0.78
1:E:84:THR:HG21	1:E:211:SER:H	1.48	0.77
1:B:24:ILE:HB	1:B:328:MET:HG3	1.67	0.77
1:C:493:ARG:HH11	1:C:493:ARG:HB3	1.49	0.77
1:E:99:ALA:O	1:E:100:VAL:HG22	1.85	0.77
1:F:396:MET:HE1	1:F:414:PRO:HG3	1.64	0.77
1:A:27:ILE:HD11	1:A:45:MET:HE1	1.67	0.76
1:A:302:MET:CE	1:A:342:VAL:HA	2.15	0.76
1:D:422:THR:HG22	1:D:424:ARG:H	1.48	0.76
1:E:180:PRO:HB3	1:E:268:GLU:OE2	1.85	0.76
1:C:223[A]:ARG:HH11	1:C:223[A]:ARG:CG	2.00	0.75
1:B:151:GLN:HB3	1:B:164:THR:HG22	1.68	0.75
1:E:87:PRO:HD2	1:E:212:PHE:HD2	1.52	0.75
1:F:260:VAL:HG22	1:F:281:LEU:HD12	1.68	0.75
1:A:396:MET:HE2	1:A:414:PRO:HG3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:422:THR:HG22	1:F:424:ARG:H	1.52	0.74
1:E:422:THR:HG22	1:E:424:ARG:H	1.54	0.72
1:C:302:MET:HE1	1:C:342:VAL:HA	1.72	0.72
1:C:15:VAL:HG11	1:C:351:LEU:HD13	1.72	0.72
1:C:223[A]:ARG:HG3	1:C:223[A]:ARG:NH1	1.95	0.72
1:C:25:CYS:HB2	1:C:45:MET:CE	2.21	0.71
1:A:404:ARG:HG2	4:A:1133:HOH:O	1.89	0.71
1:A:100:VAL:HA	1:A:170:THR:HB	1.71	0.70
1:B:136:ARG:HG2	1:B:136:ARG:HH21	1.55	0.70
1:E:110:THR:HG22	1:E:160:THR:HG23	1.72	0.70
1:B:396:MET:HE2	1:B:414:PRO:HG3	1.73	0.70
1:D:24:ILE:HG12	1:D:47:VAL:HB	1.74	0.70
1:A:12:PHE:HZ	1:B:242:HIS:HB2	1.56	0.70
1:B:147:ILE:HD11	4:B:1066:HOH:O	1.91	0.69
1:C:99:ALA:O	1:C:100:VAL:HG22	1.93	0.69
1:C:25:CYS:HB2	1:C:45:MET:HE3	1.74	0.69
1:B:215:SER:HB3	1:B:218:GLN:H	1.58	0.69
1:B:494:ILE:HD12	1:D:380:VAL:HG23	1.74	0.69
1:C:261:ALA:HA	1:C:295:ALA:HB3	1.75	0.69
1:D:109:VAL:HG11	1:D:126:ILE:HD12	1.75	0.68
1:E:396:MET:CE	1:E:414:PRO:HG3	2.23	0.68
1:B:396:MET:HE1	1:B:414:PRO:HG3	1.75	0.68
1:C:84:THR:HG22	1:C:211:SER:HB2	1.75	0.68
1:B:338:TYR:O	1:B:342:VAL:HG23	1.94	0.68
1:E:169:HIS:HB3	4:E:3012:HOH:O	1.92	0.68
1:F:103:ARG:O	1:F:165:VAL:HB	1.94	0.67
1:A:402:THR:HG22	1:A:424:ARG:HH22	1.60	0.67
1:B:158:GLU:HG3	1:B:159:GLN:HG3	1.77	0.67
1:B:302:MET:HB3	1:B:342:VAL:HG22	1.75	0.67
1:B:401:ASN:HA	1:B:422:THR:HG23	1.77	0.66
1:A:108:TYR:HB2	1:A:123:LYS:HB2	1.77	0.66
1:E:120:THR:HG23	1:E:123:LYS:H	1.59	0.66
1:A:260:VAL:O	1:A:295:ALA:HB3	1.96	0.66
1:F:99:ALA:O	1:F:100:VAL:HG22	1.94	0.66
1:B:261:ALA:HA	1:B:295:ALA:HB3	1.75	0.66
1:B:278:GLN:HG2	1:B:282:ILE:HD12	1.76	0.66
1:E:151:GLN:HB3	1:E:164:THR:HG22	1.79	0.66
1:F:400:SER:O	1:F:422:THR:HG23	1.96	0.65
1:B:169:HIS:HB3	4:B:1066:HOH:O	1.95	0.65
1:E:-1:HIS:ND1	4:E:3071:HOH:O	2.30	0.65
1:A:151:GLN:HB3	1:A:164:THR:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ILE:HG12	1:C:47:VAL:HB	1.79	0.65
1:F:47:VAL:HG22	1:F:79:ALA:HB3	1.79	0.65
1:A:89:ILE:HG22	1:A:177:VAL:HB	1.79	0.64
1:A:259:MET:HG2	1:A:295:ALA:HB2	1.80	0.64
1:C:400:SER:O	1:C:422:THR:HG23	1.98	0.64
1:A:248:ILE:HG12	1:A:281:LEU:HD22	1.80	0.64
1:D:378:GLU:HA	1:D:408:LEU:HD21	1.80	0.64
1:A:47:VAL:HG22	1:A:79:ALA:HB3	1.80	0.64
1:A:100:VAL:HG23	1:A:100:VAL:O	1.98	0.63
1:F:81:ALA:HB2	1:F:207:MET:HE2	1.79	0.63
1:C:263:GLY:HA2	1:D:310:ARG:HH12	1.63	0.63
1:D:103:ARG:O	1:D:105:ALA:N	2.30	0.63
1:E:25:CYS:HB2	1:E:45:MET:CE	2.28	0.63
1:E:103:ARG:O	1:E:165:VAL:HB	1.99	0.63
1:E:248:ILE:HG12	1:E:281:LEU:HD22	1.79	0.63
1:B:276:VAL:HG12	1:B:280:ILE:HD11	1.81	0.63
1:C:493:ARG:HB3	1:C:493:ARG:NH1	2.14	0.63
1:D:260:VAL:O	1:D:295:ALA:HB3	1.99	0.63
1:D:298:MET:HE3	1:D:327:VAL:HB	1.79	0.63
1:A:399:LEU:HD12	1:A:453:LYS:HD2	1.82	0.62
1:E:84:THR:HG22	1:E:211:SER:H	1.61	0.62
1:A:7:LEU:HD11	1:B:287:VAL:HG21	1.82	0.62
1:E:298:MET:HE1	1:E:327:VAL:HG12	1.81	0.62
1:C:120:THR:HG23	1:C:123:LYS:H	1.65	0.62
1:C:248:ILE:HG12	1:C:281:LEU:HD22	1.82	0.62
1:F:189:VAL:CG1	1:F:221:ASP:HB3	2.30	0.62
1:F:385:VAL:HG21	1:F:412:TYR:HB2	1.82	0.62
1:A:25:CYS:HB2	1:A:45:MET:HE2	1.81	0.61
1:B:298:MET:HE1	1:B:327:VAL:HG12	1.82	0.61
1:F:396:MET:HE2	1:F:414:PRO:HG3	1.80	0.61
1:E:377:ASP:OD2	1:E:404[B]:ARG:NH1	2.26	0.61
1:E:400:SER:O	1:E:422:THR:HG23	2.01	0.61
1:A:422:THR:HG21	1:A:427:THR:HB	1.81	0.61
1:A:84:THR:HG22	1:A:211:SER:H	1.64	0.61
1:C:83:ASP:HA	1:C:209:PHE:HB2	1.82	0.61
1:E:87:PRO:HD2	1:E:212:PHE:CD2	2.35	0.61
1:E:396:MET:HE2	1:E:414:PRO:HG3	1.82	0.60
1:A:83:ASP:HA	1:A:209:PHE:HB2	1.84	0.60
1:F:258:ILE:O	1:F:292:VAL:HA	2.01	0.60
1:B:458:ALA:O	1:B:462:GLU:HG2	2.01	0.60
1:D:140:TYR:HE2	1:D:151:GLN:HE21	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:ARG:HH12	1:F:263:GLY:HA2	1.67	0.59
1:E:27:ILE:HD12	1:E:37:LEU:HD21	1.83	0.59
1:C:189:VAL:HG12	1:C:221:ASP:HB3	1.85	0.59
1:E:84:THR:CG2	1:E:211:SER:N	2.59	0.59
1:D:298:MET:CE	1:D:327:VAL:HB	2.32	0.59
1:F:83:ASP:HA	1:F:209:PHE:HB2	1.84	0.59
1:F:144:ASP:O	1:F:147:ILE:HG12	2.03	0.59
1:E:24:ILE:HG23	1:E:47:VAL:HG12	1.85	0.59
1:E:99:ALA:O	1:E:100:VAL:CG2	2.51	0.59
1:D:169:HIS:HB3	4:D:2001:HOH:O	2.03	0.58
1:B:47:VAL:HG22	1:B:79:ALA:HB3	1.86	0.58
1:A:428:CYS:SG	1:A:439:SER:HB3	2.44	0.58
1:C:297:GLN:OE1	1:D:310:ARG:NH1	2.37	0.58
1:C:126:ILE:HD13	1:C:177:VAL:HG11	1.85	0.58
1:B:294:CYS:HB3	1:B:298:MET:HE1	1.84	0.58
1:D:248:ILE:HG12	1:D:281:LEU:HD22	1.86	0.58
1:E:238:LYS:HE3	1:E:259:MET:SD	2.43	0.58
1:C:129:GLN:HA	1:C:129:GLN:NE2	2.18	0.58
1:D:109:VAL:CG1	1:D:126:ILE:HD12	2.33	0.58
1:E:27:ILE:HD11	1:E:45:MET:HE1	1.85	0.58
1:D:53:SER:HA	1:D:85:LYS:HG3	1.86	0.57
1:D:380:VAL:HG21	1:D:490:ASN:HB3	1.85	0.57
1:B:27:ILE:HD11	1:B:45:MET:HE1	1.87	0.57
1:E:20:ALA:HB1	1:E:435:GLN:HG2	1.86	0.57
1:C:307:ARG:HG2	1:C:345:TYR:OH	2.04	0.57
1:F:455:HIS:CE1	4:F:3015:HOH:O	2.57	0.57
1:C:151:GLN:HB3	1:C:164:THR:HG22	1.87	0.57
1:E:385:VAL:HG21	1:E:412:TYR:HB2	1.87	0.56
1:D:422:THR:HG21	1:D:427:THR:HB	1.87	0.56
1:C:302:MET:HE3	1:C:342:VAL:HA	1.86	0.56
1:D:84:THR:HG22	1:D:211:SER:H	1.71	0.56
1:F:262:ARG:NH2	1:F:315:ASP:OD2	2.36	0.56
1:D:259:MET:HG2	1:D:295:ALA:HB2	1.86	0.56
1:E:261:ALA:HA	1:E:295:ALA:HB3	1.87	0.56
1:E:259:MET:HG2	1:E:295:ALA:HB2	1.87	0.56
1:E:396:MET:HE1	1:E:409:VAL:HG13	1.87	0.56
1:C:178:ASN:HB3	2:C:505:SO4:O2	2.05	0.56
1:A:396:MET:HE1	1:A:414:PRO:HG3	1.87	0.55
1:B:98:ASP:HB2	1:B:171:ILE:O	2.07	0.55
1:F:100:VAL:HA	1:F:170:THR:HB	1.88	0.55
1:F:135:VAL:HG11	1:F:152:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:CYS:O	1:E:298:MET:HE2	2.07	0.55
1:A:110:THR:HB	1:A:112:ASP:H	1.70	0.55
1:B:108:TYR:HB2	1:B:123:LYS:HB2	1.87	0.55
1:A:110:THR:HA	1:A:159:GLN:O	2.07	0.55
1:C:189:VAL:CG1	1:C:221:ASP:HB3	2.36	0.55
1:D:103:ARG:C	1:D:105:ALA:H	2.10	0.55
1:D:24:ILE:HB	1:D:328:MET:HG3	1.88	0.55
1:C:147:ILE:O	1:C:167:ASN:ND2	2.39	0.55
1:B:180:PRO:HB3	1:B:268:GLU:OE2	2.07	0.55
1:A:99:ALA:O	1:A:100:VAL:HG22	2.06	0.55
1:D:25:CYS:HB2	1:D:45:MET:HE2	1.88	0.54
1:D:153:GLN:HE21	1:D:164:THR:CG2	2.20	0.54
1:E:396:MET:HE3	1:E:414:PRO:HG3	1.89	0.54
1:A:265:LEU:O	1:A:269:ILE:HB	2.06	0.54
1:A:302:MET:HE3	1:A:342:VAL:HG13	1.90	0.54
1:F:374:MET:HE2	1:F:378:GLU:HG3	1.90	0.54
1:E:215:SER:HB2	1:E:218:GLN:H	1.72	0.54
1:F:108:TYR:HB2	1:F:123:LYS:HB2	1.90	0.54
1:E:26:THR:OG1	1:E:49:ARG:HD3	2.08	0.53
1:C:396:MET:HE3	1:C:418:ILE:HG12	1.90	0.53
1:D:1:SER:HA	1:D:361:VAL:HG21	1.90	0.53
1:E:129:GLN:HE21	1:E:129:GLN:HA	1.74	0.53
1:F:260:VAL:O	1:F:295:ALA:HB3	2.09	0.53
1:C:87:PRO:HD2	1:C:212:PHE:HD2	1.73	0.53
1:B:400:SER:O	1:B:422:THR:HG23	2.09	0.53
1:C:25:CYS:HB2	1:C:45:MET:HE2	1.91	0.53
1:A:25:CYS:CB	1:A:45:MET:HE3	2.26	0.53
1:B:20:ALA:HB1	1:B:435:GLN:HG2	1.91	0.53
1:F:108:TYR:O	1:F:123:LYS:HA	2.09	0.53
1:F:137:PRO:HB3	1:F:153:GLN:O	2.09	0.53
1:A:98:ASP:HB3	1:A:172:SER:HA	1.91	0.52
1:D:84:THR:CG2	1:D:211:SER:H	2.22	0.52
1:E:25:CYS:HB2	1:E:45:MET:HE3	1.90	0.52
1:B:268:GLU:HG2	4:B:1049:HOH:O	2.09	0.52
1:E:210:ALA:HB1	1:E:213:ILE:HD11	1.90	0.52
1:C:260:VAL:O	1:C:295:ALA:HB3	2.09	0.52
1:F:263:GLY:N	1:F:296:THR:OG1	2.33	0.52
1:F:298:MET:HE1	1:F:327:VAL:HG12	1.92	0.52
1:C:103:ARG:O	1:C:165:VAL:HB	2.09	0.52
1:C:283:SER:HA	4:C:2071:HOH:O	2.09	0.52
1:D:481:ALA:O	1:D:482:ASP:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HD23	1:D:45:MET:HE3	1.92	0.52
1:B:371:HIS:HE1	4:B:1026:HOH:O	1.91	0.52
1:F:129:GLN:HE21	1:F:129:GLN:HA	1.75	0.52
1:F:449:HIS:CD2	1:F:451:TRP:CZ2	2.97	0.52
1:C:396:MET:HE2	1:C:414:PRO:HG3	1.90	0.52
1:D:332:GLU:O	1:D:336:GLY:HA3	2.09	0.52
1:F:190:SER:N	1:F:193:ASP:HB2	2.24	0.52
1:B:258:ILE:O	1:B:292:VAL:HA	2.10	0.51
1:A:217:GLU:HG2	1:A:217:GLU:O	2.10	0.51
1:E:242:HIS:HB2	1:F:12:PHE:CZ	2.45	0.51
1:A:89:ILE:CG2	1:A:177:VAL:HB	2.40	0.51
1:A:422:THR:HG22	1:A:424:ARG:N	2.21	0.51
1:B:376:ALA:O	1:B:380:VAL:HG23	2.09	0.51
1:C:109:VAL:HG11	1:C:126:ILE:HD12	1.93	0.51
1:B:103:ARG:O	1:B:165:VAL:O	2.29	0.51
1:B:289:GLY:HA3	1:B:411:LYS:HD2	1.93	0.51
1:C:47:VAL:HG22	1:C:79:ALA:HB3	1.93	0.51
1:C:231:ARG:HD2	4:C:2023:HOH:O	2.11	0.51
1:E:40:LEU:HD23	1:E:45:MET:HE3	1.93	0.51
1:E:84:THR:HG22	1:E:211:SER:N	2.23	0.51
1:E:242:HIS:HB2	1:F:12:PHE:HZ	1.76	0.51
1:B:426:GLN:O	1:B:430:GLN:HG3	2.10	0.50
1:A:76:VAL:HG23	1:A:78:ILE:HG12	1.93	0.50
1:C:261:ALA:HA	1:C:295:ALA:CB	2.41	0.50
3:E:508:GOL:H32	4:E:3046:HOH:O	2.11	0.50
1:B:25:CYS:HB2	1:B:45:MET:CE	2.41	0.50
1:B:278:GLN:HG2	1:B:282:ILE:CD1	2.41	0.50
1:D:299:LEU:HA	1:D:312:GLU:HG2	1.93	0.50
1:E:131:LEU:HD11	1:E:179:LEU:HD21	1.94	0.50
1:A:302:MET:SD	1:A:308:PRO:HD3	2.52	0.50
1:C:259:MET:HG2	1:C:295:ALA:HB2	1.94	0.50
1:C:316:VAL:HB	1:C:349:ILE:HG21	1.93	0.50
1:E:170:THR:HG22	4:E:4111:HOH:O	2.11	0.50
1:F:47:VAL:HG11	1:F:207:MET:HE1	1.94	0.50
1:B:24:ILE:CB	1:B:328:MET:HG3	2.41	0.50
1:C:17:ASN:O	1:C:18[A]:TYR:HB3	2.12	0.50
1:C:84:THR:HG22	1:C:211:SER:H	1.77	0.50
1:A:12:PHE:CZ	1:B:242:HIS:HB2	2.42	0.49
1:D:83:ASP:HA	1:D:209:PHE:HB2	1.94	0.49
1:F:275:VAL:O	1:F:278:GLN:HB3	2.12	0.49
1:C:81:ALA:HB2	1:C:207:MET:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:TYR:O	1:C:123:LYS:HA	2.12	0.49
1:D:108:TYR:O	1:D:123:LYS:HA	2.13	0.49
1:E:109:VAL:HG11	1:E:126:ILE:HD12	1.94	0.49
1:F:218:GLN:O	1:F:221:ASP:HB2	2.12	0.49
1:B:24:ILE:HG12	1:B:47:VAL:HB	1.92	0.49
1:B:135:VAL:HG11	1:B:152:VAL:HG21	1.92	0.49
1:C:100:VAL:HG12	1:C:170:THR:HB	1.94	0.49
1:C:15:VAL:CG1	1:C:351:LEU:HD13	2.42	0.49
1:F:18:TYR:CG	1:F:18:TYR:O	2.66	0.49
1:F:214:ARG:O	1:F:251:ILE:HD11	2.12	0.49
1:C:167:ASN:HD21	1:D:307:ARG:HH12	1.61	0.49
1:F:302:MET:HE1	1:F:342:VAL:HA	1.93	0.49
1:E:471:GLN:H	1:E:474:ASP:HB2	1.78	0.49
1:F:142:TYR:CE1	1:F:180:PRO:HG3	2.47	0.49
1:B:108:TYR:O	1:B:123:LYS:HA	2.12	0.48
1:D:260:VAL:HG22	1:D:281:LEU:HD12	1.93	0.48
1:B:110:THR:HG22	1:B:160:THR:OG1	2.13	0.48
1:B:136:ARG:HG2	1:B:136:ARG:NH2	2.26	0.48
1:B:302:MET:SD	1:B:308:PRO:HD3	2.53	0.48
1:F:302:MET:HB3	1:F:342:VAL:HG23	1.95	0.48
1:B:376:ALA:HB2	1:D:475:TYR:CE1	2.48	0.48
1:B:261:ALA:HA	1:B:295:ALA:HB1	1.91	0.48
1:D:260:VAL:O	1:D:295:ALA:CB	2.62	0.48
1:C:407:ARG:HG3	1:C:434:THR:HG21	1.95	0.48
1:F:99:ALA:O	1:F:100:VAL:CG2	2.60	0.48
1:B:482:ASP:HB2	4:B:1132:HOH:O	2.13	0.48
1:C:422:THR:HG21	1:C:427:THR:HB	1.95	0.48
1:F:189:VAL:HG11	1:F:221:ASP:HB3	1.94	0.48
1:D:129:GLN:HA	1:D:129:GLN:NE2	2.28	0.48
1:D:253:GLU:O	1:D:253:GLU:HG3	2.13	0.48
1:F:479:ILE:HG12	1:F:480:HIS:N	2.28	0.48
1:D:27:ILE:HG21	1:D:63:THR:HG23	1.96	0.48
1:A:396:MET:HG2	1:A:477:VAL:HB	1.95	0.48
1:C:378:GLU:HA	1:C:408:LEU:HD21	1.94	0.48
1:E:11:ILE:HD11	1:F:245:VAL:HG11	1.96	0.48
1:E:378:GLU:OE1	1:E:408:LEU:HD11	2.14	0.48
1:F:248:ILE:HG12	1:F:281:LEU:HD22	1.96	0.48
1:D:386:ASN:O	1:D:390:GLU:HG3	2.14	0.48
1:E:214:ARG:O	1:E:251:ILE:HD11	2.13	0.48
1:C:-1:HIS:CE1	1:C:5:HIS:HB2	2.49	0.47
1:B:41:ILE:HG12	1:B:78:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:GLN:CB	4:D:2149:HOH:O	2.62	0.47
1:C:418:ILE:HB	1:C:437:VAL:HG22	1.95	0.47
1:D:261:ALA:HA	1:D:295:ALA:CB	2.39	0.47
1:F:120:THR:HG23	1:F:123:LYS:H	1.79	0.47
1:F:413:ARG:NH1	1:F:435:GLN:HG3	2.30	0.47
1:C:431:LEU:HD13	1:C:437:VAL:HG11	1.96	0.47
1:D:398:VAL:O	1:D:420:CYS:HA	2.13	0.47
1:E:24:ILE:HG12	1:E:47:VAL:HB	1.96	0.47
1:E:246:GLN:HG3	1:F:12:PHE:CE2	2.50	0.47
1:B:99:ALA:O	1:B:100:VAL:CG2	2.51	0.47
1:A:275:VAL:O	1:A:278:GLN:HB3	2.14	0.47
1:A:345:TYR:O	1:A:349:ILE:HG13	2.13	0.47
1:D:396:MET:HG2	1:D:477:VAL:HB	1.96	0.47
1:A:27:ILE:CD1	1:A:45:MET:HE1	2.40	0.47
1:B:293:ILE:HG12	1:B:326:CYS:HB2	1.96	0.47
1:C:40:LEU:HD11	1:C:339:PRO:HB2	1.97	0.47
1:C:103:ARG:O	1:C:105:ALA:N	2.47	0.47
1:F:5:HIS:CD2	1:F:358:ASN:HB2	2.50	0.47
1:A:285:CYS:HB3	1:A:290:LYS:O	2.15	0.47
1:D:307:ARG:HD2	4:D:2123:HOH:O	2.14	0.47
1:E:341:GLU:OE1	1:E:341:GLU:N	2.42	0.47
1:B:238:LYS:HE3	1:B:259:MET:SD	2.55	0.47
1:D:120:THR:HG23	1:D:123:LYS:H	1.79	0.47
1:A:100:VAL:O	1:A:100:VAL:CG2	2.63	0.47
1:A:370:GLN:HG3	1:A:412:TYR:OH	2.15	0.47
1:A:390:GLU:HB3	1:C:374:MET:SD	2.55	0.47
1:E:450:ASP:CG	1:E:455:HIS:HB2	2.35	0.47
1:A:289:GLY:HA3	1:A:411:LYS:HD2	1.96	0.46
1:C:54:HIS:ND1	2:C:503:SO4:O2	2.46	0.46
1:F:126:ILE:HG22	1:F:128:TYR:H	1.80	0.46
1:F:282:ILE:HA	1:F:292:VAL:HG11	1.97	0.46
1:B:425:LEU:HD13	1:B:441:PHE:CD1	2.49	0.46
1:C:87:PRO:HG3	1:C:188:ALA:HA	1.96	0.46
1:C:103:ARG:C	1:C:105:ALA:H	2.18	0.46
1:D:299:LEU:HD23	1:D:312:GLU:HB3	1.96	0.46
1:A:338:TYR:O	1:A:342:VAL:CG2	2.47	0.46
1:D:370:GLN:HG3	1:D:412:TYR:OH	2.16	0.46
1:D:422:THR:HG21	1:D:427:THR:CB	2.46	0.46
1:D:144:ASP:OD2	1:D:175:ARG:HD3	2.16	0.46
1:F:165:VAL:HG12	1:F:167:ASN:O	2.15	0.46
1:E:451:TRP:HA	1:E:451:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:THR:CG2	1:C:211:SER:H	2.29	0.45
1:E:94:PHE:HE1	1:E:124:PHE:HB3	1.80	0.45
1:C:240:GLU:HG2	1:C:264:ASP:HB2	1.98	0.45
1:D:153:GLN:HE21	1:D:164:THR:HG22	1.81	0.45
1:E:278:GLN:HG2	1:E:282:ILE:HD12	1.97	0.45
1:F:207:MET:CE	1:F:433:ILE:HG21	2.47	0.45
1:B:265:LEU:HB3	1:B:269:ILE:HD12	1.98	0.45
1:C:2:GLN:HB2	4:D:2149:HOH:O	2.17	0.45
1:E:89:ILE:HD11	1:E:184:VAL:HG11	1.98	0.45
1:F:180:PRO:HB3	1:F:268:GLU:OE2	2.17	0.45
1:E:246:GLN:HG3	1:F:12:PHE:HE2	1.81	0.45
1:F:458:ALA:O	1:F:462[A]:GLU:HG2	2.16	0.45
1:A:429:ARG:O	1:A:432:ASN:HB2	2.16	0.45
1:B:481:ALA:O	1:B:482:ASP:HB3	2.17	0.45
1:C:403:GLY:O	1:C:404:ARG:C	2.55	0.45
1:C:426:GLN:O	1:C:430:GLN:HG3	2.16	0.45
1:D:46:SER:HB3	1:D:432:ASN:HB3	1.99	0.45
1:E:25:CYS:HB2	1:E:45:MET:HE2	1.98	0.45
1:F:289:GLY:HA3	1:F:411:LYS:HD2	1.98	0.45
1:D:400:SER:O	1:D:422:THR:HG23	2.16	0.45
1:F:110:THR:CG2	1:F:123:LYS:HD3	2.47	0.45
1:B:294:CYS:O	1:B:298:MET:HE2	2.17	0.45
1:D:17:ASN:O	1:D:18:TYR:HB3	2.17	0.45
1:B:298:MET:HE3	1:B:327:VAL:HB	1.99	0.45
1:B:488:TYR:HB3	4:B:1008:HOH:O	2.16	0.45
1:C:271:ALA:O	1:C:274:VAL:HB	2.17	0.45
1:F:374:MET:HE3	1:F:378:GLU:HG2	1.99	0.45
1:C:218:GLN:O	1:C:221:ASP:HB2	2.17	0.45
1:F:47:VAL:HG21	1:F:433:ILE:HG22	1.99	0.45
1:B:403:GLY:HA3	1:B:407:ARG:NH2	2.32	0.44
1:C:416:CYS:HB2	1:C:417:PRO:CD	2.47	0.44
1:A:180:PRO:HB3	1:A:268:GLU:OE2	2.16	0.44
1:C:458:ALA:O	1:C:462:GLU:HB2	2.16	0.44
1:F:112:ASP:HA	1:F:113:PRO:HD2	1.85	0.44
1:A:85:LYS:O	1:A:88:GLU:HG3	2.17	0.44
1:D:211:SER:HA	1:D:238:LYS:HB2	2.00	0.44
1:A:297:GLN:OE1	1:B:310:ARG:NH1	2.51	0.44
1:A:422:THR:HG21	1:A:427:THR:CB	2.47	0.44
1:B:201:VAL:HG22	1:B:233:ILE:HD12	1.99	0.44
1:C:332:GLU:O	1:C:336:GLY:HA3	2.18	0.44
1:C:376:ALA:O	1:C:380:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:VAL:HG11	1:D:80:ILE:HG12	1.99	0.44
1:E:6:ASN:ND2	1:F:279:LYS:HB3	2.33	0.44
1:F:98:ASP:HB2	1:F:171:ILE:O	2.17	0.44
1:C:5:HIS:CD2	1:C:358:ASN:HB2	2.53	0.44
1:C:23:ILE:HG12	1:C:346:MET:HG2	1.99	0.44
1:C:57:HIS:O	1:C:61:GLN:N	2.41	0.44
1:D:103:ARG:O	1:D:165:VAL:HB	2.17	0.44
1:B:248:ILE:HG12	1:B:281:LEU:CD2	2.41	0.44
1:E:108:TYR:O	1:E:123:LYS:HA	2.18	0.44
1:F:45:MET:HE2	1:F:48:ALA:HA	1.99	0.44
1:C:87:PRO:HD2	1:C:212:PHE:CD2	2.51	0.44
1:D:140:TYR:O	1:D:180:PRO:HD2	2.18	0.44
1:D:293:ILE:HG23	1:D:326:CYS:HB2	2.00	0.44
1:E:24:ILE:HG23	1:E:47:VAL:CG1	2.48	0.44
1:B:422:THR:HG22	1:B:424:ARG:N	2.25	0.44
1:A:216:ALA:HB3	4:A:1073:HOH:O	2.18	0.43
1:B:385:VAL:HG11	1:B:412:TYR:O	2.18	0.43
1:C:139:ASN:HD22	1:C:139:ASN:N	2.14	0.43
1:D:302:MET:HB3	1:D:342:VAL:HG23	2.00	0.43
1:F:340:ASN:HB3	1:F:344:GLN:HE21	1.83	0.43
1:E:422:THR:HG21	1:E:427:THR:HB	2.00	0.43
1:F:214:ARG:HD2	1:F:218:GLN:HE22	1.83	0.43
1:A:454:GLU:HG2	1:A:455:HIS:N	2.33	0.43
1:C:96:GLY:O	1:C:97:GLY:C	2.56	0.43
1:D:6:ASN:HA	1:D:9:LEU:HD12	2.00	0.43
1:D:332:GLU:CD	1:D:332:GLU:H	2.20	0.43
1:E:51:ASN:HA	1:E:83:ASP:HB3	1.98	0.43
1:A:24:ILE:HG23	1:A:47:VAL:HG12	2.00	0.43
1:D:84:THR:HB	1:D:210:ALA:HA	2.00	0.43
1:D:453:LYS:O	1:D:457:VAL:HG23	2.17	0.43
1:E:365:SER:HB3	1:F:3:LEU:HD22	1.99	0.43
1:A:279:LYS:HB3	1:B:6:ASN:ND2	2.34	0.43
1:B:165:VAL:HG12	1:B:167:ASN:O	2.18	0.43
1:B:310:ARG:HG2	1:B:310:ARG:HH11	1.84	0.43
1:F:189:VAL:HG12	1:F:221:ASP:HB3	1.98	0.43
1:A:493:ARG:HD2	4:A:1005:HOH:O	2.18	0.43
1:B:339:PRO:HD2	4:B:1095:HOH:O	2.18	0.43
1:F:138:GLY:HA2	1:F:151:GLN:HE21	1.84	0.43
1:E:100:VAL:HG12	1:E:170:THR:HB	2.00	0.43
1:F:262:ARG:NH1	1:F:278:GLN:OE1	2.50	0.43
1:F:425:LEU:HD22	1:F:441:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HG21	1:A:328:MET:HE2	2.01	0.43
1:A:84:THR:HG22	1:A:211:SER:N	2.32	0.43
1:B:56:SER:O	1:B:60:HIS:CD2	2.72	0.43
1:B:186:LEU:HA	1:B:187:PRO:HD3	1.88	0.43
1:D:302:MET:CB	1:D:342:VAL:HG23	2.48	0.43
1:A:54:HIS:ND1	2:A:503:SO4:O3	2.44	0.42
1:A:63:THR:O	1:A:67:VAL:HG23	2.19	0.42
1:A:156:GLU:HB3	1:A:160:THR:HB	2.01	0.42
1:A:109:VAL:HG11	1:A:126:ILE:HD12	2.01	0.42
1:A:113:PRO:C	1:A:115:PHE:H	2.22	0.42
1:C:186:LEU:HA	1:C:187:PRO:HD3	1.91	0.42
1:D:431:LEU:HD23	1:D:431:LEU:HA	1.88	0.42
1:F:259:MET:HG2	1:F:295:ALA:HB2	2.00	0.42
1:F:298:MET:HE3	1:F:327:VAL:HB	2.01	0.42
1:F:354:GLN:C	1:F:356:ALA:H	2.22	0.42
1:F:417:PRO:HG2	1:F:469:TYR:CG	2.54	0.42
1:C:282:ILE:HG23	1:C:292:VAL:HG11	2.00	0.42
1:D:18:TYR:O	1:D:18:TYR:CG	2.72	0.42
1:A:109:VAL:O	1:A:160:THR:HA	2.20	0.42
1:A:129:GLN:HA	1:A:129:GLN:NE2	2.21	0.42
1:A:461:VAL:O	1:A:464:ALA:HB3	2.19	0.42
1:C:83:ASP:CG	1:C:238:LYS:HZ2	2.22	0.42
1:E:384:ALA:O	1:E:387:SER:HB2	2.19	0.42
1:A:1:SER:HA	1:A:361:VAL:HG21	2.02	0.42
1:E:293:ILE:HG23	1:E:326:CYS:HB2	2.02	0.42
1:F:143:ILE:HB	1:F:148:LEU:HD23	2.02	0.42
1:F:367:LYS:C	1:F:369:LEU:H	2.22	0.42
1:A:380:VAL:HG21	1:A:490:ASN:HB3	2.01	0.42
1:A:385:VAL:HG21	1:A:412:TYR:HB2	2.00	0.42
1:B:0:MET:HG2	1:B:1:SER:H	1.85	0.42
1:C:142:TYR:CE1	1:C:180:PRO:HG3	2.54	0.42
1:E:12:PHE:HZ	1:F:242:HIS:HB2	1.84	0.42
1:A:337:LYS:O	1:A:337:LYS:HG2	2.20	0.42
1:B:260:VAL:O	1:B:295:ALA:CB	2.68	0.42
1:C:215:SER:HB2	1:C:218:GLN:HG3	2.01	0.42
1:E:398:VAL:HG11	1:E:406:ALA:HA	2.00	0.42
1:C:99:ALA:O	1:C:100:VAL:CG2	2.63	0.42
1:D:110:THR:HB	1:D:160:THR:HG23	2.00	0.42
1:F:110:THR:HG22	1:F:160:THR:CG2	2.35	0.42
1:F:134:VAL:HG22	1:F:134:VAL:O	2.20	0.42
1:A:239:ILE:HG13	1:A:248:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:THR:HA	1:C:159:GLN:O	2.20	0.42
1:E:407:ARG:HG3	1:E:434:THR:HG21	2.01	0.42
1:C:361:VAL:O	1:C:365:SER:HB2	2.20	0.41
1:C:452:GLY:C	1:C:454:GLU:H	2.22	0.41
1:A:52:PHE:CE1	1:A:82:LEU:HG	2.55	0.41
1:A:84:THR:CG2	1:A:211:SER:H	2.30	0.41
1:C:223[B]:ARG:HG3	1:C:235:ILE:HD12	2.02	0.41
1:E:47:VAL:HG22	1:E:79:ALA:HB3	2.01	0.41
1:B:341:GLU:OE1	4:B:1095:HOH:O	2.22	0.41
1:C:144:ASP:O	1:C:147:ILE:HG12	2.20	0.41
1:C:150:LEU:HD22	1:C:165:VAL:HG22	2.01	0.41
1:D:27:ILE:HD11	1:D:45:MET:HE1	2.01	0.41
1:F:140:TYR:HA	1:F:150:LEU:O	2.20	0.41
1:F:171:ILE:HB	1:F:175:ARG:HG3	2.02	0.41
1:F:425:LEU:HD13	1:F:441:PHE:CD1	2.55	0.41
1:B:494:ILE:O	1:D:490:ASN:ND2	2.53	0.41
1:C:26:THR:HA	1:C:49:ARG:HB3	2.01	0.41
1:F:405:SER:O	1:F:409:VAL:HG23	2.20	0.41
1:A:264:ASP:HA	1:A:267:VAL:HG23	2.02	0.41
1:A:299:LEU:HD21	1:A:316:VAL:HG21	2.02	0.41
1:B:34:VAL:HG23	1:B:35:GLU:H	1.85	0.41
1:B:251:ILE:O	1:B:255:SER:HB3	2.20	0.41
1:C:312:GLU:O	1:C:316:VAL:HG23	2.21	0.41
1:D:258:ILE:O	1:D:292:VAL:HA	2.19	0.41
1:E:422:THR:HG21	1:E:427:THR:CB	2.50	0.41
1:A:332:GLU:HB3	1:A:342:VAL:HG11	2.03	0.41
1:D:64:ILE:O	1:D:68:ARG:HB2	2.21	0.41
1:F:261:ALA:HA	1:F:295:ALA:HB3	2.01	0.41
1:A:132:SER:HB3	1:A:161:LEU:HD21	2.03	0.41
1:A:348:ARG:HH11	1:A:348:ARG:HD2	1.75	0.41
1:C:2:GLN:HB3	4:D:2149:HOH:O	2.21	0.41
1:C:309:THR:O	1:C:310:ARG:C	2.59	0.41
1:E:38:LYS:HD2	1:E:74:LEU:HD21	2.03	0.41
1:E:94:PHE:HE1	1:E:124:PHE:CB	2.33	0.41
1:F:169:HIS:HB3	4:F:3002:HOH:O	2.20	0.41
1:E:12:PHE:HE2	1:F:246:GLN:HG3	1.86	0.41
1:E:108:TYR:HB2	1:E:123:LYS:CB	2.50	0.41
1:E:131:LEU:CD1	1:E:179:LEU:HD21	2.51	0.41
1:E:186:LEU:HA	1:E:187:PRO:HD3	1.92	0.41
1:E:240:GLU:HG2	1:E:264:ASP:HB2	2.02	0.41
1:A:402:THR:HG22	1:A:424:ARG:NH2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:VAL:HB	1:B:497:VAL:HG21	2.02	0.41
1:C:239:ILE:HG22	1:C:265:LEU:HD21	2.03	0.41
1:C:258:ILE:HB	1:C:285:CYS:SG	2.61	0.41
1:D:59:TYR:O	1:D:62:THR:HB	2.21	0.41
1:E:15:VAL:O	1:E:16:ALA:C	2.58	0.41
1:F:389:TYR:CE1	1:F:415:ASN:ND2	2.89	0.41
1:F:455:HIS:HE1	4:F:3015:HOH:O	2.00	0.41
1:B:89:ILE:HG23	1:B:128:TYR:HB2	2.03	0.41
1:B:129:GLN:HE21	1:B:129:GLN:HA	1.85	0.41
1:B:276:VAL:HG12	1:B:280:ILE:CD1	2.49	0.41
1:B:298:MET:HE3	1:B:328:MET:H	1.86	0.41
1:D:215:SER:HB2	1:D:218:GLN:HG3	2.03	0.41
1:E:47:VAL:HG21	1:E:433:ILE:HG23	2.03	0.41
1:A:331:GLY:HA2	1:A:334:ALA:HB3	2.02	0.40
1:D:144:ASP:O	1:D:147:ILE:HG12	2.22	0.40
1:D:298:MET:CE	1:D:327:VAL:CB	2.99	0.40
1:F:413:ARG:HH12	1:F:435:GLN:HG3	1.86	0.40
1:B:25:CYS:HB2	1:B:45:MET:HE2	2.02	0.40
1:C:95:VAL:HG23	1:C:119:GLY:O	2.21	0.40
1:C:298:MET:HE3	1:C:327:VAL:HB	2.03	0.40
1:D:400:SER:HB2	1:D:405:SER:HB2	2.04	0.40
1:E:12:PHE:CZ	1:F:242:HIS:HB2	2.56	0.40
1:B:112:ASP:HA	1:B:113:PRO:HD2	1.94	0.40
1:C:45:MET:HE1	1:C:48:ALA:HA	2.04	0.40
1:A:396:MET:HE3	1:A:418:ILE:HG12	2.04	0.40
1:C:431:LEU:HD23	1:C:431:LEU:HA	1.97	0.40
1:D:328:MET:HB3	1:D:328:MET:HE3	1.81	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	492/539 (91%)	448 (91%)	37 (8%)	7 (1%)	11	38
1	B	494/539 (92%)	437 (88%)	51 (10%)	6 (1%)	13	42
1	C	494/539 (92%)	454 (92%)	32 (6%)	8 (2%)	9	36
1	D	492/539 (91%)	452 (92%)	33 (7%)	7 (1%)	11	38
1	E	494/539 (92%)	445 (90%)	44 (9%)	5 (1%)	15	46
1	F	495/539 (92%)	456 (92%)	36 (7%)	3 (1%)	25	57
All	All	2961/3234 (92%)	2692 (91%)	233 (8%)	36 (1%)	13	42

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLY
1	B	490	ASN
1	D	18	TYR
1	D	100	VAL
1	D	103	ARG
1	D	490	ASN
1	E	103	ARG
1	F	103	ARG
1	A	103	ARG
1	B	100	VAL
1	C	18[A]	TYR
1	C	18[B]	TYR
1	C	174	ARG
1	D	104	GLY
1	A	356	ALA
1	B	2	GLN
1	C	103	ARG
1	D	450	ASP
1	E	128	TYR
1	E	330	SER
1	F	331	GLY
1	A	174	ARG
1	A	472	THR
1	B	174	ARG
1	C	104	GLY
1	A	145	ASP
1	B	14	PRO
1	A	100	VAL
1	C	253	GLU
1	E	472	THR

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Mol	Chain	Res	Type
1	C	497	VAL
1	D	497	VAL
1	E	100	VAL
1	C	100	VAL
1	F	100	VAL
1	B	44	GLY

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	415/451 (92%)	381 (92%)	34 (8%)	11	36
1	B	416/451 (92%)	370 (89%)	46 (11%)	6	23
1	C	417/451 (92%)	383 (92%)	34 (8%)	11	36
1	D	415/451 (92%)	380 (92%)	35 (8%)	11	35
1	E	417/451 (92%)	375 (90%)	42 (10%)	7	27
1	F	417/451 (92%)	378 (91%)	39 (9%)	8	30
All	All	2497/2706 (92%)	2267 (91%)	230 (9%)	9	31

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	35	GLU
1	A	40	LEU
1	A	69	GLN
1	A	84	THR
1	A	101	MET
1	A	110	THR
1	A	117	ASP
1	A	120	THR
1	A	121	LYS
1	A	123	LYS
1	A	129	GLN

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Mol	Chain	Res	Type
1	A	132	SER
1	A	134	VAL
1	A	166	THR
1	A	170	THR
1	A	217	GLU
1	A	243	GLN
1	A	253	GLU
1	A	262	ARG
1	A	268	GLU
1	A	287	VAL
1	A	296	THR
1	A	298	MET
1	A	345	TYR
1	A	351	LEU
1	A	362	PHE
1	A	364	ASN
1	A	401	ASN
1	A	424	ARG
1	A	434	THR
1	A	435	GLN
1	A	445	ASP
1	A	479	ILE
1	B	0	MET
1	B	3	LEU
1	B	15	VAL
1	B	34	VAL
1	B	35	GLU
1	B	40	LEU
1	B	42	GLN
1	B	46	SER
1	B	68	ARG
1	B	101	MET
1	B	106	THR
1	B	117	ASP
1	B	120	THR
1	B	121	LYS
1	B	123	LYS
1	B	129	GLN
1	B	132	SER
1	B	136	ARG
1	B	145	ASP
1	B	147	ILE

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Mol	Chain	Res	Type
1	B	164	THR
1	B	166	THR
1	B	183	ASP
1	B	214	ARG
1	B	215	SER
1	B	231	ARG
1	B	253	GLU
1	B	262	ARG
1	B	281	LEU
1	B	296	THR
1	B	328	MET
1	B	345	TYR
1	B	351	LEU
1	B	357	LEU
1	B	362	PHE
1	B	401	ASN
1	B	402	THR
1	B	404	ARG
1	B	425	LEU
1	B	434	THR
1	B	435	GLN
1	B	439	SER
1	B	445	ASP
1	B	479	ILE
1	B	490	ASN
1	B	496	LEU
1	C	0	MET
1	C	68	ARG
1	C	69	GLN
1	C	84	THR
1	C	101	MET
1	C	110	THR
1	C	121	LYS
1	C	145	ASP
1	C	164	THR
1	C	170	THR
1	C	223[A]	ARG
1	C	223[B]	ARG
1	C	231	ARG
1	C	242	HIS
1	C	243	GLN
1	C	253	GLU

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Mol	Chain	Res	Type
1	C	262	ARG
1	C	281	LEU
1	C	296	THR
1	C	351	LEU
1	C	357	LEU
1	C	361	VAL
1	C	362	PHE
1	C	365	SER
1	C	404	ARG
1	C	434	THR
1	C	435	GLN
1	C	439	SER
1	C	445	ASP
1	C	454	GLU
1	C	462	GLU
1	C	479	ILE
1	C	492	THR
1	C	493	ARG
1	D	0	MET
1	D	3	LEU
1	D	45	MET
1	D	84	THR
1	D	101	MET
1	D	103	ARG
1	D	110	THR
1	D	120	THR
1	D	121	LYS
1	D	123	LYS
1	D	129	GLN
1	D	132	SER
1	D	135	VAL
1	D	166	THR
1	D	170	THR
1	D	183	ASP
1	D	243	GLN
1	D	253	GLU
1	D	254	GLU
1	D	296	THR
1	D	314	SER
1	D	335	LYS
1	D	342	VAL
1	D	345	TYR

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Mol	Chain	Res	Type
1	D	351	LEU
1	D	357	LEU
1	D	362	PHE
1	D	377	ASP
1	D	422	THR
1	D	424	ARG
1	D	435	GLN
1	D	439	SER
1	D	479	ILE
1	D	490	ASN
1	D	491	GLN
1	E	0	MET
1	E	1	SER
1	E	40	LEU
1	E	42	GLN
1	E	68	ARG
1	E	69	GLN
1	E	95	VAL
1	E	98	ASP
1	E	101	MET
1	E	121	LYS
1	E	129	GLN
1	E	147	ILE
1	E	159	GLN
1	E	164	THR
1	E	166	THR
1	E	167	ASN
1	E	172	SER
1	E	183	ASP
1	E	231	ARG
1	E	253	GLU
1	E	262	ARG
1	E	268	GLU
1	E	281	LEU
1	E	283	SER
1	E	296	THR
1	E	298	MET
1	E	314	SER
1	E	342	VAL
1	E	345	TYR
1	E	351	LEU
1	E	357	LEU

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Mol	Chain	Res	Type
1	E	380	VAL
1	E	396	MET
1	E	422	THR
1	E	425	LEU
1	E	434	THR
1	E	435	GLN
1	E	449	HIS
1	E	454	GLU
1	E	479	ILE
1	E	491	GLN
1	E	492	THR
1	F	0	MET
1	F	40	LEU
1	F	101	MET
1	F	106	THR
1	F	117	ASP
1	F	120	THR
1	F	121	LYS
1	F	123	LYS
1	F	129	GLN
1	F	132	SER
1	F	164	THR
1	F	166	THR
1	F	169	HIS
1	F	170	THR
1	F	183	ASP
1	F	186	LEU
1	F	231	ARG
1	F	262	ARG
1	F	268	GLU
1	F	287	VAL
1	F	314	SER
1	F	342	VAL
1	F	345[A]	TYR
1	F	345[B]	TYR
1	F	351	LEU
1	F	357	LEU
1	F	365	SER
1	F	380	VAL
1	F	401	ASN
1	F	422	THR
1	F	425	LEU

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Mol	Chain	Res	Type
1	F	426	GLN
1	F	434	THR
1	F	435	GLN
1	F	439	SER
1	F	445	ASP
1	F	454	GLU
1	F	479	ILE
1	F	490	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	69	GLN
1	A	129	GLN
1	A	139	ASN
1	A	243	GLN
1	A	286	ASN
1	A	322	ASN
1	A	370	GLN
1	A	401	ASN
1	B	129	GLN
1	B	159	GLN
1	B	178	ASN
1	B	401	ASN
1	B	491	GLN
1	C	5	HIS
1	C	129	GLN
1	C	139	ASN
1	C	243	GLN
1	C	286	ASN
1	C	305	ASN
1	C	322	ASN
1	C	401	ASN
1	C	435	GLN
1	C	491	GLN
1	D	6	ASN
1	D	129	GLN
1	D	151	GLN
1	D	153	GLN
1	D	243	GLN
1	D	286	ASN

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Mol	Chain	Res	Type
1	D	305	ASN
1	E	129	GLN
1	E	159	GLN
1	E	178	ASN
1	E	401	ASN
1	F	129	GLN
1	F	139	ASN
1	F	151	GLN
1	F	159	GLN
1	F	344	GLN
1	F	386	ASN
1	F	401	ASN
1	F	449	HIS
1	F	491	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

44 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	SO4	C	507	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	F	508	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	E	507	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	502	-	4,4,4	0.16	0	6,6,6	0.20	0
2	SO4	D	504	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	E	504	-	4,4,4	0.14	0	6,6,6	0.21	0
2	SO4	D	507	-	4,4,4	0.17	0	6,6,6	0.28	0
2	SO4	C	505	-	4,4,4	0.13	0	6,6,6	0.18	0
2	SO4	E	501	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	F	507	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	B	503	-	4,4,4	0.12	0	6,6,6	0.15	0
2	SO4	F	503	-	4,4,4	0.11	0	6,6,6	0.15	0
3	GOL	A	510	-	5,5,5	0.36	0	5,5,5	0.35	0
2	SO4	B	507	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	D	501	-	4,4,4	0.18	0	6,6,6	0.15	0
3	GOL	E	508	-	5,5,5	0.43	0	5,5,5	0.45	0
2	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	A	501	-	4,4,4	0.18	0	6,6,6	0.29	0
2	SO4	C	506	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	C	501	-	4,4,4	0.17	0	6,6,6	0.23	0
2	SO4	E	506	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	D	506	-	4,4,4	0.15	0	6,6,6	0.27	0
3	GOL	A	509	-	5,5,5	0.43	0	5,5,5	0.31	0
2	SO4	A	506	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	C	508	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	F	501	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	B	506[A]	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	B	501	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	D	502	-	4,4,4	0.22	0	6,6,6	0.25	0
2	SO4	E	502	-	4,4,4	0.11	0	6,6,6	0.25	0
2	SO4	B	504	-	4,4,4	0.11	0	6,6,6	0.24	0
2	SO4	F	502	-	4,4,4	0.16	0	6,6,6	0.30	0
2	SO4	B	508	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	A	502	-	4,4,4	0.12	0	6,6,6	0.31	0
2	SO4	C	502	-	4,4,4	0.15	0	6,6,6	0.32	0
2	SO4	C	503	-	4,4,4	0.11	0	6,6,6	0.29	0
2	SO4	F	506	-	4,4,4	0.14	0	6,6,6	0.29	0
2	SO4	B	506[B]	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	E	503	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	A	507	-	4,4,4	0.17	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.24	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
3	GOL	A	510	-	-	4/4/4/4	-
3	GOL	A	509	-	-	0/4/4/4	-
3	GOL	E	508	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	510	GOL	C1-C2-C3-O3
3	E	508	GOL	C1-C2-C3-O3
3	E	508	GOL	O2-C2-C3-O3
3	E	508	GOL	O1-C1-C2-O2
3	A	510	GOL	O1-C1-C2-C3
3	E	508	GOL	O1-C1-C2-C3
3	A	510	GOL	O2-C2-C3-O3
3	A	510	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	505	SO4	1	0
3	E	508	GOL	1	0
2	C	503	SO4	1	0
2	A	503	SO4	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	494/539 (91%)	0.50	4 (0%)	86	86	59, 74, 84, 92	11 (2%)
1	B	497/539 (92%)	0.53	10 (2%)	65	64	60, 74, 83, 97	8 (1%)
1	C	494/539 (91%)	0.47	1 (0%)	95	96	61, 73, 83, 90	16 (3%)
1	D	495/539 (91%)	0.51	10 (2%)	65	64	62, 73, 84, 96	11 (2%)
1	E	495/539 (91%)	0.49	5 (1%)	82	82	60, 74, 83, 95	13 (2%)
1	F	496/539 (92%)	0.54	12 (2%)	59	56	62, 74, 84, 93	16 (3%)
All	All	2971/3234 (91%)	0.51	42 (1%)	75	75	59, 74, 84, 97	75 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	-2	SER	4.3
1	F	-3	GLY	3.6
1	B	488	TYR	3.2
1	B	-2	SER	3.1
1	D	-2	SER	2.8
1	B	451	TRP	2.8
1	E	210	ALA	2.8
1	B	487	GLY	2.8
1	F	451	TRP	2.7
1	F	452	GLY	2.6
1	F	198	GLN	2.6
1	B	476	CYS	2.5
1	E	186	LEU	2.5
1	D	210	ALA	2.4
1	B	197	LEU	2.4
1	F	399	LEU	2.4
1	F	218	GLN	2.4
1	D	382	SER	2.3
1	E	199	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	237	CYS	2.3
1	B	358	ASN	2.3
1	C	215	SER	2.2
1	A	374	MET	2.2
1	F	197	LEU	2.2
1	D	451	TRP	2.2
1	A	237	CYS	2.2
1	F	382	SER	2.2
1	A	261	ALA	2.2
1	F	449	HIS	2.2
1	F	-2	SER	2.2
1	D	183	ASP	2.2
1	D	82	LEU	2.1
1	F	237	CYS	2.1
1	A	194	ARG	2.1
1	B	214	ARG	2.1
1	B	210	ALA	2.1
1	D	79	ALA	2.0
1	B	447	LEU	2.0
1	F	380	VAL	2.0
1	D	235	ILE	2.0
1	D	447	LEU	2.0
1	E	213	ILE	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, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	E	508	6/6	0.69	0.51	81,84,85,85	0
2	SO4	F	503	5/5	0.70	0.27	146,147,147,147	0
2	SO4	C	508	5/5	0.73	0.21	142,143,143,143	0
2	SO4	C	503	5/5	0.74	0.33	125,125,125,126	0
2	SO4	B	505	5/5	0.76	0.28	140,141,141,141	0
2	SO4	D	504	5/5	0.77	0.25	128,128,129,129	0
2	SO4	F	508	5/5	0.77	0.19	153,153,154,154	0
2	SO4	E	506	5/5	0.77	0.27	117,117,118,118	0
2	SO4	D	505	5/5	0.78	0.25	150,151,152,152	0
3	GOL	A	509	6/6	0.78	0.32	83,87,89,89	0
2	SO4	F	506	5/5	0.78	0.29	100,101,102,102	0
2	SO4	C	505	5/5	0.79	0.28	137,137,138,138	0
2	SO4	A	503	5/5	0.80	0.22	123,123,123,124	0
2	SO4	E	503	5/5	0.80	0.23	151,152,152,152	0
2	SO4	A	506	5/5	0.81	0.28	110,111,111,111	0
2	SO4	A	508	5/5	0.82	0.17	129,130,130,130	0
2	SO4	B	508	5/5	0.82	0.24	147,147,147,148	0
2	SO4	D	503	5/5	0.83	0.24	135,136,137,137	0
2	SO4	D	506	5/5	0.85	0.27	105,105,105,105	0
2	SO4	F	501	5/5	0.86	0.22	101,101,102,103	0
2	SO4	B	503	5/5	0.86	0.24	140,140,140,141	0
2	SO4	B	506[A]	5/5	0.87	0.38	63,63,64,64	5
2	SO4	C	506	5/5	0.87	0.20	102,103,103,103	0
2	SO4	B	506[B]	5/5	0.87	0.38	80,81,81,81	5
2	SO4	C	501	5/5	0.89	0.26	105,105,106,106	0
2	SO4	D	501	5/5	0.90	0.21	104,105,105,106	0
2	SO4	A	501	5/5	0.90	0.21	99,100,100,100	0
2	SO4	E	501	5/5	0.91	0.21	98,99,99,100	0
2	SO4	E	504	5/5	0.92	0.14	112,112,113,113	0
2	SO4	B	504	5/5	0.92	0.18	123,123,124,125	0
2	SO4	E	502	5/5	0.93	0.23	87,87,87,88	0
2	SO4	B	501	5/5	0.93	0.22	102,103,103,104	0
3	GOL	A	510	6/6	0.94	0.17	76,78,81,81	0
2	SO4	A	507	5/5	0.94	0.20	77,78,78,79	0
2	SO4	B	507	5/5	0.95	0.16	84,84,85,85	0
2	SO4	E	507	5/5	0.95	0.16	77,78,79,80	0
2	SO4	C	507	5/5	0.95	0.19	77,77,78,79	0
2	SO4	A	502	5/5	0.96	0.26	77,78,78,79	0
2	SO4	C	502	5/5	0.96	0.27	85,87,89,89	0
2	SO4	B	502	5/5	0.96	0.25	82,83,83,84	0
2	SO4	F	502	5/5	0.96	0.25	83,84,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	507	5/5	0.96	0.23	68,68,68,70	0
2	SO4	D	502	5/5	0.97	0.22	80,81,81,82	0
2	SO4	F	507	5/5	0.97	0.21	78,78,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.