



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:15 pm GMT

PDB ID : 3OOJ
Title : C1A mutant of E. coli GlnS in complex with glucose-6P and glutamate
Authors : Mouilleron, S.; Golinelli-Pimpaneau, B.
Deposited on : 2010-08-31
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28986

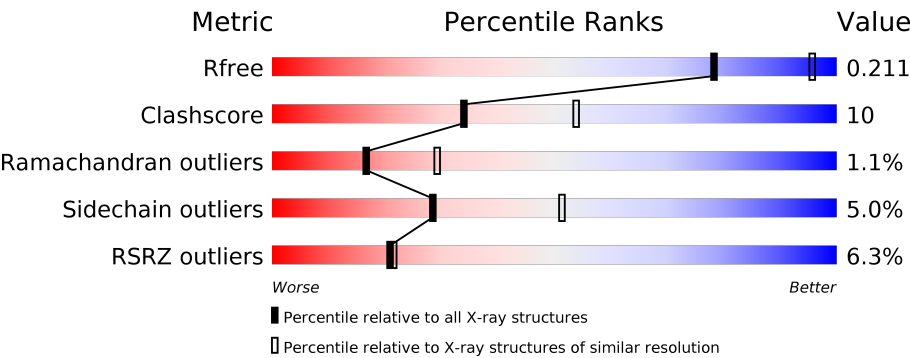
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	608	<div><div>3%</div><div><div></div><div>84%</div><div>15%</div><div>.</div></div></div>
1	B	608	<div><div>5%</div><div><div></div><div>77%</div><div>20%</div><div>.</div></div></div>
1	C	608	<div><div>4%</div><div><div></div><div>78%</div><div>19%</div><div>..</div></div></div>
1	D	608	<div><div>4%</div><div><div></div><div>76%</div><div>21%</div><div>..</div></div></div>
1	E	608	<div><div>4%</div><div><div></div><div>77%</div><div>19%</div><div>..</div></div></div>
1	F	608	<div><div>16%</div><div><div></div><div>69%</div><div>25%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	608	
1	H	608	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	F	701	-	-	X	-
4	GOL	C	609	-	-	-	X
4	GOL	F	609	-	-	-	X
4	GOL	G	609	-	-	-	X
5	G6Q	A	610	-	-	-	X
5	G6Q	B	610	-	-	-	X
5	G6Q	C	611	-	-	-	X
5	G6Q	D	611	-	-	-	X
5	G6Q	E	610	-	-	-	X
5	G6Q	F	610	-	-	-	X
5	G6Q	G	610	-	-	-	X
5	G6Q	H	610	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39092 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.

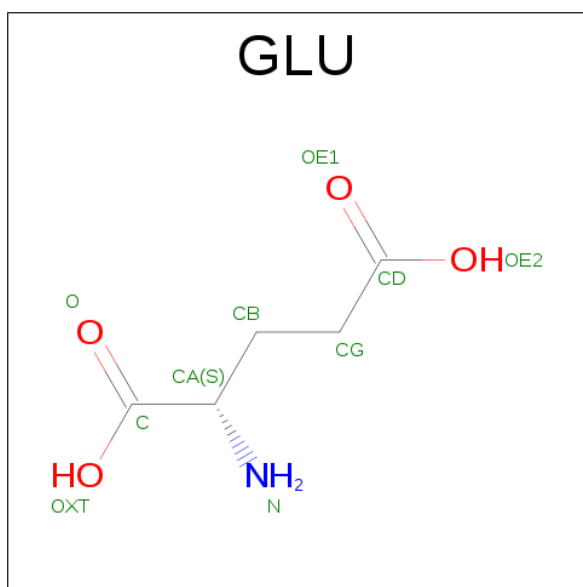
- Molecule 1 is a protein called Glucosamine/fructose-6-phosphate aminotransferase, isomerizing.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	5	0
			4718	2966	838	898	16			
1	B	608	Total	C	N	O	S	0	2	0
			4697	2953	834	894	16			
1	C	601	Total	C	N	O	S	0	2	0
			4631	2915	819	881	16			
1	D	602	Total	C	N	O	S	0	3	0
			4634	2915	821	882	16			
1	E	602	Total	C	N	O	S	0	2	0
			4647	2925	826	880	16			
1	F	594	Total	C	N	O	S	0	0	0
			4583	2887	811	869	16			
1	G	605	Total	C	N	O	S	0	1	0
			4653	2929	823	885	16			
1	H	608	Total	C	N	O	S	0	2	0
			4692	2954	828	894	16			

There are 8 discrepancies between the modelled and reference sequences:

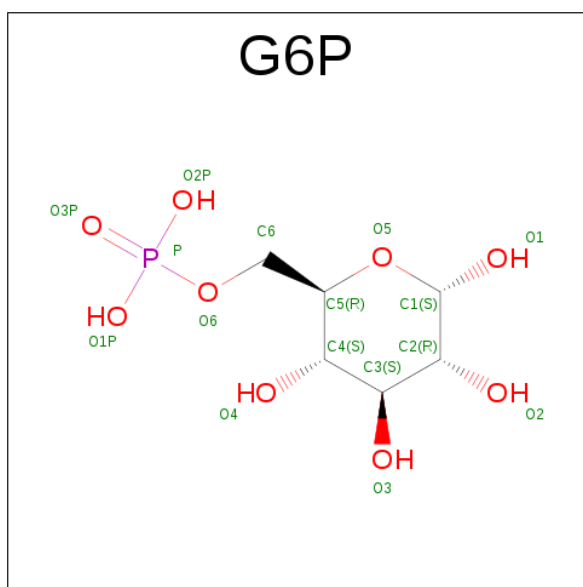
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
B	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
C	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
D	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
E	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
F	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
G	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7
H	1	ALA	CYS	ENGINEERED MUTATION	UNP C9QXA7

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		
2	H	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: C₆H₁₃O₉P).



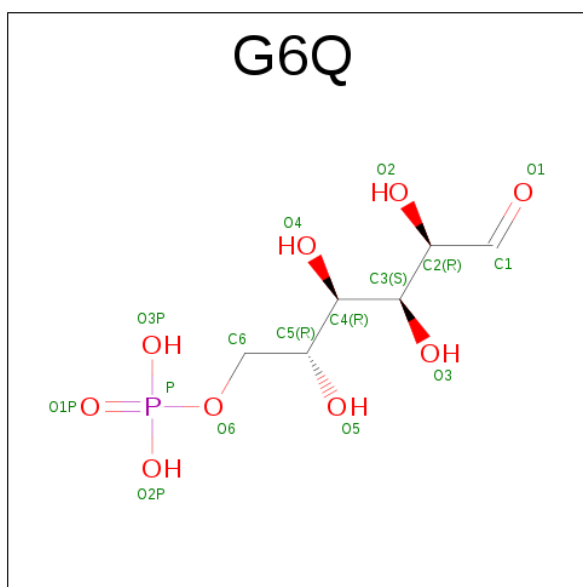
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		
3	E	1	Total	C	O	P	0	0
			16	6	9	1		
3	F	1	Total	C	O	P	0	0
			16	6	9	1		
3	G	1	Total	C	O	P	0	0
			16	6	9	1		
3	H	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SUGAR (GLUCOSE-6-PHOSPHATE) (three-letter code: G6Q) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			16	6	9	1		
5	B	1	Total	C	O	P	0	0
			16	6	9	1		
5	C	1	Total	C	O	P	0	0
			16	6	9	1		
5	D	1	Total	C	O	P	0	0
			16	6	9	1		
5	E	1	Total	C	O	P	0	0
			16	6	9	1		
5	F	1	Total	C	O	P	0	0
			16	6	9	1		
5	G	1	Total	C	O	P	0	0
			16	6	9	1		
5	H	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	231	Total	O	0	0
			231	231		
6	B	192	Total	O	0	0
			192	192		
6	C	196	Total	O	0	0
			196	196		
6	D	244	Total	O	0	0
			244	244		

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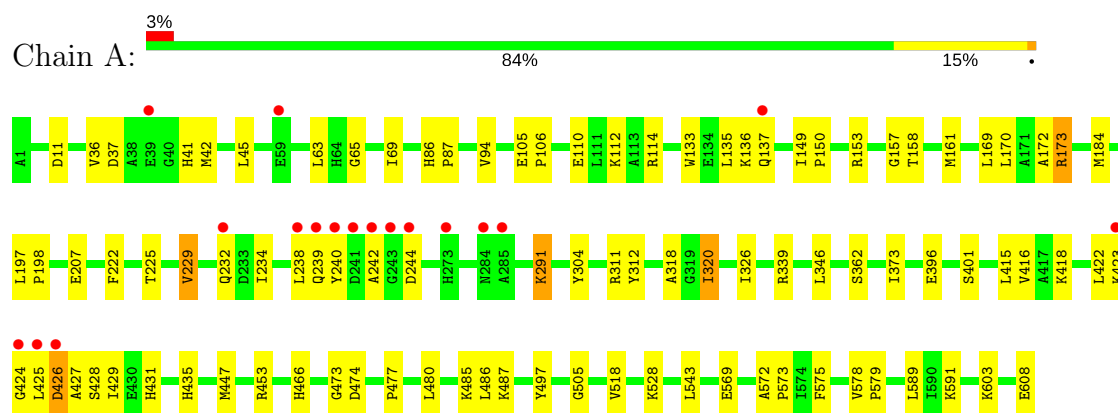
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	123	Total 123	O 123	0	0
6	F	123	Total 123	O 123	0	0
6	G	175	Total 175	O 175	0	0
6	H	169	Total 169	O 169	0	0

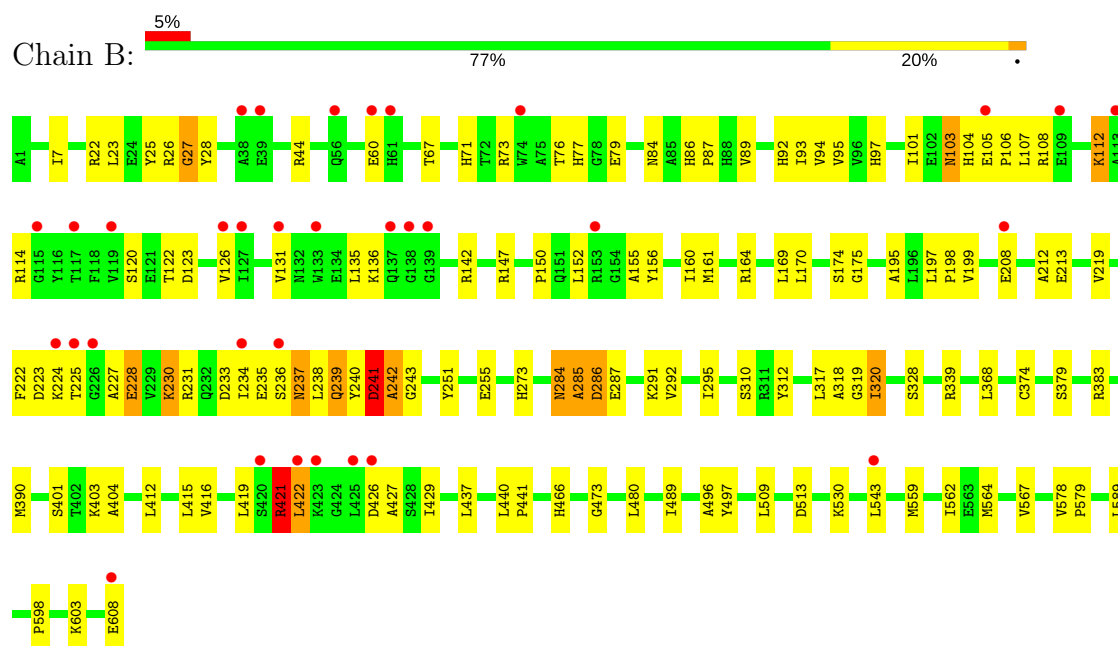
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

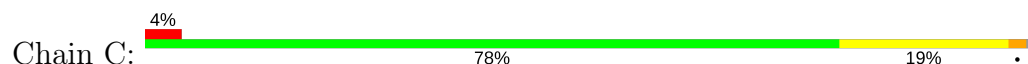
- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing

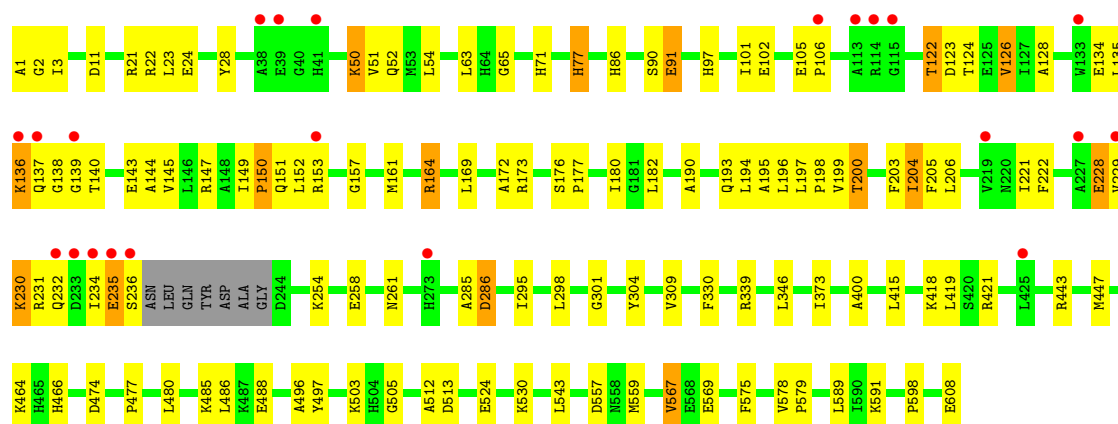


- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing

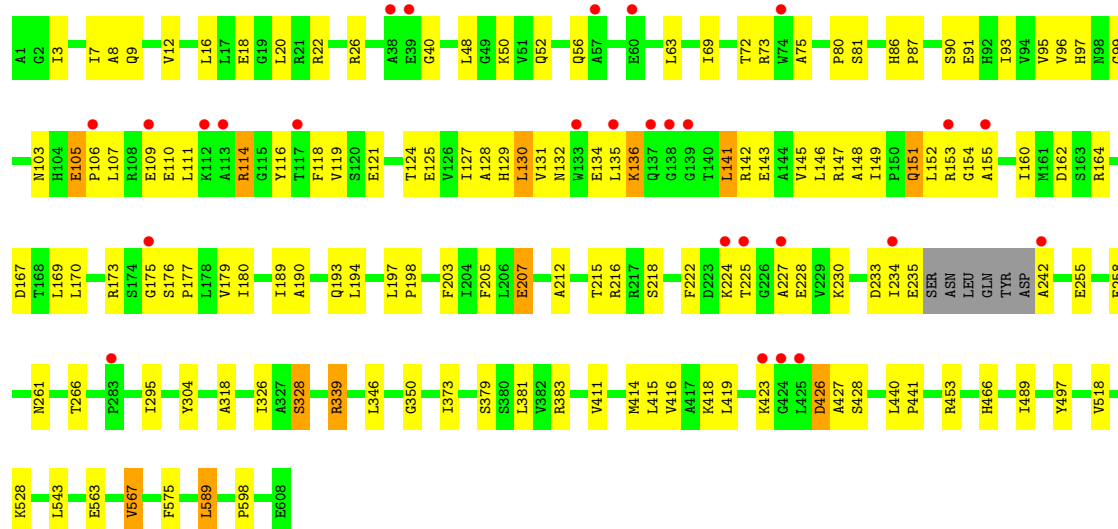
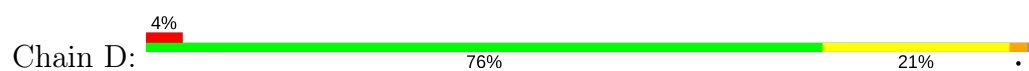


- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing

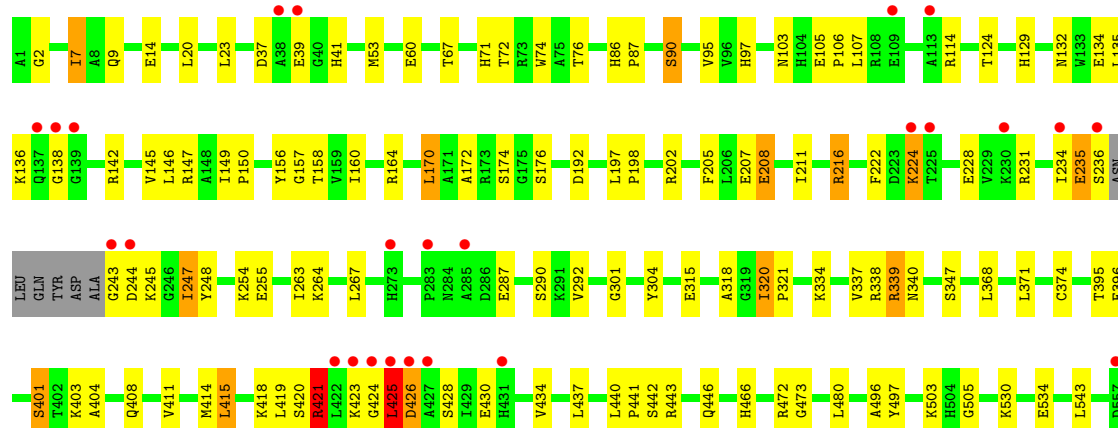
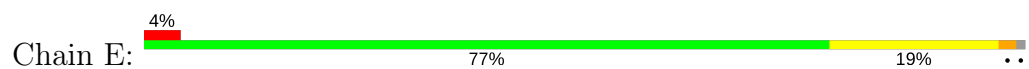




• Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing



• Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing

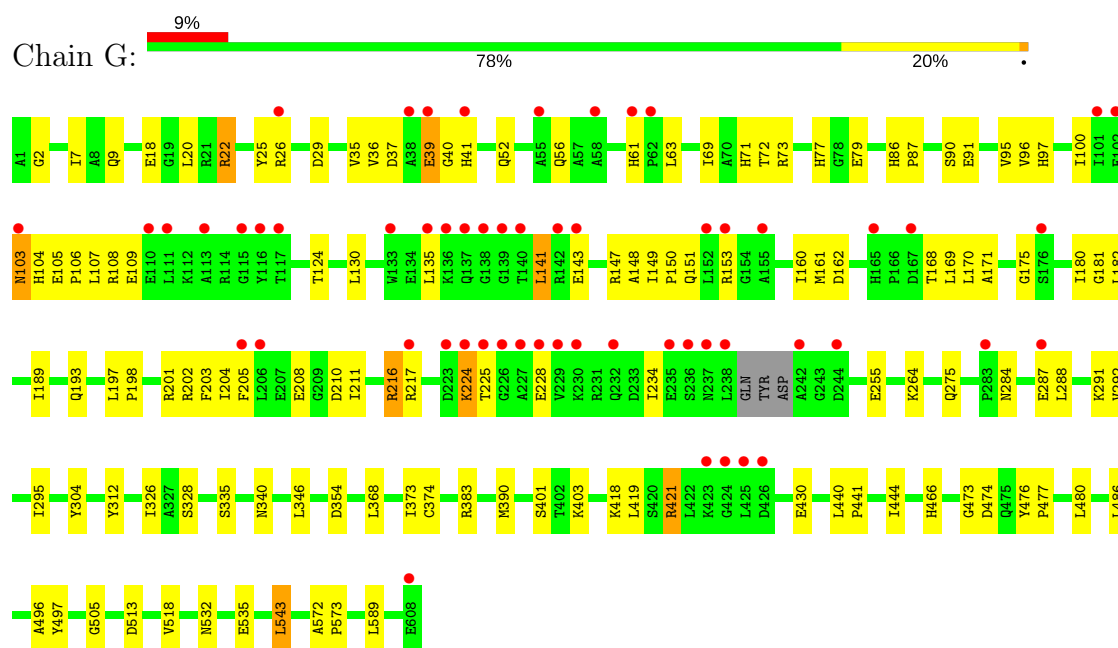




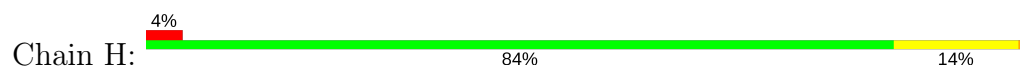
- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing

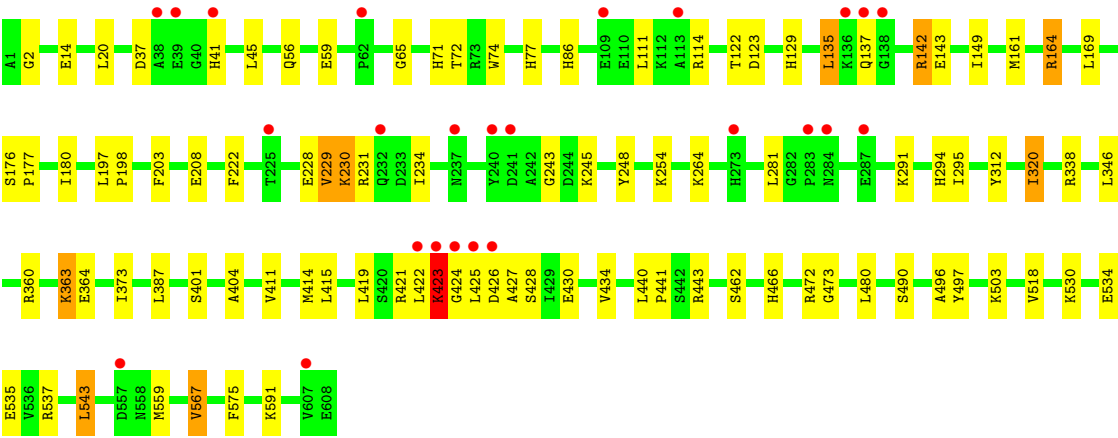


- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing



- Molecule 1: Glucosamine/fructose-6-phosphate aminotransferase, isomerizing





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	247.60Å 247.60Å 630.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.99-2.50) 98.5 (19.99-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.178 , 0.220 0.163 , 0.211	Depositor DCC
R_{free} test set	12636 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.000 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.000 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	39092	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, G6P, G6Q

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	0.44	0/4805	0.61	1/6510 (0.0%)
1	B	0.41	0/4783	0.59	1/6478 (0.0%)
1	C	0.43	0/4714	0.59	0/6384
1	D	0.42	0/4712	0.59	1/6380 (0.0%)
1	E	0.41	0/4734	0.58	2/6409 (0.0%)
1	F	0.40	0/4662	0.57	1/6312 (0.0%)
1	G	0.41	0/4736	0.56	0/6414
1	H	0.42	0/4780	0.57	0/6475
All	All	0.42	0/37926	0.58	6/51362 (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	E	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	567	VAL	CB-CA-C	-6.09	99.84	111.40
1	E	157	GLY	N-CA-C	-5.81	98.57	113.10
1	B	421	ARG	N-CA-C	5.72	126.44	111.00
1	D	518	VAL	CB-CA-C	-5.54	100.87	111.40
1	A	320	ILE	CB-CA-C	-5.25	101.09	111.60
1	E	567	VAL	CB-CA-C	-5.06	101.78	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	425	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4718	0	4704	61	0
1	B	4697	0	4698	106	0
1	C	4631	0	4638	99	0
1	D	4634	0	4640	89	0
1	E	4647	0	4666	81	0
1	F	4583	0	4617	149	0
1	G	4653	0	4669	72	0
1	H	4692	0	4703	68	0
2	A	10	0	5	0	0
2	B	10	0	5	2	0
2	C	10	0	5	2	0
2	D	10	0	5	1	0
2	E	10	0	5	2	0
2	F	10	0	5	4	0
2	G	10	0	5	0	0
2	H	10	0	5	1	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	0	0
3	D	16	0	11	0	0
3	E	16	0	11	0	0
3	F	16	0	11	0	0
3	G	16	0	11	0	0
3	H	16	0	11	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	E	6	0	8	1	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	6	0	8	0	0
5	A	16	0	11	3	0
5	B	16	0	11	0	0
5	C	16	0	11	3	0
5	D	16	0	11	1	0
5	E	16	0	11	1	0
5	F	16	0	11	4	0
5	G	16	0	11	2	0
5	H	16	0	11	0	0
6	A	231	0	0	2	0
6	B	192	0	0	3	0
6	C	196	0	0	3	0
6	D	244	0	0	5	0
6	E	123	0	0	1	0
6	F	123	0	0	2	0
6	G	175	0	0	2	0
6	H	169	0	0	2	0
All	All	39092	0	37615	720	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 10.

All (720) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ALA:HB3	1:B:243:GLY:HA3	1.32	1.10
1:H:230:LYS:HE3	1:H:231:ARG:H	1.11	1.10
1:B:236:SER:HA	1:B:237:ASN:HB2	1.14	1.07
1:B:236:SER:HA	1:B:237:ASN:CB	1.92	0.97
1:F:569:GLU:HG3	5:F:610:G6Q:O2	1.66	0.94
1:F:99:GLY:O	2:F:701:GLU:HB2	1.67	0.93
1:B:242:ALA:CB	1:B:243:GLY:HA3	1.99	0.92
1:H:424:GLY:HA3	1:H:425:LEU:HB3	1.51	0.91
1:F:86:HIS:HD2	1:F:97:HIS:H	1.14	0.89
1:G:9:GLN:HB2	1:G:216:ARG:HH21	1.38	0.89
1:C:485:LYS:HE3	1:C:488:GLU:OE1	1.74	0.87
1:B:236:SER:CA	1:B:237:ASN:HB2	2.04	0.86
1:D:328[A]:SER:OG	6:D:1385:HOH:O	1.94	0.85
1:H:423:LYS:CB	1:H:424:GLY:HA2	2.06	0.84
1:D:9:GLN:HB2	1:D:216:ARG:NH1	1.93	0.84
1:A:239:GLN:O	1:A:240:TYR:HD1	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:GLY:HA3	1:B:422:LEU:HD13	1.59	0.83
1:F:71:HIS:HB2	1:F:96:VAL:HG23	1.60	0.82
1:C:105:GLU:HB2	1:C:106:PRO:HD3	1.60	0.82
1:H:222:PHE:HA	1:H:229:VAL:HG13	1.62	0.81
1:H:230:LYS:HE3	1:H:231:ARG:N	1.95	0.81
1:D:153:ARG:HG2	1:D:154:GLY:H	1.45	0.81
1:C:24:GLU:OE1	1:C:28:TYR:OH	1.98	0.80
1:B:292:VAL:O	1:B:421:ARG:NH2	2.15	0.80
1:D:136:LYS:HE2	1:D:136:LYS:HA	1.64	0.79
1:H:423:LYS:HB2	1:H:424:GLY:HA2	1.66	0.78
1:A:425:LEU:HB2	1:A:427:ALA:H	1.50	0.77
1:F:73:ARG:NH2	1:F:78:GLY:O	2.17	0.77
1:F:480:LEU:HD23	1:F:496:ALA:HB3	1.66	0.76
1:B:27:GLY:HA3	1:B:28:TYR:HB3	1.66	0.76
1:D:69:ILE:HD12	1:D:96:VAL:HG13	1.68	0.76
1:C:149:ILE:HB	1:C:150:PRO:HD3	1.68	0.75
1:D:135:LEU:HD21	1:D:164:ARG:HH22	1.51	0.75
1:B:150:PRO:HG3	1:B:224:LYS:HD2	1.69	0.75
1:E:426:ASP:HB3	1:E:428:SER:HB3	1.68	0.74
1:A:425:LEU:HA	1:A:426:ASP:CB	2.16	0.74
1:F:530:LYS:NZ	1:F:534:GLU:OE2	2.19	0.74
1:D:143:GLU:HA	1:D:146:LEU:HD12	1.69	0.74
1:B:230:LYS:HE2	1:B:230:LYS:HA	1.68	0.74
1:C:204:ILE:HD11	1:C:221:ILE:HD11	1.70	0.74
1:G:7:ILE:HG12	1:G:216:ARG:HB3	1.69	0.73
1:E:224:LYS:H	1:E:224:LYS:HD2	1.53	0.73
1:F:86:HIS:CD2	1:F:97:HIS:H	2.03	0.73
1:D:130:LEU:O	1:D:130:LEU:HD12	1.88	0.72
1:A:239:GLN:C	1:A:240:TYR:HD1	1.93	0.72
1:E:443:ARG:HH11	1:E:446:GLN:HE22	1.36	0.72
1:F:71:HIS:HB2	1:F:96:VAL:CG2	2.20	0.72
1:A:425:LEU:CB	1:A:427:ALA:H	2.03	0.72
1:G:105:GLU:O	1:G:109:GLU:HG2	1.90	0.72
1:D:93:ILE:HG21	1:D:131:VAL:HG23	1.71	0.71
1:G:20:LEU:HD22	1:G:72:THR:HG23	1.71	0.70
1:H:208:GLU:OE2	6:H:1507:HOH:O	2.08	0.70
1:B:240:TYR:HB2	1:B:241:ASP:HB2	1.73	0.70
1:F:285:ALA:O	1:F:286:ASP:CB	2.40	0.70
1:H:424:GLY:CA	1:H:425:LEU:HB3	2.21	0.70
1:G:71:HIS:HE1	1:G:73:ARG:HB2	1.57	0.69
1:C:231:ARG:HH11	1:C:231:ARG:HG2	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:GLY:HA3	1:F:41:HIS:HB2	1.75	0.69
1:B:318:ALA:HB1	1:B:320:ILE:HD11	1.74	0.69
1:C:261:ASN:OD1	6:C:809:HOH:O	2.11	0.69
1:H:142:ARG:HG3	1:H:143:GLU:N	2.08	0.68
1:A:477:PRO:HA	1:A:480:LEU:HD12	1.76	0.68
1:H:567:VAL:HG11	1:H:575:PHE:CD1	2.29	0.68
1:D:234:ILE:HG22	1:D:235:GLU:H	1.59	0.68
1:C:138:GLY:HA3	1:C:147:ARG:NH2	2.09	0.68
1:F:291:LYS:N	1:F:291:LYS:HD2	2.09	0.68
1:E:222:PHE:HB3	1:E:228:GLU:HA	1.76	0.67
1:G:284:ASN:O	1:G:287:GLU:HB2	1.93	0.67
1:F:4:VAL:HG12	1:F:16:LEU:HD23	1.77	0.67
1:F:149:ILE:HG21	1:F:224:LYS:HZ2	1.60	0.67
1:F:97:HIS:HB3	1:F:124:THR:HG23	1.77	0.67
1:B:230:LYS:HE2	1:B:231:ARG:H	1.60	0.67
1:F:3:ILE:HG12	1:F:96:VAL:HG22	1.76	0.67
1:B:223:ASP:OD1	1:B:225:THR:HG22	1.95	0.66
1:D:7:ILE:HD13	1:D:215:THR:HA	1.77	0.66
1:H:423:LYS:CG	1:H:424:GLY:HA2	2.25	0.66
1:G:210:ASP:O	1:G:211:ILE:HD13	1.95	0.66
1:F:93:ILE:HD13	1:F:131:VAL:HG22	1.76	0.66
5:A:610:G6Q:O3	5:A:610:G6Q:O5	2.10	0.66
1:E:425:LEU:O	1:E:426:ASP:HB2	1.96	0.66
1:B:236:SER:CA	1:B:237:ASN:CB	2.69	0.65
1:D:339:ARG:NH1	6:D:743:HOH:O	2.28	0.65
1:F:40:GLY:CA	1:F:41:HIS:HB2	2.27	0.65
1:F:140:THR:HG22	1:F:141:LEU:H	1.60	0.65
1:C:21:ARG:O	1:C:24:GLU:HG3	1.96	0.65
1:G:9:GLN:HB2	1:G:216:ARG:NH2	2.10	0.65
1:B:255:GLU:HG2	1:B:403:LYS:HE2	1.77	0.65
1:F:188:PHE:CE2	1:F:199:VAL:HG11	2.31	0.65
1:E:576:TYR:O	1:E:579:PRO:HD2	1.97	0.64
1:B:161:MET:HB3	1:B:169:LEU:HD23	1.79	0.64
1:E:426:ASP:HB3	1:E:428:SER:CB	2.28	0.64
1:D:95:VAL:HG22	1:D:160:ILE:HG12	1.80	0.64
1:E:426:ASP:C	1:E:428:SER:H	2.00	0.64
1:F:136:LYS:O	1:F:137:GLN:HG3	1.96	0.64
1:A:173:ARG:HG2	1:A:207:GLU:O	1.97	0.64
1:B:240:TYR:CA	1:B:241:ASP:HB2	2.28	0.64
1:B:240:TYR:CZ	1:H:243:GLY:HA3	2.33	0.63
1:H:426:ASP:OD2	1:H:427:ALA:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ARG:HG3	1:D:176:SER:O	1.98	0.63
1:C:400:ALA:HB1	1:C:485:LYS:HE2	1.80	0.63
1:A:431[B]:HIS:NE2	1:A:435[B]:HIS:CD2	2.67	0.63
1:E:95:VAL:HG22	1:E:160:ILE:HG12	1.80	0.63
1:E:207:GLU:HG3	1:E:231:ARG:NH1	2.14	0.63
1:F:138:GLY:O	1:F:143:GLU:HB3	1.99	0.63
1:H:422:LEU:O	1:H:423:LYS:HG2	1.97	0.63
1:C:204:ILE:HD11	1:C:221:ILE:CD1	2.28	0.63
1:F:28:TYR:CB	1:F:72:THR:HG23	2.28	0.62
1:A:63:LEU:N	1:A:63:LEU:HD12	2.13	0.62
1:F:162:ASP:OD1	1:F:163:SER:N	2.32	0.62
1:C:608:GLU:O	1:D:528:LYS:HE3	1.99	0.62
1:B:222:PHE:CE1	1:B:228:GLU:HG2	2.34	0.62
1:C:138:GLY:HA3	1:C:147:ARG:HH22	1.63	0.62
1:H:480:LEU:HD23	1:H:496:ALA:HB3	1.80	0.62
1:A:425:LEU:HB2	1:A:427:ALA:N	2.14	0.62
1:C:77:HIS:O	1:C:122:THR:HA	1.99	0.62
1:F:149:ILE:HG23	1:F:156:TYR:OH	1.99	0.62
1:B:95:VAL:HG22	1:B:160:ILE:HG12	1.82	0.61
1:F:71:HIS:CG	1:F:96:VAL:HG23	2.35	0.61
1:G:71:HIS:CE1	1:G:73:ARG:HB2	2.35	0.61
1:E:263:ILE:HG21	1:E:440:LEU:HD23	1.82	0.61
1:D:118:PHE:HA	1:D:125:GLU:OE2	2.00	0.61
1:E:243:GLY:O	1:E:245:LYS:N	2.33	0.61
1:B:230:LYS:HA	1:B:230:LYS:CE	2.31	0.61
1:F:569:GLU:HG3	5:F:610:G6Q:HO2	1.60	0.61
1:F:71:HIS:CB	1:F:96:VAL:HG23	2.29	0.61
1:B:285:ALA:C	1:B:287:GLU:H	2.04	0.61
1:H:530:LYS:HD3	1:H:559:MET:SD	2.41	0.61
1:F:7:ILE:HD13	1:F:215:THR:HA	1.83	0.61
1:B:242:ALA:CB	1:B:243:GLY:CA	2.77	0.61
1:E:103:ASN:ND2	1:E:107:LEU:HD11	2.16	0.61
1:B:285:ALA:O	1:B:287:GLU:N	2.33	0.61
1:C:477:PRO:HA	1:C:480:LEU:HD12	1.81	0.61
1:G:180:ILE:O	1:G:203:PHE:HA	2.01	0.60
1:D:107:LEU:HD13	1:D:152:LEU:HD23	1.82	0.60
1:F:346:LEU:HD23	1:F:373:ILE:HB	1.84	0.60
1:G:480:LEU:HD23	1:G:496:ALA:HB3	1.83	0.60
1:E:235:GLU:OE2	1:E:236:SER:N	2.34	0.60
1:D:86:HIS:HB3	1:D:87:PRO:HA	1.84	0.60
1:G:105:GLU:HB2	1:G:106:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:SER:HB2	1:D:128:ALA:HB1	1.82	0.60
1:F:112:LYS:HE2	1:F:117:THR:HA	1.83	0.60
1:B:76:THR:HG1	2:B:701:GLU:N	2.00	0.60
5:C:611:G6Q:O3	5:C:611:G6Q:O5	2.11	0.60
1:F:15:ILE:HD13	1:F:188:PHE:CE1	2.37	0.59
1:A:346:LEU:HD23	1:A:373:ILE:HB	1.84	0.59
1:C:101:ILE:HD12	1:C:152:LEU:HD22	1.84	0.59
1:C:513:ASP:HB3	6:C:1513:HOH:O	2.02	0.59
1:B:320:ILE:CD1	1:B:421:ARG:HG2	2.32	0.59
1:H:222:PHE:HB3	1:H:228:GLU:HA	1.84	0.59
1:D:22:ARG:HD3	6:D:1429:HOH:O	2.01	0.59
1:B:105:GLU:HG3	1:B:106:PRO:HD3	1.84	0.59
1:B:427:ALA:N	6:B:631:HOH:O	2.34	0.58
1:B:480:LEU:HD23	1:B:496:ALA:HB3	1.84	0.58
1:G:255:GLU:HG2	1:G:403:LYS:HE2	1.83	0.58
1:F:76:THR:O	1:F:77:HIS:HB2	2.02	0.58
1:B:240:TYR:CB	1:B:241:ASP:HB2	2.32	0.58
1:E:292:VAL:O	1:E:421:ARG:NH1	2.33	0.58
1:F:4:VAL:HG11	1:F:16:LEU:HA	1.85	0.58
1:F:92:HIS:CD2	1:F:93:ILE:HG13	2.38	0.58
1:H:37:ASP:OD2	1:H:41[A]:HIS:HB2	2.03	0.58
1:B:240:TYR:HA	1:B:241:ASP:CB	2.33	0.58
1:F:71:HIS:CB	1:F:86:HIS:HB2	2.34	0.58
1:F:1:ALA:HB3	1:F:72:THR:HG22	1.85	0.58
1:A:239:GLN:C	1:A:240:TYR:CD1	2.76	0.57
1:F:28:TYR:HB3	1:F:72:THR:HG23	1.85	0.57
1:F:95:VAL:HG22	1:F:160:ILE:HG23	1.86	0.57
1:B:318:ALA:HB2	1:B:416:VAL:HG13	1.85	0.57
1:F:149:ILE:HG21	1:F:224:LYS:NZ	2.19	0.57
1:C:229:VAL:CG2	1:C:231:ARG:HH12	2.17	0.57
1:E:567:VAL:HG11	1:E:575:PHE:CD1	2.39	0.57
1:C:149:ILE:C	1:C:151:GLN:H	2.07	0.57
1:C:474:ASP:OD2	5:C:611:G6Q:H3	2.05	0.57
5:G:610:G6Q:O3	5:G:610:G6Q:O5	2.13	0.57
1:H:534:GLU:OE1	1:H:537:ARG:NH1	2.38	0.57
1:C:161:MET:HB3	1:C:169:LEU:CD2	2.34	0.57
1:G:513:ASP:HB3	6:G:1354:HOH:O	2.04	0.56
1:A:425:LEU:HA	1:A:426:ASP:HB3	1.88	0.56
1:C:285:ALA:O	1:C:286:ASP:CB	2.53	0.56
1:F:139:GLY:HA3	1:F:143:GLU:OE1	2.04	0.56
1:F:22:ARG:NE	1:F:198:PRO:HG3	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:ILE:HD12	1:G:96:VAL:HG22	1.86	0.56
1:F:71:HIS:CD2	1:F:96:VAL:HG23	2.40	0.56
1:G:466:HIS:CE1	1:H:466:HIS:CE1	2.93	0.56
1:E:146:LEU:HD23	1:E:211:ILE:HD12	1.86	0.56
1:A:86:HIS:HB3	1:A:87:PRO:HA	1.87	0.56
1:E:142:ARG:HA	1:E:170:LEU:HD11	1.88	0.56
1:E:530:LYS:NZ	1:E:534:GLU:OE2	2.35	0.56
1:C:466:HIS:CE1	1:D:466:HIS:CE1	2.94	0.56
1:F:106:PRO:O	1:F:110:GLU:HB2	2.06	0.56
1:F:76:THR:OG1	1:F:76:THR:O	2.19	0.56
1:A:431[B]:HIS:CD2	1:A:435[B]:HIS:HD2	2.23	0.56
1:A:466:HIS:CE1	1:B:466:HIS:CE1	2.94	0.56
1:C:197:LEU:N	1:C:198:PRO:HD2	2.21	0.56
1:D:225:THR:HA	6:D:694:HOH:O	2.06	0.56
1:E:466:HIS:CE1	1:F:466:HIS:CE1	2.94	0.56
1:F:474:ASP:OD1	5:F:610:G6Q:H3	2.05	0.56
1:H:423:LYS:HG2	1:H:424:GLY:HA2	1.87	0.56
1:C:196:LEU:HB2	1:C:203:PHE:HE1	1.70	0.56
1:E:90:SER:OG	1:E:129:HIS:ND1	2.30	0.56
1:G:86:HIS:HB3	1:G:87:PRO:HA	1.87	0.56
1:D:93:ILE:HG21	1:D:131:VAL:CG2	2.35	0.55
1:F:71:HIS:HB3	1:F:86:HIS:HB2	1.87	0.55
1:A:426:ASP:H	1:A:429:ILE:HD12	1.70	0.55
1:C:149:ILE:O	1:C:151:GLN:N	2.38	0.55
1:B:240:TYR:HA	1:B:241:ASP:HB2	1.89	0.55
1:F:93:ILE:HD12	1:F:132:ASN:HA	1.88	0.55
1:C:50:LYS:HB3	1:C:50:LYS:NZ	2.22	0.55
1:F:167:ASP:O	1:F:215:THR:HG22	2.07	0.55
1:F:440:LEU:HB3	1:F:441:PRO:HD3	1.88	0.55
1:A:291:LYS:N	1:A:291:LYS:HD2	2.21	0.55
1:D:411:VAL:HA	1:D:414:MET:CE	2.37	0.55
1:F:69:ILE:HD12	1:F:96:VAL:HG12	1.89	0.55
1:B:84:ASN:OD1	1:B:120:SER:HB2	2.07	0.55
1:C:339:ARG:NH1	6:D:743:HOH:O	2.40	0.55
1:E:301:GLY:O	1:E:304:TYR:HB3	2.07	0.55
1:E:76:THR:HG1	2:E:701:GLU:N	2.04	0.55
1:D:222:PHE:HA	1:D:228:GLU:CA	2.37	0.54
1:F:450:GLN:OE1	1:F:453:ARG:NH2	2.37	0.54
1:G:103:ASN:OD1	1:G:153:ARG:HB2	2.06	0.54
1:F:63:LEU:H	1:F:63:LEU:HD12	1.72	0.54
1:G:149:ILE:HB	1:G:150:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:ILE:HD11	1:G:419:LEU:HD13	1.90	0.54
1:E:103:ASN:O	1:E:107:LEU:HD12	2.08	0.54
1:F:141:LEU:HD23	1:F:170:LEU:HD23	1.88	0.54
1:D:127:ILE:O	1:D:131:VAL:HG22	2.07	0.54
1:D:63:LEU:HD12	1:D:63:LEU:N	2.23	0.54
1:A:425:LEU:CA	1:A:427:ALA:H	2.21	0.54
1:B:174:SER:HA	1:B:208:GLU:OE2	2.08	0.54
1:C:285:ALA:O	1:C:286:ASP:HB2	2.08	0.54
1:F:77:HIS:HB2	2:F:701:GLU:N	2.23	0.54
1:G:95:VAL:HG22	1:G:160:ILE:HG23	1.89	0.54
1:B:319:GLY:CA	1:B:422:LEU:HD13	2.35	0.54
1:F:105:GLU:HB3	1:F:106:PRO:HD3	1.88	0.54
1:F:199:VAL:HG12	1:F:200:THR:HG22	1.88	0.54
1:F:188:PHE:CZ	1:F:199:VAL:HG11	2.43	0.54
1:B:241:ASP:O	1:B:242:ALA:CB	2.56	0.53
1:G:141:LEU:HD11	1:G:162:ASP:HB2	1.90	0.53
1:G:2:GLY:O	1:G:71:HIS:HA	2.08	0.53
1:D:48:LEU:HD13	1:D:81:SER:HA	1.90	0.53
1:C:222:PHE:HB3	1:C:228:GLU:HA	1.88	0.53
1:B:71:HIS:HE1	1:B:73:ARG:HB2	1.74	0.53
1:D:20:LEU:HD22	1:D:72:THR:HG23	1.91	0.53
1:F:79:GLU:HG2	1:F:84:ASN:ND2	2.23	0.53
1:B:320:ILE:HD12	1:B:421:ARG:HG2	1.91	0.53
1:D:170:LEU:HD13	1:D:212:ALA:O	2.08	0.53
1:F:183:GLY:HA2	1:F:186:GLU:O	2.09	0.53
1:G:22:ARG:HG2	1:G:22:ARG:HH11	1.74	0.53
1:C:197:LEU:HD23	1:C:203:PHE:HZ	1.73	0.53
1:E:149:ILE:HB	1:E:150:PRO:HD3	1.90	0.53
1:E:39:GLU:HB3	1:E:41[A]:HIS:CE1	2.44	0.53
1:H:422:LEU:O	1:H:424:GLY:HA3	2.08	0.53
1:D:90:SER:OG	1:D:129:HIS:HA	2.09	0.53
1:C:105:GLU:HA	1:C:105:GLU:OE2	2.09	0.53
1:B:92:HIS:CD2	1:B:93:ILE:HD12	2.44	0.52
1:B:285:ALA:C	1:B:287:GLU:N	2.62	0.52
1:F:285:ALA:O	1:F:286:ASP:HB2	2.10	0.52
1:B:234:ILE:HG12	1:B:235:GLU:N	2.24	0.52
1:H:360:ARG:O	1:H:363:LYS:HB2	2.08	0.52
1:A:222:PHE:HA	1:A:229:VAL:HG13	1.92	0.52
1:E:426:ASP:C	1:E:428:SER:N	2.61	0.52
1:E:86:HIS:HB3	1:E:87:PRO:HA	1.92	0.52
1:F:4:VAL:O	1:F:16:LEU:HD22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:401:SER:HB2	6:G:1455:HOH:O	2.09	0.52
1:H:2:GLY:O	1:H:71:HIS:HA	2.10	0.52
1:B:241:ASP:O	1:B:242:ALA:HB3	2.09	0.52
1:F:127:ILE:O	1:F:131:VAL:HG12	2.09	0.52
1:F:576:TYR:O	1:F:579:PRO:HD2	2.09	0.52
1:F:472:ARG:HG2	1:F:473:GLY:N	2.24	0.52
1:G:201:ARG:HA	1:G:203:PHE:HE1	1.75	0.52
1:G:61:HIS:CG	1:G:61:HIS:O	2.63	0.52
1:B:104:HIS:HD2	1:B:108:ARG:HH12	1.58	0.52
1:B:108:ARG:O	1:B:112:LYS:HB2	2.10	0.52
1:E:480:LEU:HD23	1:E:496:ALA:HB3	1.92	0.52
1:F:90:SER:O	1:F:91:GLU:HB3	2.09	0.51
1:H:530:LYS:NZ	1:H:534:GLU:OE2	2.31	0.51
1:E:339:ARG:NE	1:F:339:ARG:NH2	2.58	0.51
1:D:145:VAL:HG13	1:D:149:ILE:HD13	1.92	0.51
1:C:123:ASP:O	1:C:126:VAL:HG13	2.10	0.51
1:C:231:ARG:NH1	1:C:231:ARG:HG2	2.23	0.51
1:D:489:ILE:HG22	1:D:598:PRO:HG3	1.92	0.51
1:H:37:ASP:OD2	1:H:41[B]:HIS:HB3	2.10	0.51
1:B:103:ASN:HD22	1:B:103:ASN:C	2.14	0.51
1:C:464:LYS:HE3	1:C:512:ALA:O	2.11	0.51
1:E:371:LEU:HD21	1:E:415:LEU:HD21	1.92	0.51
1:E:7:ILE:HD12	1:E:67:THR:OG1	2.11	0.51
1:F:22:ARG:CZ	1:F:198:PRO:HG3	2.40	0.51
1:H:77:HIS:O	1:H:122:THR:HA	2.10	0.51
1:D:155:ALA:HA	1:D:175:GLY:HA3	1.93	0.51
1:F:8:ALA:HB2	1:F:186:GLU:HB2	1.92	0.51
1:F:1:ALA:O	1:F:26:ARG:HD3	2.11	0.51
1:H:411:VAL:HA	1:H:414:MET:HE2	1.93	0.51
1:H:518:VAL:HG23	1:H:543:LEU:HD21	1.92	0.51
1:H:86:HIS:CD2	1:H:86:HIS:N	2.79	0.51
1:G:346:LEU:HD23	1:G:373:ILE:HB	1.93	0.51
1:A:304:TYR:CD1	1:A:326:ILE:HD13	2.45	0.51
1:E:255:GLU:HG2	1:E:403:LYS:HE2	1.93	0.50
1:H:422:LEU:O	1:H:425:LEU:HB3	2.11	0.50
1:B:170:LEU:HD13	1:B:212:ALA:O	2.11	0.50
1:B:197:LEU:N	1:B:198:PRO:CD	2.74	0.50
1:G:143:GLU:HB3	1:G:147:ARG:NH1	2.26	0.50
1:B:23:LEU:HD21	1:B:195:ALA:HB2	1.93	0.50
1:C:2:GLY:O	1:C:71:HIS:HA	2.11	0.50
1:E:105:GLU:HB2	1:E:106:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:TYR:N	1:F:175:GLY:HA3	2.25	0.50
1:H:490:SER:O	1:H:591:LYS:NZ	2.40	0.50
1:G:161:MET:HB3	1:G:169:LEU:CD2	2.41	0.50
1:D:86:HIS:HE1	1:D:97:HIS:HB3	1.77	0.50
2:F:701:GLU:HG2	2:F:701:GLU:O	2.11	0.50
1:B:147:ARG:O	1:B:150:PRO:HD2	2.11	0.50
1:G:77:HIS:HE1	1:G:100:ILE:HD13	1.76	0.50
1:A:425:LEU:HD12	1:A:425:LEU:O	2.11	0.50
1:B:97:HIS:NE2	1:B:156:TYR:HB2	2.26	0.50
1:D:105:GLU:HA	1:D:105:GLU:OE2	2.12	0.50
1:E:136:LYS:C	1:E:138:GLY:H	2.15	0.50
1:E:248:TYR:CD2	1:E:254:LYS:HB2	2.47	0.50
1:B:284:ASN:O	1:B:286:ASP:N	2.44	0.50
1:C:254:LYS:HE2	1:C:258:GLU:OE2	2.12	0.50
1:E:224:LYS:H	1:E:224:LYS:CD	2.21	0.50
1:F:140:THR:HG22	1:F:141:LEU:N	2.27	0.50
1:G:107:LEU:HD11	1:G:151:GLN:O	2.12	0.50
1:H:248:TYR:CD2	1:H:254:LYS:HB2	2.47	0.50
1:E:20:LEU:HD22	1:E:72:THR:HG23	1.94	0.50
1:B:320:ILE:CD1	1:B:419:LEU:O	2.60	0.49
1:C:145:VAL:O	1:C:149:ILE:HG12	2.12	0.49
1:D:346:LEU:HD23	1:D:373:ILE:HB	1.94	0.49
1:H:161:MET:HB3	1:H:169:LEU:CD2	2.42	0.49
1:C:137:GLN:HG2	1:C:137:GLN:O	2.12	0.49
1:H:20:LEU:HD22	1:H:72:THR:HG23	1.94	0.49
1:B:103:ASN:O	1:B:107:LEU:HG	2.13	0.49
1:F:71:HIS:CD2	1:F:96:VAL:CG2	2.96	0.49
1:C:102:GLU:N	1:C:153:ARG:O	2.41	0.49
1:D:103:ASN:O	1:D:107:LEU:HD12	2.13	0.49
1:D:426:ASP:O	1:D:427:ALA:HB3	2.12	0.49
1:G:35:VAL:HG21	1:G:63:LEU:HB3	1.95	0.49
1:E:2:GLY:O	1:E:71:HIS:HA	2.12	0.49
1:G:36:VAL:HG12	1:G:37:ASP:O	2.13	0.49
1:B:77:HIS:O	1:B:122:THR:HA	2.11	0.49
1:C:569:GLU:HB3	5:C:611:G6Q:O2	2.12	0.49
1:D:12:VAL:O	1:D:16:LEU:HG	2.13	0.49
1:G:171:ALA:O	1:G:211:ILE:HA	2.12	0.49
1:H:401:SER:OG	1:H:404:ALA:HB3	2.13	0.49
1:B:421:ARG:H	1:B:422:LEU:HB3	1.77	0.49
1:C:235:GLU:HG3	1:C:236:SER:N	2.25	0.49
1:H:423:LYS:CB	1:H:424:GLY:CA	2.87	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:VAL:HG11	1:C:575:PHE:CG	2.47	0.49
1:E:129:HIS:O	1:E:132:ASN:HB3	2.13	0.49
1:F:204:ILE:HG21	1:F:221:ILE:HD11	1.94	0.49
1:G:205:PHE:HE1	1:G:234:ILE:HD11	1.77	0.49
1:G:328:SER:HB3	1:G:354:ASP:OD2	2.12	0.49
1:G:86:HIS:CE1	1:G:124:THR:HG21	2.48	0.48
1:H:312:TYR:CE2	1:H:473:GLY:HA2	2.48	0.48
1:A:431[B]:HIS:CD2	1:A:435[B]:HIS:CD2	3.01	0.48
5:D:611:G6Q:O5	5:D:611:G6Q:O3	2.25	0.48
1:F:214:ILE:HG23	1:F:219:VAL:HG22	1.95	0.48
1:F:225:THR:OG1	1:F:226:GLY:HA2	2.13	0.48
1:H:567:VAL:HG11	1:H:575:PHE:CG	2.47	0.48
1:C:591:LYS:NZ	6:C:1346:HOH:O	2.38	0.48
1:C:295:ILE:HD11	1:C:419:LEU:HD13	1.94	0.48
1:F:76:THR:O	1:F:77:HIS:CB	2.61	0.48
1:F:285:ALA:O	1:F:286:ASP:HB3	2.11	0.48
1:H:281:LEU:HD22	1:H:387:LEU:HB3	1.95	0.48
1:H:430:GLU:O	1:H:434:VAL:HG23	2.13	0.48
1:H:472:ARG:HG2	1:H:473:GLY:N	2.28	0.48
1:B:93:ILE:HG12	1:B:131:VAL:HG12	1.95	0.48
1:C:480:LEU:HD23	1:C:496:ALA:HB3	1.96	0.48
1:E:135:LEU:HD23	1:E:135:LEU:HA	1.56	0.48
1:E:567:VAL:HG11	1:E:575:PHE:CG	2.49	0.48
1:G:275:GLN:HG3	1:G:430:GLU:OE2	2.14	0.48
1:A:234:ILE:HD12	1:A:234:ILE:C	2.33	0.48
1:B:44:ARG:NH1	1:B:89:VAL:HG13	2.29	0.48
1:E:7:ILE:HG23	1:E:7:ILE:O	2.14	0.48
1:C:137:GLN:N	1:C:137:GLN:OE1	2.47	0.48
1:C:63:LEU:HD12	1:C:63:LEU:N	2.29	0.48
1:D:52:GLN:NE2	1:D:56:GLN:OE1	2.46	0.48
4:E:609:GOL:H12	6:E:1521:HOH:O	2.13	0.48
1:F:89:VAL:HG22	1:F:90:SER:N	2.28	0.48
1:H:111:LEU:HD13	1:H:129:HIS:HB2	1.93	0.48
1:D:148:ALA:O	1:D:151:GLN:HG3	2.14	0.48
1:D:304:TYR:CD1	1:D:326:ILE:HD13	2.49	0.48
1:A:110:GLU:O	1:A:114:ARG:HG3	2.14	0.48
1:D:453:ARG:NH2	1:D:563:GLU:O	2.36	0.47
1:F:15:ILE:HG21	1:F:188:PHE:CE1	2.48	0.47
1:H:245:LYS:NZ	6:H:891:HOH:O	2.47	0.47
1:E:145:VAL:O	1:E:149:ILE:HG12	2.14	0.47
1:F:513:ASP:HB3	6:F:1392:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:GLN:HA	1:H:59:GLU:HG2	1.95	0.47
1:B:89:VAL:HG12	1:B:94:VAL:HG13	1.95	0.47
1:C:90:SER:O	1:C:91:GLU:HB3	2.14	0.47
1:D:73:ARG:NH1	1:D:75:ALA:HB2	2.29	0.47
1:E:205:PHE:HD1	1:E:234:ILE:HD11	1.79	0.47
1:E:396:GLU:OE1	1:E:401:SER:HB2	2.14	0.47
1:F:522:ASN:ND2	6:F:694:HOH:O	2.47	0.47
1:F:457:LEU:HD22	1:F:562:ILE:HD13	1.95	0.47
1:G:104:HIS:CD2	1:G:108:ARG:HH22	2.33	0.47
1:A:240:TYR:N	1:A:240:TYR:CD1	2.83	0.47
1:B:155:ALA:HA	1:B:175:GLY:HA3	1.96	0.47
1:C:447:MET:HG2	1:C:578:VAL:HB	1.97	0.47
1:D:173:ARG:NH2	1:D:177:PRO:HB3	2.29	0.47
1:B:320:ILE:HD13	1:B:421:ARG:HG2	1.97	0.47
1:C:400:ALA:HB1	1:C:485:LYS:CE	2.44	0.47
1:E:37:ASP:OD2	1:E:41[A]:HIS:HB2	2.15	0.47
1:E:9:GLN:HB2	1:E:216:ARG:HH21	1.79	0.47
1:F:149:ILE:N	1:F:150:PRO:CD	2.77	0.47
1:G:39:GLU:CD	1:G:39:GLU:H	2.18	0.47
1:H:295:ILE:HD11	1:H:320:ILE:HD12	1.97	0.47
1:A:591:LYS:HE3	6:A:1520:HOH:O	2.14	0.47
1:D:142:ARG:HG2	1:D:146:LEU:HD11	1.96	0.47
1:C:234:ILE:C	1:C:234:ILE:HD12	2.34	0.47
1:D:134:GLU:OE2	1:D:147:ARG:NH2	2.43	0.47
1:F:188:PHE:CE2	1:F:199:VAL:CG1	2.97	0.47
1:H:518:VAL:CG2	1:H:543:LEU:HD21	2.45	0.47
1:B:440:LEU:HB3	1:B:441:PRO:HD3	1.95	0.47
1:E:197:LEU:N	1:E:198:PRO:CD	2.77	0.47
1:F:174:SER:OG	1:F:224:LYS:NZ	2.48	0.47
1:B:71:HIS:CE1	1:B:73:ARG:HB2	2.50	0.47
1:F:503:LYS:HG3	1:F:503:LYS:O	2.14	0.47
1:C:567:VAL:HG11	1:C:575:PHE:CD1	2.50	0.46
1:E:411:VAL:HA	1:E:414:MET:HE2	1.97	0.46
1:F:23:LEU:HG	1:F:195:ALA:HB2	1.96	0.46
1:F:489:ILE:HG22	1:F:598:PRO:HG3	1.97	0.46
1:H:426:ASP:CG	1:H:427:ALA:H	2.17	0.46
1:A:161:MET:HB3	1:A:169:LEU:CD2	2.44	0.46
1:C:90:SER:HB2	1:C:128:ALA:HB1	1.95	0.46
1:A:474:ASP:OD2	5:A:610:G6Q:H3	2.15	0.46
1:E:267:LEU:HD21	1:E:437:LEU:HD22	1.97	0.46
1:D:119:VAL:N	1:D:125:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:VAL:HA	1:D:414:MET:HE2	1.97	0.46
1:F:223:ASP:O	1:F:226:GLY:HA3	2.14	0.46
1:B:240:TYR:CE2	1:H:243:GLY:HA3	2.51	0.46
1:C:97:HIS:HB3	1:C:124:THR:HG23	1.97	0.46
1:E:74:TRP:CG	1:E:264:LYS:HE2	2.50	0.46
1:F:401:SER:OG	1:F:404:ALA:HB3	2.16	0.46
1:F:40:GLY:HA3	1:F:41:HIS:CB	2.38	0.46
1:B:401:SER:OG	1:B:404:ALA:HB3	2.15	0.46
1:C:346:LEU:HD23	1:C:373:ILE:HB	1.97	0.46
1:C:578:VAL:N	1:C:579:PRO:HD2	2.31	0.46
1:E:9:GLN:HB2	1:E:216:ARG:NH2	2.30	0.46
1:F:3:ILE:HG12	1:F:96:VAL:CG2	2.44	0.46
1:A:447:MET:HG2	1:A:575:PHE:CE1	2.51	0.46
1:F:227:ALA:O	1:F:229:VAL:HG23	2.15	0.46
1:F:20:LEU:HD11	1:F:71:HIS:C	2.36	0.46
1:B:86:HIS:HB3	1:B:87:PRO:HA	1.98	0.46
1:C:229:VAL:O	1:C:230:LYS:HD2	2.16	0.46
1:B:7:ILE:HD13	1:B:67:THR:OG1	2.15	0.46
1:D:142:ARG:HD3	1:D:222:PHE:CE2	2.51	0.46
1:G:474:ASP:OD1	5:G:610:G6Q:H3	2.16	0.46
1:C:105:GLU:HB2	1:C:106:PRO:CD	2.40	0.46
1:C:105:GLU:CB	1:C:106:PRO:HD3	2.38	0.46
1:D:197:LEU:N	1:D:198:PRO:CD	2.79	0.46
1:D:255:GLU:HA	1:D:258:GLU:HG2	1.97	0.46
1:C:135:LEU:O	1:C:136:LYS:C	2.55	0.45
1:C:199:VAL:HG23	1:C:200:THR:HG22	1.99	0.45
1:F:149:ILE:N	1:F:150:PRO:HD2	2.31	0.45
1:H:423:LYS:HB2	1:H:424:GLY:CA	2.42	0.45
1:D:295:ILE:HD11	1:D:419:LEU:HD13	1.98	0.45
1:E:371:LEU:CD2	1:E:415:LEU:HD21	2.46	0.45
1:F:15:ILE:HD13	1:F:188:PHE:HE1	1.79	0.45
1:B:241:ASP:HB3	1:B:251:TYR:HE1	1.80	0.45
1:H:164:ARG:HB2	1:H:164:ARG:HE	1.57	0.45
1:B:295:ILE:HD11	1:B:419:LEU:HD13	1.97	0.45
1:B:562:ILE:HG22	1:B:564:MET:CE	2.47	0.45
1:C:298:LEU:HD11	1:C:330:PHE:CD2	2.51	0.45
1:H:346:LEU:HD23	1:H:373:ILE:HB	1.99	0.45
1:D:567:VAL:HG11	1:D:575:PHE:CD1	2.52	0.45
1:E:76:THR:OG1	2:E:701:GLU:N	2.50	0.45
1:C:222:PHE:CB	1:C:228:GLU:HA	2.46	0.45
1:D:194:LEU:HD11	1:D:383:ARG:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ILE:HG23	1:E:156:TYR:OH	2.16	0.45
1:F:190:ALA:HB2	1:F:196:LEU:HD21	1.99	0.45
1:F:28:TYR:CG	1:F:72:THR:HG23	2.52	0.45
1:D:193:GLN:OE1	1:D:205:PHE:HZ	2.00	0.45
1:E:97:HIS:HB3	1:E:124:THR:HG23	1.99	0.45
1:F:136:LYS:HE2	1:F:136:LYS:HB2	1.70	0.45
1:F:196:LEU:HB2	1:F:203:PHE:HE1	1.81	0.45
1:F:457:LEU:CD2	1:F:562:ILE:HD13	2.47	0.45
1:G:476:TYR:HB3	1:G:477:PRO:HD3	1.99	0.45
1:H:135:LEU:HA	1:H:135:LEU:HD23	1.61	0.45
1:H:180:ILE:O	1:H:203:PHE:HA	2.17	0.45
1:C:557:ASP:OD1	1:C:557:ASP:N	2.49	0.45
1:E:472:ARG:HG2	1:E:473:GLY:N	2.31	0.45
1:G:440:LEU:HB3	1:G:441:PRO:HD3	1.98	0.45
1:G:486:LEU:HD12	1:G:486:LEU:HA	1.70	0.45
1:A:425:LEU:HA	1:A:427:ALA:H	1.81	0.45
1:B:291:LYS:HD3	1:B:291:LYS:HA	1.82	0.45
1:G:175:GLY:N	1:G:208:GLU:OE2	2.50	0.45
1:C:3:ILE:O	1:C:190:ALA:HA	2.17	0.45
1:F:123:ASP:OD1	1:F:124:THR:N	2.50	0.45
1:H:74:TRP:CG	1:H:264:LYS:HE2	2.52	0.45
1:B:225:THR:HG23	1:B:227:ALA:H	1.81	0.44
1:B:240:TYR:CA	1:B:241:ASP:CB	2.92	0.44
1:B:578:VAL:HB	1:B:579:PRO:HD3	1.99	0.44
1:D:203:PHE:O	1:D:233:ASP:HA	2.16	0.44
1:D:350:GLY:HA2	1:D:381:LEU:HD12	1.99	0.44
1:E:247:ILE:HG13	1:E:247:ILE:O	2.16	0.44
1:E:334:LYS:HB3	1:E:334:LYS:HE2	1.76	0.44
1:F:118:PHE:CE2	1:F:126:VAL:HG12	2.52	0.44
1:H:503:LYS:O	1:H:503:LYS:HG3	2.17	0.44
1:D:207:GLU:HA	1:D:207:GLU:OE1	2.18	0.44
1:G:205:PHE:CE1	1:G:234:ILE:HD11	2.51	0.44
1:H:440:LEU:HB3	1:H:441:PRO:HD3	1.98	0.44
1:A:63:LEU:HD12	1:A:63:LEU:H	1.82	0.44
1:C:503:LYS:HG3	1:C:503:LYS:O	2.18	0.44
1:E:340:ASN:HA	1:E:368:LEU:HG	1.99	0.44
1:B:320:ILE:HD11	1:B:419:LEU:O	2.17	0.44
1:E:430:GLU:O	1:E:434:VAL:HG23	2.18	0.44
1:F:531:SER:O	1:F:534:GLU:HB2	2.16	0.44
1:G:18:GLU:O	1:G:22:ARG:HD2	2.18	0.44
1:G:224:LYS:HD2	1:G:225:THR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:N	1:A:198:PRO:CD	2.81	0.44
1:A:239:GLN:O	1:A:240:TYR:CD1	2.53	0.44
1:C:1:ALA:N	2:C:701:GLU:OE1	2.44	0.44
1:D:3:ILE:O	1:D:190:ALA:HA	2.17	0.44
1:F:441:PRO:O	1:F:445:GLU:HG3	2.18	0.44
1:G:141:LEU:CD1	1:G:162:ASP:HB2	2.47	0.44
1:H:294:HIS:CD2	1:H:338:ARG:HG2	2.52	0.44
1:A:572:ALA:N	1:A:573:PRO:CD	2.81	0.44
1:B:237:ASN:N	1:B:239:GLN:OE1	2.45	0.44
1:C:51:VAL:O	1:C:54:LEU:N	2.51	0.44
1:D:105:GLU:H	1:D:106:PRO:HD2	1.83	0.44
1:D:440:LEU:HB3	1:D:441:PRO:HD3	1.98	0.44
1:A:318:ALA:HB2	1:A:416:VAL:HG13	1.99	0.44
1:G:97:HIS:HB3	1:G:124:THR:HG23	2.00	0.44
1:H:320:ILE:HG23	1:H:421:ARG:HG3	1.99	0.44
1:B:312:TYR:CE2	1:B:473:GLY:HA2	2.52	0.44
1:B:489:ILE:HG22	1:B:598:PRO:HG3	2.00	0.44
1:C:180:ILE:HD12	1:C:206:LEU:HD21	2.00	0.44
1:C:232:GLN:HE21	1:C:234:ILE:HG22	1.83	0.44
1:D:99:GLY:O	2:D:701:GLU:N	2.51	0.44
1:G:25:TYR:CD2	1:G:383:ARG:HB3	2.52	0.44
1:B:22:ARG:CZ	1:B:198:PRO:HG3	2.48	0.44
1:D:167:ASP:O	1:D:215:THR:HG22	2.18	0.44
1:G:264:LYS:HB2	1:G:264:LYS:HE3	1.75	0.44
1:B:92:HIS:CD2	1:B:164:ARG:NE	2.85	0.43
1:D:318:ALA:HB2	1:D:416:VAL:HG13	1.98	0.43
1:D:379:SER:O	1:D:383:ARG:HG3	2.17	0.43
1:H:176:SER:HA	1:H:177:PRO:HD3	1.85	0.43
1:H:426:ASP:O	1:H:427:ALA:HB3	2.18	0.43
1:A:234:ILE:HD12	1:A:234:ILE:O	2.18	0.43
1:B:230:LYS:HE2	1:B:231:ARG:N	2.31	0.43
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.78	0.43
1:C:86:HIS:CE1	1:C:124:THR:HG21	2.52	0.43
1:H:295:ILE:CD1	1:H:320:ILE:HD12	2.48	0.43
1:A:242:ALA:HA	1:D:242:ALA:N	2.33	0.43
1:C:140:THR:OG1	1:C:143:GLU:OE1	2.37	0.43
1:C:530:LYS:HG2	1:C:559:MET:SD	2.58	0.43
1:G:104:HIS:HD2	1:G:108:ARG:HH12	1.67	0.43
1:B:123:ASP:O	1:B:126:VAL:HG22	2.18	0.43
1:C:229:VAL:HG23	1:C:231:ARG:HH12	1.83	0.43
1:D:141:LEU:HD21	1:D:162:ASP:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:ASP:OD1	1:F:41:HIS:HB3	2.19	0.43
1:A:149:ILE:HB	1:A:150:PRO:HD3	2.00	0.43
1:A:69:ILE:HD11	1:A:94:VAL:HG12	2.00	0.43
1:D:411:VAL:HA	1:D:414:MET:HE3	1.99	0.43
1:A:423:LYS:HA	1:A:423:LYS:HD3	1.80	0.43
1:C:157:GLY:HA2	1:C:172:ALA:O	2.18	0.43
1:C:196:LEU:HB2	1:C:203:PHE:CE1	2.53	0.43
1:F:77:HIS:O	1:F:122:THR:HA	2.18	0.43
1:G:518:VAL:CG2	1:G:543:LEU:HD21	2.49	0.43
1:C:11:ASP:HA	1:C:65:GLY:O	2.19	0.43
5:E:610:G6Q:O5	5:E:610:G6Q:O3	2.24	0.43
1:F:284:ASN:O	1:F:285:ALA:C	2.55	0.43
1:H:443:ARG:HD2	1:H:567:VAL:HG12	2.00	0.43
1:F:3:ILE:HD12	1:F:98:ASN:ND2	2.34	0.43
1:A:157:GLY:HA2	1:A:172:ALA:O	2.19	0.43
1:C:204:ILE:CD1	1:C:221:ILE:HD11	2.43	0.43
1:E:425:LEU:HD13	1:E:426:ASP:OD2	2.18	0.43
1:F:178:LEU:HB3	1:F:189:ILE:HD11	2.01	0.43
1:G:130:LEU:HD23	1:G:148:ALA:HB1	2.01	0.43
1:G:292:VAL:O	1:G:421:ARG:NH1	2.52	0.43
1:H:37:ASP:HA	1:H:65:GLY:HA2	2.01	0.43
1:B:76:THR:OG1	2:B:701:GLU:N	2.52	0.43
1:C:197:LEU:HD23	1:C:203:PHE:CZ	2.53	0.43
1:D:8:ALA:HA	1:D:216:ARG:HG2	2.00	0.43
1:E:440:LEU:HB3	1:E:441:PRO:HD3	2.00	0.43
1:E:86:HIS:N	1:E:86:HIS:CD2	2.85	0.43
1:B:320:ILE:H	1:B:320:ILE:HG12	1.67	0.42
1:C:193:GLN:O	1:C:195:ALA:N	2.52	0.42
1:D:110:GLU:HG3	1:D:114:ARG:NH2	2.34	0.42
1:D:567:VAL:HG11	1:D:575:PHE:CG	2.53	0.42
1:D:86:HIS:CE1	1:D:97:HIS:HB3	2.53	0.42
1:E:315:GLU:HG2	1:E:320:ILE:O	2.19	0.42
1:E:424:GLY:O	1:E:425:LEU:HB2	2.19	0.42
1:F:196:LEU:HB2	1:F:203:PHE:CE1	2.53	0.42
1:F:221:ILE:O	1:F:229:VAL:HB	2.18	0.42
1:F:35:VAL:CG2	1:F:63:LEU:HB3	2.49	0.42
1:G:572:ALA:N	1:G:573:PRO:CD	2.82	0.42
1:A:133:TRP:O	1:A:136:LYS:HB2	2.19	0.42
1:B:174:SER:OG	1:B:174:SER:O	2.28	0.42
1:E:425:LEU:HA	1:E:425:LEU:HD23	1.74	0.42
1:F:530:LYS:HD3	1:F:559:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:LEU:HA	1:B:437:LEU:HD23	1.90	0.42
1:G:197:LEU:N	1:G:198:PRO:CD	2.82	0.42
1:A:11:ASP:HA	1:A:65:GLY:O	2.19	0.42
1:A:396:GLU:OE1	1:A:401:SER:HB2	2.20	0.42
1:B:513:ASP:HB3	6:B:618:HOH:O	2.20	0.42
1:E:321:PRO:HB3	1:F:338:ARG:CZ	2.49	0.42
1:G:304:TYR:CD1	1:G:326:ILE:HD13	2.54	0.42
1:A:173:ARG:O	1:A:173:ARG:HG3	2.12	0.42
1:A:425:LEU:HD13	1:A:428:SER:CB	2.50	0.42
1:A:487:LYS:HG2	1:B:509:LEU:HD11	2.02	0.42
1:E:134:GLU:O	1:E:147:ARG:NH2	2.52	0.42
1:E:174:SER:HA	1:E:208:GLU:OE2	2.19	0.42
1:E:337:VAL:HG12	1:E:338:ARG:O	2.18	0.42
1:F:125:GLU:HG2	1:F:129:HIS:CD2	2.54	0.42
1:F:175:GLY:N	1:F:208:GLU:OE2	2.53	0.42
1:B:379:SER:O	1:B:383:ARG:HG3	2.20	0.42
1:D:90:SER:HB2	1:D:128:ALA:CB	2.48	0.42
1:F:136:LYS:C	1:F:137:GLN:HG3	2.40	0.42
1:F:4:VAL:CG1	1:F:16:LEU:HA	2.50	0.42
1:F:374:CYS:O	1:F:390:MET:HA	2.20	0.42
1:F:35:VAL:HG21	1:F:63:LEU:HB3	2.00	0.42
1:A:431[B]:HIS:NE2	1:A:435[B]:HIS:HD2	2.16	0.42
1:B:603:LYS:HD2	1:B:603:LYS:HA	1.80	0.42
1:C:309:VAL:HG23	1:C:477:PRO:HB2	2.02	0.42
1:D:130:LEU:C	1:D:130:LEU:HD12	2.40	0.42
1:F:71:HIS:CG	1:F:86:HIS:HB2	2.54	0.42
1:B:142:ARG:NE	1:B:213:GLU:OE1	2.52	0.42
1:A:528:LYS:HE3	1:B:608:GLU:O	2.20	0.42
1:F:223:ASP:OD2	1:F:224:LYS:N	2.49	0.42
1:G:182:LEU:HD11	1:G:204:ILE:HD11	2.02	0.42
1:H:197:LEU:N	1:H:198:PRO:CD	2.82	0.42
1:A:311:ARG:HD3	6:A:707:HOH:O	2.19	0.42
1:C:134:GLU:HB3	1:C:144:ALA:HA	2.02	0.42
1:C:488:GLU:O	1:C:598:PRO:HB3	2.19	0.42
1:D:111:LEU:HD22	1:D:116:TYR:CE2	2.55	0.42
1:D:86:HIS:CE1	1:D:124:THR:HG21	2.55	0.42
1:D:18:GLU:O	1:D:22:ARG:HG3	2.20	0.42
1:E:404:ALA:O	1:E:408:GLN:HG3	2.19	0.42
1:H:530:LYS:O	1:H:534:GLU:HG2	2.20	0.42
1:C:486:LEU:HD12	1:C:486:LEU:HA	1.89	0.42
1:F:420:SER:HB2	1:F:426:ASP:CG	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:ASN:OD1	1:G:368:LEU:HD21	2.20	0.42
1:C:23:LEU:HA	1:C:23:LEU:HD23	1.82	0.41
1:G:217:ARG:HD3	1:G:217:ARG:HA	1.60	0.41
1:A:569:GLU:HB2	5:A:610:G6Q:O2	2.20	0.41
1:C:193:GLN:OE1	1:C:205:PHE:HZ	2.03	0.41
1:E:158:THR:HG22	1:E:172:ALA:HB3	2.02	0.41
1:F:3:ILE:HG21	1:F:159:VAL:HG21	2.02	0.41
1:F:24:GLU:HG2	1:F:28:TYR:CE1	2.55	0.41
1:F:569:GLU:HG2	5:F:610:G6Q:O4	2.19	0.41
1:B:25:TYR:CE2	1:B:26:ARG:HG3	2.55	0.41
1:C:301:GLY:O	1:C:304:TYR:HB3	2.20	0.41
1:E:164:ARG:HE	1:E:164:ARG:HB2	1.54	0.41
1:F:287:GLU:O	1:F:291:LYS:HD3	2.21	0.41
1:F:34:ALA:HB2	1:F:87:PRO:HG2	2.02	0.41
1:F:557:ASP:N	1:F:557:ASP:OD1	2.53	0.41
1:F:567:VAL:CG2	1:F:575:PHE:CD2	3.03	0.41
1:G:181:GLY:HA2	1:G:202:ARG:O	2.20	0.41
1:G:90:SER:O	1:G:91:GLU:HB2	2.20	0.41
1:A:37:ASP:OD2	1:A:41[A]:HIS:HB2	2.20	0.41
1:B:101:ILE:HG21	1:B:152:LEU:HD22	2.02	0.41
1:B:368:LEU:HD23	1:B:368:LEU:HA	1.83	0.41
1:F:476:TYR:HB3	1:F:477:PRO:HD3	2.02	0.41
1:H:423:LYS:HD2	1:H:423:LYS:N	2.35	0.41
1:C:164:ARG:HB2	1:C:164:ARG:HE	1.42	0.41
1:D:90:SER:O	1:D:132:ASN:ND2	2.54	0.41
1:F:47:ARG:HD3	1:F:47:ARG:HA	1.83	0.41
1:G:374:CYS:O	1:G:390:MET:HA	2.20	0.41
1:C:443:ARG:HD2	1:C:567:VAL:HG12	2.03	0.41
1:D:179:VAL:HG22	1:D:180:ILE:N	2.36	0.41
1:E:287:GLU:O	1:E:290:SER:OG	2.34	0.41
1:E:318:ALA:HB1	1:E:420:SER:HA	2.02	0.41
1:D:107:LEU:CD1	1:D:152:LEU:HD23	2.50	0.41
1:F:145:VAL:C	1:F:147:ARG:H	2.24	0.41
1:F:3:ILE:HG13	1:F:98:ASN:ND2	2.35	0.41
1:B:101:ILE:HD12	1:B:152:LEU:HB3	2.01	0.41
1:B:230:LYS:HE2	1:B:230:LYS:CA	2.45	0.41
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.74	0.41
1:E:347:SER:O	1:E:374:CYS:HA	2.21	0.41
1:F:130:LEU:HD23	1:F:130:LEU:C	2.41	0.41
1:A:105:GLU:HB2	1:A:106:PRO:HD3	2.03	0.41
1:A:486:LEU:HA	1:A:486:LEU:HD12	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:VAL:N	1:A:579:PRO:HD2	2.36	0.41
1:C:176:SER:HA	1:C:177:PRO:HD3	1.83	0.41
1:C:309:VAL:CG2	1:C:477:PRO:HB2	2.50	0.41
1:C:71:HIS:ND1	1:C:86:HIS:HB2	2.36	0.41
1:D:80:PRO:O	1:D:81:SER:HB3	2.20	0.41
1:D:95:VAL:HG22	1:D:160:ILE:CG1	2.50	0.41
1:F:197:LEU:N	1:F:198:PRO:CD	2.83	0.41
1:F:281:LEU:HA	1:F:281:LEU:HD23	1.93	0.41
1:F:486:LEU:HD12	1:F:486:LEU:HA	1.91	0.41
1:A:312:TYR:CE2	1:A:473:GLY:HA2	2.55	0.41
1:C:149:ILE:C	1:C:151:GLN:N	2.73	0.41
1:F:224:LYS:HE2	1:F:224:LYS:HB2	1.89	0.41
1:B:401:SER:HB2	6:B:659:HOH:O	2.20	0.41
1:F:196:LEU:HD12	1:F:203:PHE:CE1	2.56	0.41
1:F:34:ALA:CB	1:F:87:PRO:HG2	2.51	0.41
1:G:193:GLN:HB2	1:G:203:PHE:CE2	2.56	0.41
1:B:310:SER:HB3	1:B:412:LEU:HD13	2.02	0.40
1:E:426:ASP:HB3	1:E:428:SER:H	1.86	0.40
1:F:84:ASN:OD1	1:F:120:SER:HB2	2.22	0.40
1:F:9:GLN:O	1:F:9:GLN:HG2	2.22	0.40
1:G:532:ASN:O	1:G:535:GLU:HB2	2.21	0.40
1:H:123:ASP:OD1	2:H:701:GLU:N	2.54	0.40
1:A:431[B]:HIS:CE1	1:A:435[B]:HIS:NE2	2.90	0.40
1:B:374:CYS:O	1:B:390:MET:HA	2.20	0.40
1:B:317:LEU:O	1:B:429:ILE:HD13	2.22	0.40
1:B:530:LYS:HD3	1:B:559:MET:SD	2.61	0.40
1:C:123:ASP:OD1	2:C:701:GLU:N	2.54	0.40
1:C:222:PHE:HA	1:C:228:GLU:HA	2.03	0.40
1:E:23:LEU:HD21	1:E:192:ASP:HB3	2.02	0.40
1:B:320:ILE:HD12	1:B:419:LEU:O	2.20	0.40
1:D:266:THR:HG22	1:D:414:MET:HE1	2.03	0.40
1:D:90:SER:HB2	1:D:128:ALA:C	2.41	0.40
1:F:141:LEU:CG	1:F:170:LEU:HD23	2.50	0.40
1:F:76:THR:HG23	2:F:701:GLU:HB3	2.02	0.40
1:G:312:TYR:CE2	1:G:473:GLY:HA2	2.56	0.40
1:G:35:VAL:CG2	1:G:63:LEU:HB3	2.52	0.40
1:A:603:LYS:HD2	1:A:603:LYS:HA	1.97	0.40
1:C:232:GLN:NE2	1:C:234:ILE:HG22	2.37	0.40
1:D:52:GLN:O	1:D:56:GLN:HG3	2.21	0.40
1:E:503:LYS:HG3	1:E:503:LYS:O	2.21	0.40
1:A:158:THR:HG22	1:A:172:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG22	1:A:42:MET:HG2	2.02	0.40
1:D:189:ILE:HG13	1:D:190:ALA:N	2.37	0.40
1:D:589:LEU:HA	1:D:589:LEU:HD23	1.95	0.40
1:F:79:GLU:HA	1:F:80:PRO:HD3	1.89	0.40
1:G:168:THR:HG22	1:G:169:LEU:N	2.37	0.40
1:G:440:LEU:O	1:G:444:ILE:HG12	2.21	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	611/608 (100%)	586 (96%)	21 (3%)	4 (1%)	25	43
1	B	608/608 (100%)	577 (95%)	21 (4%)	10 (2%)	11	19
1	C	599/608 (98%)	572 (96%)	20 (3%)	7 (1%)	15	27
1	D	601/608 (99%)	576 (96%)	18 (3%)	7 (1%)	15	27
1	E	600/608 (99%)	566 (94%)	28 (5%)	6 (1%)	18	32
1	F	590/608 (97%)	531 (90%)	47 (8%)	12 (2%)	9	14
1	G	602/608 (99%)	576 (96%)	22 (4%)	4 (1%)	25	43
1	H	608/608 (100%)	587 (96%)	19 (3%)	2 (0%)	44	66
All	All	4819/4864 (99%)	4571 (95%)	196 (4%)	52 (1%)	17	29

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	ASN
1	B	241	ASP
1	B	242	ALA
1	B	284	ASN

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Mol	Chain	Res	Type
1	B	285	ALA
1	C	139	GLY
1	E	114	ARG
1	E	426	ASP
1	F	77	HIS
1	F	114	ARG
1	F	286	ASP
1	A	424	GLY
1	B	228	GLU
1	B	286	ASP
1	B	426	ASP
1	C	286	ASP
1	D	114	ARG
1	D	227	ALA
1	D	426	ASP
1	E	244	ASP
1	E	419	LEU
1	F	40	GLY
1	A	238	LEU
1	A	244	ASP
1	C	194	LEU
1	D	224	LYS
1	F	41	HIS
1	G	41	HIS
1	G	228	GLU
1	B	114	ARG
1	C	91	GLU
1	C	136	LYS
1	E	421	ARG
1	F	138	GLY
1	F	222	PHE
1	G	40	GLY
1	H	423	LYS
1	H	535	GLU
1	D	91	GLU
1	F	79	GLU
1	F	92	HIS
1	F	146	LEU
1	F	183	GLY
1	F	505	GLY
1	G	505	GLY
1	C	505	GLY

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Mol	Chain	Res	Type
1	D	40	GLY
1	D	105	GLU
1	E	505	GLY
1	A	505	GLY
1	B	27	GLY
1	C	150	PRO

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	498/499 (100%)	472 (95%)	26 (5%)	27	49
1	B	497/499 (100%)	474 (95%)	23 (5%)	31	55
1	C	490/499 (98%)	469 (96%)	21 (4%)	33	58
1	D	488/499 (98%)	464 (95%)	24 (5%)	29	52
1	E	492/499 (99%)	466 (95%)	26 (5%)	26	48
1	F	487/499 (98%)	453 (93%)	34 (7%)	18	33
1	G	493/499 (99%)	471 (96%)	22 (4%)	32	56
1	H	497/499 (100%)	474 (95%)	23 (5%)	31	55
All	All	3942/3992 (99%)	3743 (95%)	199 (5%)	28	51

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	112	LYS
1	A	135	LEU
1	A	137	GLN
1	A	153	ARG
1	A	170	LEU
1	A	173	ARG
1	A	184	MET
1	A	225	THR

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Mol	Chain	Res	Type
1	A	229	VAL
1	A	232	GLN
1	A	291	LYS
1	A	320	ILE
1	A	339	ARG
1	A	362	SER
1	A	415	LEU
1	A	418	LYS
1	A	422	LEU
1	A	426	ASP
1	A	453	ARG
1	A	485	LYS
1	A	497	TYR
1	A	518	VAL
1	A	543	LEU
1	A	589	LEU
1	A	608	GLU
1	B	60	GLU
1	B	79	GLU
1	B	103	ASN
1	B	112	LYS
1	B	135	LEU
1	B	136	LYS
1	B	199	VAL
1	B	219	VAL
1	B	230	LYS
1	B	233	ASP
1	B	238	LEU
1	B	239	GLN
1	B	241	ASP
1	B	320	ILE
1	B	328	SER
1	B	339	ARG
1	B	415	LEU
1	B	421	ARG
1	B	422	LEU
1	B	497	TYR
1	B	543	LEU
1	B	567	VAL
1	B	589	LEU
1	C	22	ARG
1	C	50	LYS

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Mol	Chain	Res	Type
1	C	52	GLN
1	C	77	HIS
1	C	122	THR
1	C	126	VAL
1	C	164	ARG
1	C	173	ARG
1	C	200	THR
1	C	204	ILE
1	C	228	GLU
1	C	230	LYS
1	C	235	GLU
1	C	415	LEU
1	C	418	LYS
1	C	421	ARG
1	C	497	TYR
1	C	524	GLU
1	C	543	LEU
1	C	567	VAL
1	C	589	LEU
1	D	26	ARG
1	D	50	LYS
1	D	109	GLU
1	D	121	GLU
1	D	130	LEU
1	D	136	LYS
1	D	141	LEU
1	D	151	GLN
1	D	169	LEU
1	D	207	GLU
1	D	218	SER
1	D	230	LYS
1	D	261	ASN
1	D	328[A]	SER
1	D	328[B]	SER
1	D	339	ARG
1	D	415	LEU
1	D	418	LYS
1	D	423	LYS
1	D	428	SER
1	D	497	TYR
1	D	543	LEU
1	D	567	VAL

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Mol	Chain	Res	Type
1	D	589	LEU
1	E	7	ILE
1	E	14	GLU
1	E	53	MET
1	E	60	GLU
1	E	90	SER
1	E	170	LEU
1	E	176	SER
1	E	202	ARG
1	E	208	GLU
1	E	216	ARG
1	E	224	LYS
1	E	235	GLU
1	E	247	ILE
1	E	320	ILE
1	E	339	ARG
1	E	395	THR
1	E	401	SER
1	E	415	LEU
1	E	418	LYS
1	E	421	ARG
1	E	423	LYS
1	E	425	LEU
1	E	442	SER
1	E	497	TYR
1	E	543	LEU
1	E	567	VAL
1	F	20	LEU
1	F	26	ARG
1	F	39	GLU
1	F	48	LEU
1	F	56	GLN
1	F	72	THR
1	F	76	THR
1	F	77	HIS
1	F	86	HIS
1	F	102	GLU
1	F	121	GLU
1	F	126	VAL
1	F	135	LEU
1	F	136	LYS
1	F	143	GLU

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Mol	Chain	Res	Type
1	F	151	GLN
1	F	160	ILE
1	F	164	ARG
1	F	165	HIS
1	F	167	ASP
1	F	184	MET
1	F	189	ILE
1	F	193	GLN
1	F	207	GLU
1	F	230	LYS
1	F	254	LYS
1	F	291	LYS
1	F	348	GLN
1	F	418	LYS
1	F	453	ARG
1	F	497	TYR
1	F	543	LEU
1	F	567	VAL
1	F	589	LEU
1	G	22	ARG
1	G	26	ARG
1	G	29	ASP
1	G	39	GLU
1	G	52	GLN
1	G	56	GLN
1	G	79	GLU
1	G	103	ASN
1	G	135	LEU
1	G	141	LEU
1	G	170	LEU
1	G	189	ILE
1	G	216	ARG
1	G	224	LYS
1	G	288	LEU
1	G	291	LYS
1	G	335	SER
1	G	418	LYS
1	G	421	ARG
1	G	497	TYR
1	G	543	LEU
1	G	589	LEU
1	H	14	GLU

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Mol	Chain	Res	Type
1	H	45	LEU
1	H	114	ARG
1	H	135	LEU
1	H	137	GLN
1	H	142	ARG
1	H	149	ILE
1	H	164	ARG
1	H	229	VAL
1	H	230	LYS
1	H	234	ILE
1	H	291	LYS
1	H	320	ILE
1	H	363	LYS
1	H	364	GLU
1	H	415	LEU
1	H	419	LEU
1	H	423	LYS
1	H	428	SER
1	H	462	SER
1	H	497	TYR
1	H	543	LEU
1	H	567	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	B	103	ASN
1	B	104	HIS
1	C	232	GLN
1	D	52	GLN
1	E	446	GLN
1	F	86	HIS
1	F	98	ASN
1	F	104	HIS
1	G	52	GLN
1	G	71	HIS
1	G	86	HIS
1	G	104	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

32 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	$\# Z > 2$
4	GOL	A	609	-	5,5,5	0.34	0	5,5,5	0.49	0
5	G6Q	A	610	-	15,15,15	1.43	3 (20%)	20,21,21	1.05	1 (5%)
3	G6P	A	611	-	16,16,16	1.41	2 (12%)	24,24,24	0.97	1 (4%)
2	GLU	A	701	-	1,9,9	0.35	0	1,11,11	0.39	0
4	GOL	B	609	-	5,5,5	0.30	0	5,5,5	0.40	0
5	G6Q	B	610	-	15,15,15	1.40	3 (20%)	20,21,21	1.17	2 (10%)
3	G6P	B	612	-	16,16,16	1.41	2 (12%)	24,24,24	0.92	1 (4%)
2	GLU	B	701	-	1,9,9	0.15	0	1,11,11	0.14	0
4	GOL	C	609	-	5,5,5	0.32	0	5,5,5	0.59	0
3	G6P	C	610	-	16,16,16	1.43	2 (12%)	24,24,24	1.06	2 (8%)
5	G6Q	C	611	-	15,15,15	1.35	3 (20%)	20,21,21	1.22	2 (10%)
2	GLU	C	701	-	1,9,9	0.44	0	1,11,11	0.19	0
3	G6P	D	609	-	16,16,16	1.44	3 (18%)	24,24,24	1.12	1 (4%)
4	GOL	D	610	-	5,5,5	0.29	0	5,5,5	0.41	0
5	G6Q	D	611	-	15,15,15	1.56	4 (26%)	20,21,21	1.24	3 (15%)
2	GLU	D	701	-	1,9,9	0.07	0	1,11,11	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	E	609	-	5,5,5	0.33	0	5,5,5	0.76	0
5	G6Q	E	610	-	15,15,15	1.37	4 (26%)	20,21,21	1.18	1 (5%)
3	G6P	E	616	-	16,16,16	1.49	2 (12%)	24,24,24	1.71	5 (20%)
2	GLU	E	701	-	1,9,9	0.02	0	1,11,11	0.58	0
4	GOL	F	609	-	5,5,5	0.27	0	5,5,5	0.50	0
5	G6Q	F	610	-	15,15,15	1.25	2 (13%)	20,21,21	1.36	4 (20%)
3	G6P	F	615	-	16,16,16	1.44	2 (12%)	24,24,24	0.93	0
2	GLU	F	701	-	1,9,9	0.34	0	1,11,11	0.07	0
4	GOL	G	609	-	5,5,5	0.33	0	5,5,5	0.52	0
5	G6Q	G	610	-	15,15,15	1.39	4 (26%)	20,21,21	1.08	2 (10%)
3	G6P	G	613	-	16,16,16	1.46	2 (12%)	24,24,24	1.27	3 (12%)
2	GLU	G	701	-	1,9,9	0.18	0	1,11,11	0.55	0
4	GOL	H	609	-	5,5,5	0.47	0	5,5,5	0.41	0
5	G6Q	H	610	-	15,15,15	1.36	2 (13%)	20,21,21	1.23	1 (5%)
3	G6P	H	614	-	16,16,16	1.43	2 (12%)	24,24,24	1.14	3 (12%)
2	GLU	H	701	-	1,9,9	0.23	0	1,11,11	0.21	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
4	GOL	A	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	A	610	-	-	0/18/20/20	0/0/0/0
3	G6P	A	611	-	-	0/6/26/26	0/1/1/1
2	GLU	A	701	-	-	0/3/9/9	0/0/0/0
4	GOL	B	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	B	610	-	-	0/18/20/20	0/0/0/0
3	G6P	B	612	-	-	0/6/26/26	0/1/1/1
2	GLU	B	701	-	-	0/3/9/9	0/0/0/0
4	GOL	C	609	-	-	0/4/4/4	0/0/0/0
3	G6P	C	610	-	-	0/6/26/26	0/1/1/1
5	G6Q	C	611	-	-	0/18/20/20	0/0/0/0
2	GLU	C	701	-	-	0/3/9/9	0/0/0/0
3	G6P	D	609	-	-	0/6/26/26	0/1/1/1
4	GOL	D	610	-	-	0/4/4/4	0/0/0/0
5	G6Q	D	611	-	-	0/18/20/20	0/0/0/0
2	GLU	D	701	-	-	0/3/9/9	0/0/0/0
4	GOL	E	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	E	610	-	-	0/18/20/20	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G6P	E	616	-	-	0/6/26/26	0/1/1/1
2	GLU	E	701	-	-	0/3/9/9	0/0/0/0
4	GOL	F	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	F	610	-	-	0/18/20/20	0/0/0/0
3	G6P	F	615	-	-	0/6/26/26	0/1/1/1
2	GLU	F	701	-	-	0/3/9/9	0/0/0/0
4	GOL	G	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	G	610	-	-	0/18/20/20	0/0/0/0
3	G6P	G	613	-	-	0/6/26/26	0/1/1/1
2	GLU	G	701	-	-	0/3/9/9	0/0/0/0
4	GOL	H	609	-	-	0/4/4/4	0/0/0/0
5	G6Q	H	610	-	-	0/18/20/20	0/0/0/0
3	G6P	H	614	-	-	0/6/26/26	0/1/1/1
2	GLU	H	701	-	-	0/3/9/9	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	610	G6Q	O2-C2	-2.93	1.37	1.43
5	D	611	G6Q	O2-C2	-2.82	1.37	1.43
5	G	610	G6Q	O2-C2	-2.74	1.38	1.43
5	B	610	G6Q	O2-C2	-2.70	1.38	1.43
5	E	610	G6Q	O2-C2	-2.66	1.38	1.43
5	H	610	G6Q	O2-C2	-2.66	1.38	1.43
5	D	611	G6Q	O4-C4	-2.51	1.37	1.43
5	F	610	G6Q	O2-C2	-2.50	1.38	1.43
5	C	611	G6Q	O2-C2	-2.43	1.38	1.43
5	H	610	G6Q	O4-C4	-2.30	1.37	1.43
5	F	610	G6Q	O4-C4	-2.30	1.37	1.43
5	B	610	G6Q	O4-C4	-2.26	1.37	1.43
5	C	611	G6Q	O5-C5	-2.23	1.38	1.43
5	A	610	G6Q	O4-C4	-2.23	1.37	1.43
5	D	611	G6Q	O5-C5	-2.22	1.38	1.43
5	B	610	G6Q	O5-C5	-2.22	1.38	1.43
5	G	610	G6Q	O4-C4	-2.19	1.37	1.43
5	E	610	G6Q	O3-C3	-2.14	1.38	1.43
5	G	610	G6Q	O5-C5	-2.12	1.38	1.43
5	E	610	G6Q	O4-C4	-2.11	1.38	1.43
5	D	611	G6Q	O3-C3	-2.10	1.38	1.43
5	A	610	G6Q	O5-C5	-2.07	1.38	1.43
5	C	611	G6Q	O4-C4	-2.05	1.38	1.43
5	G	610	G6Q	O3-C3	-2.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	610	G6Q	O5-C5	-2.01	1.38	1.43
3	D	609	G6P	C1-C2	2.15	1.57	1.52
3	A	611	G6P	P-O1P	2.24	1.64	1.54
3	C	610	G6P	P-O1P	2.25	1.64	1.54
3	D	609	G6P	P-O1P	2.32	1.64	1.54
3	F	615	G6P	P-O1P	2.33	1.64	1.54
3	A	611	G6P	P-O2P	2.37	1.64	1.54
3	G	613	G6P	P-O1P	2.44	1.64	1.54
3	E	616	G6P	P-O1P	2.49	1.65	1.54
3	B	612	G6P	P-O1P	2.52	1.65	1.54
3	H	614	G6P	P-O1P	2.52	1.65	1.54
3	C	610	G6P	P-O2P	2.54	1.65	1.54
3	H	614	G6P	P-O2P	2.55	1.65	1.54
3	B	612	G6P	P-O2P	2.56	1.65	1.54
3	F	615	G6P	P-O2P	2.64	1.65	1.54
3	D	609	G6P	P-O2P	2.65	1.65	1.54
3	E	616	G6P	P-O2P	2.65	1.65	1.54
3	G	613	G6P	P-O2P	2.67	1.65	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	609	G6P	C6-C5-C4	-2.70	106.25	112.00
5	D	611	G6Q	C5-C4-C3	-2.61	108.25	112.46
5	F	610	G6Q	O2-C2-C1	-2.51	104.34	110.30
3	A	611	G6P	C6-C5-C4	-2.48	106.72	112.00
5	C	611	G6Q	C5-C4-C3	-2.45	108.51	112.46
3	C	610	G6P	C6-C5-C4	-2.19	107.32	112.00
5	B	610	G6Q	O1-C1-C2	-2.13	119.32	125.13
3	H	614	G6P	C6-C5-C4	-2.11	107.51	112.00
5	G	610	G6Q	O2-C2-C1	-2.02	105.49	110.30
5	F	610	G6Q	O1-C1-C2	-2.02	119.62	125.13
5	D	611	G6Q	O1-C1-C2	-2.02	119.64	125.13
3	B	612	G6P	C1-O5-C5	2.04	117.07	113.39
3	H	614	G6P	P-O6-C6	2.13	124.17	118.30
3	E	616	G6P	O6-P-O3P	2.15	112.50	106.47
3	C	610	G6P	O6-P-O3P	2.19	112.62	106.47
5	F	610	G6Q	C4-C3-C2	2.19	117.42	113.54
3	G	613	G6P	O6-P-O3P	2.28	112.88	106.47
5	D	611	G6Q	O6-C6-C5	2.41	115.80	109.36
3	G	613	G6P	O3-C3-C2	2.42	115.62	110.36
3	E	616	G6P	O3-C3-C2	2.58	115.98	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	610	G6Q	O6-C6-C5	2.62	116.35	109.36
3	H	614	G6P	O3-C3-C4	2.66	116.15	110.36
3	E	616	G6P	O3-C3-C4	2.91	116.70	110.36
3	G	613	G6P	C1-O5-C5	3.09	118.97	113.39
3	E	616	G6P	O5-C1-C2	3.13	115.23	110.04
5	G	610	G6Q	O6-C6-C5	3.15	117.76	109.36
5	F	610	G6Q	O6-C6-C5	3.17	117.81	109.36
5	E	610	G6Q	O6-C6-C5	3.43	118.52	109.36
5	B	610	G6Q	O6-C6-C5	3.46	118.59	109.36
5	C	611	G6Q	O6-C6-C5	3.54	118.82	109.36
5	H	610	G6Q	O6-C6-C5	3.74	119.33	109.36
3	E	616	G6P	C1-O5-C5	4.66	121.79	113.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	610	G6Q	3	0
2	B	701	GLU	2	0
5	C	611	G6Q	3	0
2	C	701	GLU	2	0
5	D	611	G6Q	1	0
2	D	701	GLU	1	0
4	E	609	GOL	1	0
5	E	610	G6Q	1	0
2	E	701	GLU	2	0
5	F	610	G6Q	4	0
2	F	701	GLU	4	0
5	G	610	G6Q	2	0
2	H	701	GLU	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	608/608 (100%)	-0.41	18 (2%)	51	53	20, 37, 72, 168	1 (0%)
1	B	608/608 (100%)	-0.15	33 (5%)	26	27	23, 43, 106, 131	1 (0%)
1	C	601/608 (98%)	-0.27	22 (3%)	42	44	18, 39, 96, 137	1 (0%)
1	D	602/608 (99%)	-0.16	27 (4%)	34	36	17, 37, 115, 142	0
1	E	602/608 (99%)	-0.23	25 (4%)	37	39	23, 47, 90, 152	2 (0%)
1	F	594/608 (97%)	0.36	95 (15%)	2	2	24, 47, 129, 158	0
1	G	605/608 (99%)	0.06	57 (9%)	9	9	20, 42, 131, 170	1 (0%)
1	H	608/608 (100%)	-0.34	25 (4%)	38	40	24, 44, 80, 135	2 (0%)
All	All	4828/4864 (99%)	-0.14	302 (6%)	21	21	17, 43, 109, 170	8 (0%)

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	10.2
1	G	138	GLY	9.6
1	B	138	GLY	9.1
1	G	238	LEU	8.5
1	A	239	GLN	8.5
1	F	100	ILE	8.2
1	A	242	ALA	7.9
1	A	243	GLY	7.5
1	F	227	ALA	7.5
1	F	1	ALA	7.0
1	G	38	ALA	6.8
1	D	113	ALA	6.7
1	F	75	ALA	6.6
1	D	138	GLY	6.5
1	G	116	TYR	6.5
1	G	227	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	425	LEU	5.9
1	A	241	ASP	5.8
1	F	220	ASN	5.7
1	H	425	LEU	5.7
1	E	426	ASP	5.7
1	G	133	TRP	5.7
1	F	109	GLU	5.7
1	F	225	THR	5.6
1	F	106	PRO	5.5
1	G	237	ASN	5.5
1	F	101	ILE	5.4
1	G	115	GLY	5.4
1	D	425	LEU	5.4
1	B	139	GLY	5.3
1	G	137	GLN	5.3
1	G	236	SER	5.1
1	E	423	LYS	5.1
1	F	121	GLU	4.9
1	G	61	HIS	4.7
1	D	117	THR	4.7
1	F	206	LEU	4.7
1	E	243	GLY	4.7
1	F	176	SER	4.6
1	F	76	THR	4.6
1	F	105	GLU	4.6
1	B	225	THR	4.5
1	E	422	LEU	4.5
1	E	225	THR	4.4
1	G	232	GLN	4.4
1	C	139	GLY	4.3
1	D	153	ARG	4.3
1	B	422	LEU	4.3
1	A	240	TYR	4.3
1	D	112	LYS	4.3
1	F	38	ALA	4.2
1	E	425	LEU	4.2
1	F	77	HIS	4.2
1	F	124	THR	4.1
1	G	140	THR	4.1
1	B	133	TRP	4.1
1	F	133	TRP	4.0
1	F	2	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	4	VAL	3.9
1	D	139	GLY	3.9
1	G	225	THR	3.9
1	G	165	HIS	3.9
1	G	39	GLU	3.9
1	D	227	ALA	3.9
1	B	38	ALA	3.8
1	F	155	ALA	3.8
1	D	133	TRP	3.8
1	F	61	HIS	3.7
1	E	424	GLY	3.7
1	G	136	LYS	3.7
1	F	138	GLY	3.7
1	F	126	VAL	3.7
1	D	424	GLY	3.7
1	C	113	ALA	3.7
1	F	60	GLU	3.7
1	G	226	GLY	3.6
1	D	224	LYS	3.6
1	F	154	GLY	3.6
1	G	223	ASP	3.6
1	F	119	VAL	3.6
1	A	284	ASN	3.6
1	F	207	GLU	3.6
1	F	144	ALA	3.6
1	E	39	GLU	3.5
1	A	244	ASP	3.5
1	B	105	GLU	3.5
1	A	273	HIS	3.5
1	F	219	VAL	3.5
1	G	229	VAL	3.5
1	F	153	ARG	3.5
1	F	211	ILE	3.5
1	D	106	PRO	3.5
1	F	135	LEU	3.4
1	F	72	THR	3.4
1	D	234	ILE	3.4
1	B	113	ALA	3.4
1	H	426	ASP	3.4
1	H	273	HIS	3.4
1	D	155	ALA	3.4
1	D	109	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	225	THR	3.3
1	H	283	PRO	3.3
1	F	183	GLY	3.3
1	A	423	LYS	3.3
1	G	224	LYS	3.3
1	G	55	ALA	3.3
1	F	169	LEU	3.3
1	C	229	VAL	3.3
1	G	423	LYS	3.3
1	G	113	ALA	3.3
1	F	175	GLY	3.3
1	F	226	GLY	3.2
1	D	175	GLY	3.2
1	G	153	ARG	3.2
1	B	115	GLY	3.2
1	F	192	ASP	3.2
1	F	208	GLU	3.2
1	B	61	HIS	3.2
1	F	137	GLN	3.2
1	H	423	LYS	3.2
1	E	138	GLY	3.2
1	F	202	ARG	3.2
1	G	244	ASP	3.2
1	G	62	PRO	3.1
1	G	143	GLU	3.1
1	F	164	ARG	3.1
1	C	133	TRP	3.1
1	F	127	ILE	3.1
1	F	189	ILE	3.1
1	B	153	ARG	3.1
1	F	217	ARG	3.1
1	B	226	GLY	3.1
1	F	141	LEU	3.1
1	C	136	LYS	3.0
1	B	39	GLU	3.0
1	F	85	ALA	3.0
1	F	165	HIS	3.0
1	H	62	PRO	3.0
1	F	160	ILE	3.0
1	C	106	PRO	3.0
1	E	234	ILE	3.0
1	G	111	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	217	ARG	3.0
1	F	273	HIS	2.9
1	B	60	GLU	2.9
1	B	426	ASP	2.9
1	F	222	PHE	2.9
1	G	425	LEU	2.9
1	C	39	GLU	2.9
1	B	236	SER	2.9
1	A	425	LEU	2.9
1	G	41	HIS	2.9
1	F	608	GLU	2.9
1	E	137	GLN	2.9
1	F	74	TRP	2.9
1	G	102	GLU	2.8
1	C	232	GLN	2.8
1	F	80	PRO	2.8
1	G	167	ASP	2.8
1	C	153	ARG	2.8
1	E	273	HIS	2.8
1	G	58	ALA	2.8
1	B	137	GLN	2.8
1	F	423	LYS	2.8
1	A	424	GLY	2.8
1	E	139	GLY	2.8
1	E	236	SER	2.8
1	B	119	VAL	2.8
1	H	607	VAL	2.8
1	H	422	LEU	2.8
1	G	230	LYS	2.8
1	F	39	GLU	2.7
1	D	423	LYS	2.7
1	D	137	GLN	2.7
1	F	112	LYS	2.7
1	C	41[A]	HIS	2.7
1	H	138	GLY	2.7
1	D	39	GLU	2.7
1	F	139	GLY	2.7
1	F	224	LYS	2.7
1	E	109	GLU	2.7
1	F	91	GLU	2.7
1	G	110	GLU	2.6
1	E	38	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	113	ALA	2.6
1	B	423	LYS	2.6
1	B	127	ILE	2.6
1	B	109	GLU	2.6
1	B	131	VAL	2.6
1	F	228	GLU	2.6
1	C	38	ALA	2.6
1	E	557	ASP	2.6
1	F	149	ILE	2.6
1	G	228	GLU	2.6
1	E	283	PRO	2.6
1	F	146	LEU	2.6
1	G	142	ARG	2.5
1	G	242	ALA	2.5
1	B	126	VAL	2.5
1	G	176	SER	2.5
1	G	135	LEU	2.5
1	B	420	SER	2.5
1	G	155	ALA	2.5
1	C	235	GLU	2.5
1	C	114	ARG	2.5
1	F	59	GLU	2.5
1	E	431[A]	HIS	2.4
1	F	89	VAL	2.4
1	F	143	GLU	2.4
1	F	230	LYS	2.4
1	B	56	GLN	2.4
1	H	137	GLN	2.4
1	D	283	PRO	2.4
1	F	425	LEU	2.4
1	G	426	ASP	2.4
1	F	53	MET	2.4
1	G	424	GLY	2.4
1	A	426	ASP	2.4
1	F	180	ILE	2.4
1	H	136	LYS	2.4
1	F	113	ALA	2.4
1	F	229	VAL	2.4
1	E	285	ALA	2.4
1	E	427	ALA	2.4
1	G	152	LEU	2.4
1	G	283	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	137	GLN	2.3
1	D	38	ALA	2.3
1	G	139	GLY	2.3
1	F	62	PRO	2.3
1	H	39	GLU	2.3
1	H	424	GLY	2.3
1	F	159	VAL	2.3
1	F	158	THR	2.3
1	F	152	LEU	2.3
1	G	26	ARG	2.3
1	G	235	GLU	2.3
1	F	73	ARG	2.3
1	A	285	ALA	2.3
1	C	236	SER	2.3
1	F	196	LEU	2.3
1	F	145	VAL	2.3
1	D	60	GLU	2.2
1	H	287	GLU	2.2
1	C	233	ASP	2.2
1	E	224	LYS	2.2
1	F	108	ARG	2.2
1	G	206	LEU	2.2
1	F	107	LEU	2.2
1	F	116	TYR	2.2
1	C	234	ILE	2.2
1	D	242	ALA	2.2
1	D	225	THR	2.2
1	F	214	ILE	2.2
1	G	101	ILE	2.2
1	B	208	GLU	2.2
1	F	197	LEU	2.2
1	F	223	ASP	2.2
1	H	240	TYR	2.2
1	C	273	HIS	2.2
1	A	59	GLU	2.2
1	D	57	ALA	2.2
1	H	232	GLN	2.2
1	B	117	THR	2.2
1	G	117	THR	2.2
1	E	244	ASP	2.2
1	H	237	ASN	2.2
1	F	30	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	137	GLN	2.2
1	A	232	GLN	2.2
1	H	241	ASP	2.2
1	B	608	GLU	2.2
1	B	224	LYS	2.1
1	D	74	TRP	2.1
1	G	205	PHE	2.1
1	H	109	GLU	2.1
1	C	425	LEU	2.1
1	B	74	TRP	2.1
1	E	113	ALA	2.1
1	B	234	ILE	2.1
1	E	230	LYS	2.1
1	F	115	GLY	2.1
1	C	219	VAL	2.1
1	G	608	GLU	2.1
1	H	557	ASP	2.1
1	C	227	ALA	2.1
1	F	156	TYR	2.1
1	D	135	LEU	2.1
1	F	41	HIS	2.1
1	G	103	ASN	2.1
1	F	177	PRO	2.1
1	B	543	LEU	2.1
1	F	102	GLU	2.0
1	A	39	GLU	2.0
1	H	41[A]	HIS	2.0
1	H	284	ASN	2.0
1	C	115	GLY	2.0
1	F	23	LEU	2.0
1	G	287	GLU	2.0
1	H	38	ALA	2.0
1	F	607	VAL	2.0
1	F	181	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	G6Q	B	610	16/16	0.87	0.31	7.89	60,86,96,100	0
5	G6Q	C	611	16/16	0.88	0.26	6.23	57,77,89,94	0
5	G6Q	F	610	16/16	0.76	0.37	6.05	63,91,104,108	0
5	G6Q	A	610	16/16	0.91	0.24	5.18	56,70,83,88	0
5	G6Q	G	610	16/16	0.86	0.26	4.71	59,90,102,107	0
5	G6Q	H	610	16/16	0.89	0.28	4.02	76,91,103,105	0
5	G6Q	E	610	16/16	0.86	0.30	3.98	95,104,115,118	0
4	GOL	C	609	6/6	0.87	0.27	3.62	56,60,64,66	0
4	GOL	F	609	6/6	0.89	0.21	3.07	55,56,57,59	0
5	G6Q	D	611	16/16	0.92	0.20	3.06	63,71,78,82	0
4	GOL	G	609	6/6	0.90	0.19	2.27	56,58,59,64	0
4	GOL	B	609	6/6	0.90	0.18	1.81	51,54,54,56	0
4	GOL	D	610	6/6	0.95	0.15	1.29	56,56,57,57	0
4	GOL	A	609	6/6	0.90	0.22	1.14	59,62,65,68	0
4	GOL	E	609	6/6	0.94	0.15	1.11	47,51,53,57	0
2	GLU	E	701	10/10	0.95	0.13	1.07	34,42,44,44	0
3	G6P	E	616	16/16	0.98	0.13	0.72	31,37,43,44	0
4	GOL	H	609	6/6	0.96	0.17	0.67	47,53,55,58	0
2	GLU	B	701	10/10	0.91	0.20	0.63	74,83,85,88	0
2	GLU	A	701	10/10	0.98	0.12	0.61	30,35,36,38	0
3	G6P	D	609	16/16	0.99	0.12	0.28	23,27,29,29	0
2	GLU	C	701	10/10	0.95	0.13	0.27	36,46,61,62	0
3	G6P	H	614	16/16	0.99	0.12	0.10	22,29,34,36	0
3	G6P	B	612	16/16	0.99	0.11	-0.02	24,28,34,39	0
2	GLU	D	701	10/10	0.93	0.17	-0.13	64,66,67,67	0
3	G6P	A	611	16/16	0.99	0.11	-0.13	22,26,31,32	0
2	GLU	H	701	10/10	0.97	0.10	-0.23	39,43,48,49	0
3	G6P	F	615	16/16	0.99	0.11	-0.27	29,32,38,39	0
3	G6P	C	610	16/16	0.98	0.11	-0.29	20,25,27,31	0
2	GLU	G	701	10/10	0.91	0.15	-0.36	68,78,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	G6P	G	613	16/16	0.99	0.10	-0.55	24,28,34,34	0
2	GLU	F	701	10/10	0.86	0.20	-0.78	73,75,80,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.