



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:16 AM UTC

PDB ID : 3TBF / pdb_00003tbf
Title : C-terminal domain of glucosamine-fructose-6-phosphate aminotransferase from *Francisella tularensis*.
Authors : Osipiuk, J.; Zhou, M.; Maltseva, N.; Kim, Y.; Papazisi, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on : 2011-08-05
Resolution : 2.28 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

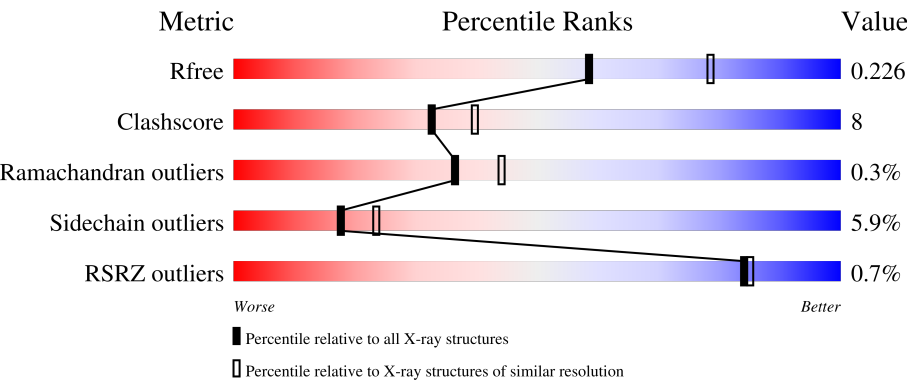
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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 $\leq 5\%$. 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	372	77%18% . .
1	B	372	% 73%19% . 5%
1	C	372	% 77%17% . .
1	D	372	78%17% . .

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Mol	Chain	Length	Quality of chain
1	E	372	78% 17%
1	F	372	% 78% 17%
1	G	372	% 72% 23%
1	H	372	2% 71% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22905 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	357	Total	C	N	O	S	Se	0	3	0
			2792	1786	456	539	5	6			
1	B	354	Total	C	N	O	S	Se	0	1	0
			2745	1755	447	532	5	6			
1	C	358	Total	C	N	O	S	Se	0	4	0
			2794	1787	455	539	7	6			
1	D	357	Total	C	N	O	S	Se	0	4	0
			2790	1785	455	537	7	6			
1	E	358	Total	C	N	O	S	Se	0	4	0
			2793	1786	455	538	8	6			
1	F	358	Total	C	N	O	S	Se	0	3	0
			2790	1786	455	536	7	6			
1	G	357	Total	C	N	O	S	Se	0	4	0
			2791	1785	454	539	7	6			
1	H	357	Total	C	N	O	S	Se	0	6	0
			2796	1786	456	541	7	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	68	Total	O	0	1
			68	68		
2	B	66	Total	O	0	0
			66	66		
2	C	97	Total	O	0	0
			97	97		
2	D	97	Total	O	0	0
			97	97		
2	E	93	Total	O	0	0
			93	93		
2	F	85	Total	O	0	0
			85	85		

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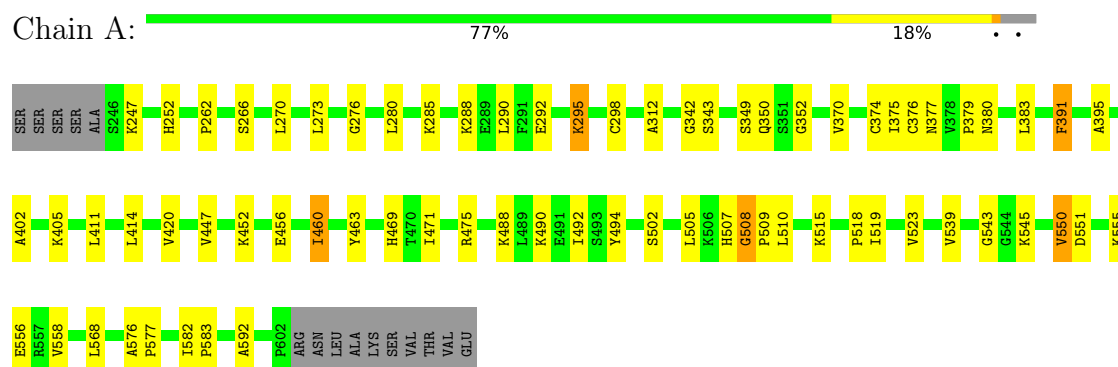
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	51	Total	O	0	0
			51	51		
2	H	57	Total	O	0	0
			57	57		

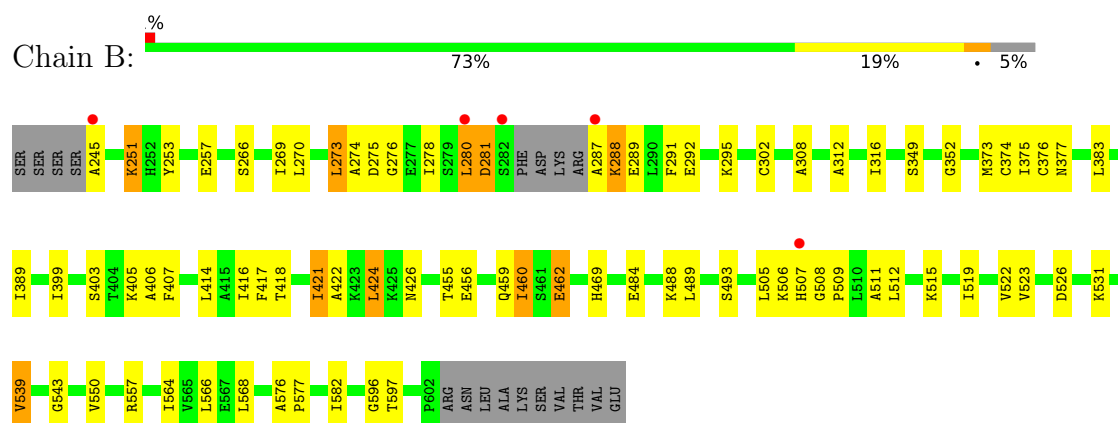
3 Residue-property plots

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.

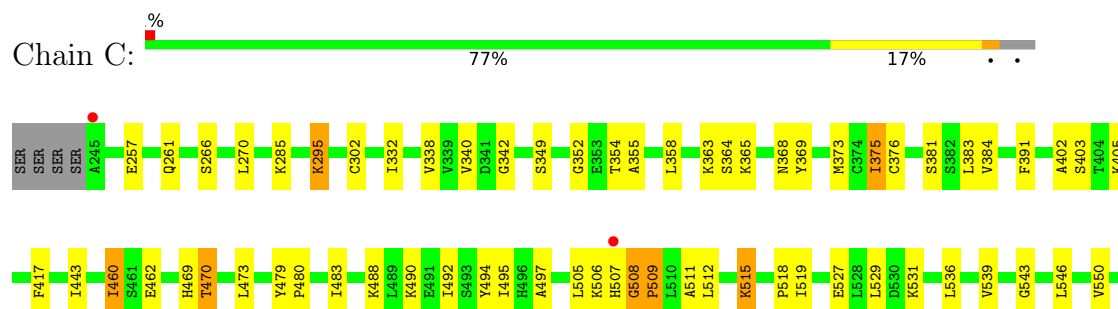
- Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]



- Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]



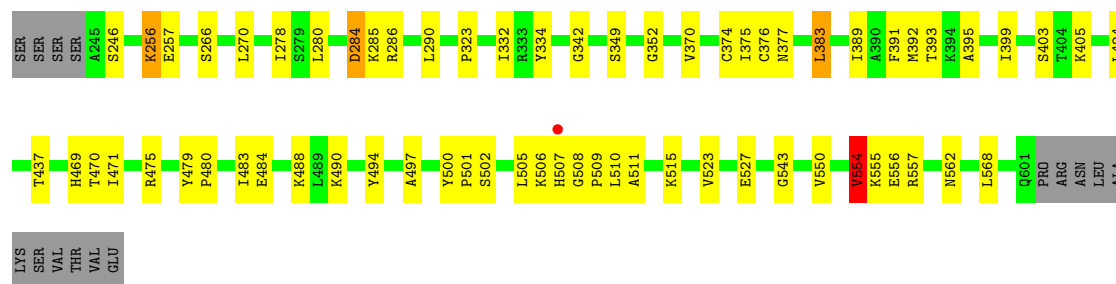
- Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]





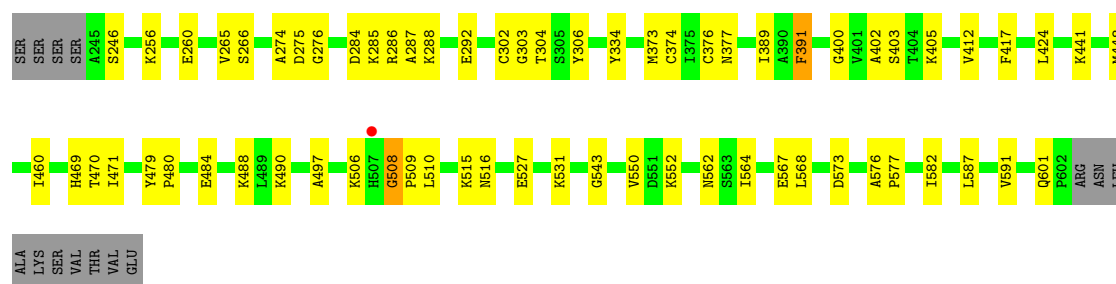
- Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

Chain D: 78% 17%



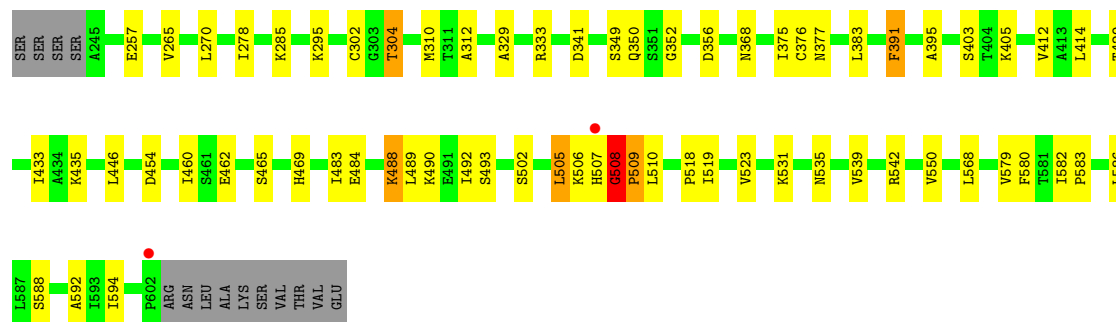
- Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

Chain E: 78% 17%



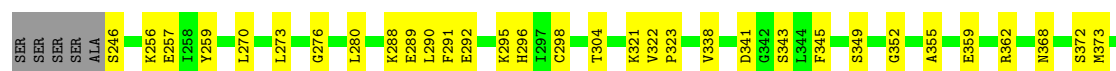
- Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

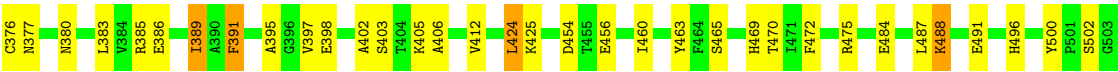
Chain F: 78% 17%



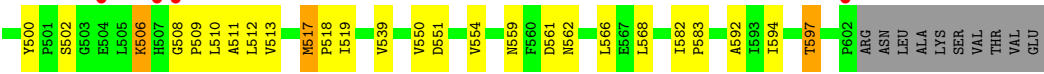
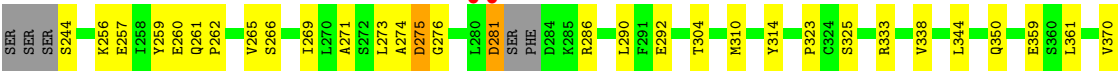
- Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]

Chain G: 72% 23%





● Molecule 1: Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.37Å 262.91Å 83.80Å 90.00° 91.32° 90.00°	Depositor
Resolution (Å)	45.80 – 2.28 45.80 – 2.28	Depositor EDS
% Data completeness (in resolution range)	74.7 (45.80-2.28) 74.7 (45.80-2.28)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.172 , 0.232 0.169 , 0.226	Depositor DCC
R_{free} test set	5213 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22905	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.10	0/2843	1.04	3/3837 (0.1%)
1	B	1.10	4/2787 (0.1%)	0.98	2/3762 (0.1%)
1	C	1.10	1/2847 (0.0%)	0.97	5/3842 (0.1%)
1	D	1.08	1/2842 (0.0%)	1.02	4/3833 (0.1%)
1	E	1.11	2/2846 (0.1%)	0.98	0/3841
1	F	1.07	0/2840	1.00	5/3833 (0.1%)
1	G	0.98	0/2844	0.98	3/3838 (0.1%)
1	H	1.04	0/2853	0.98	2/3849 (0.1%)
All	All	1.07	8/22702 (0.0%)	0.99	24/30635 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	582	ILE	C-O	-6.83	1.18	1.24
1	E	582	ILE	CA-CB	6.14	1.57	1.54
1	B	316	ILE	CA-CB	-5.91	1.47	1.54
1	B	308	ALA	CA-CB	-5.49	1.44	1.53
1	E	471	ILE	CA-CB	-5.23	1.48	1.54
1	C	582	ILE	CA-CB	-5.16	1.51	1.54
1	B	422	ALA	CA-CB	-5.12	1.45	1.53
1	D	471	ILE	CA-CB	-5.01	1.48	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	508	GLY	CA-C-N	9.77	129.53	119.56
1	G	508	GLY	C-N-CA	9.77	129.53	119.56
1	A	508	GLY	CA-C-N	9.12	128.86	119.56
1	A	508	GLY	C-N-CA	9.12	128.86	119.56
1	H	508	GLY	CA-C-N	7.07	128.68	119.84
1	H	508	GLY	C-N-CA	7.07	128.68	119.84
1	B	302	CYS	N-CA-C	6.88	119.87	109.41
1	C	375	ILE	N-CA-C	-6.00	97.76	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	508	GLY	CA-C-N	5.91	127.23	119.84
1	D	508	GLY	C-N-CA	5.91	127.23	119.84
1	D	286	ARG	N-CA-C	5.89	119.29	111.75
1	F	460	ILE	CB-CA-C	-5.86	104.36	112.04
1	D	554	VAL	N-CA-CB	-5.84	105.38	112.33
1	F	460	ILE	N-CA-C	5.67	117.08	110.62
1	F	508	GLY	CA-C-N	5.67	126.92	119.84
1	F	508	GLY	C-N-CA	5.67	126.92	119.84
1	G	509	PRO	N-CA-C	5.55	121.05	113.84
1	B	460	ILE	CB-CA-C	-5.36	104.91	112.14
1	C	508	GLY	CA-C-N	5.27	126.42	119.84
1	C	508	GLY	C-N-CA	5.27	126.42	119.84
1	C	460	ILE	CB-CA-C	-5.23	104.06	112.16
1	F	375	ILE	N-CA-C	-5.22	99.65	107.37
1	C	355	ALA	N-CA-C	5.13	116.56	111.07
1	A	460	ILE	CB-CA-C	-5.11	105.24	112.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2792	0	2840	39	0
1	B	2745	0	2792	47	0
1	C	2794	0	2847	42	0
1	D	2790	0	2850	38	0
1	E	2793	0	2847	41	0
1	F	2790	0	2847	47	0
1	G	2791	0	2841	62	0
1	H	2796	0	2852	62	0
2	A	68	0	0	0	0
2	B	66	0	0	2	0
2	C	97	0	0	0	0
2	D	97	0	0	2	0
2	E	93	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	85	0	0	2	0
2	G	51	0	0	1	0
2	H	57	0	0	0	0
All	All	22905	0	22716	355	0

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

All (355) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302[B]:CYS:SG	1:F:507:HIS:NE2	2.35	0.99
1:E:302[B]:CYS:HG	1:F:507:HIS:HE2	0.88	0.88
1:H:257:GLU:HG2	1:H:405:LYS:HE2	1.63	0.81
1:D:374[A]:CYS:SG	1:D:376[A]:CYS:HB2	2.23	0.79
1:G:484:GLU:OE2	1:G:488:LYS:NZ	2.16	0.79
1:B:273:LEU:HD23	1:B:276:GLY:HA2	1.65	0.78
1:B:257:GLU:HG2	1:B:405:LYS:HE2	1.66	0.76
1:H:373:MSE:HE1	1:H:417:PHE:CE1	2.21	0.76
1:F:395:ALA:O	1:F:405:LYS:NZ	2.20	0.74
1:H:373:MSE:HE1	1:H:417:PHE:CD1	2.22	0.74
1:A:505:LEU:HA	1:A:509:PRO:HG2	1.69	0.73
1:B:374:CYS:SG	1:B:376:CYS:HB2	2.28	0.73
1:A:374:CYS:SG	1:A:376:CYS:HB2	2.29	0.72
1:F:391:PHE:HD1	1:F:391:PHE:C	1.97	0.72
1:G:380:ASN:O	1:G:385:ARG:NH1	2.23	0.72
1:H:273:LEU:HD13	1:H:276:GLY:HA2	1.71	0.72
1:D:523:VAL:HB	1:D:550:VAL:HG22	1.73	0.71
1:F:350:GLN:HE21	1:F:377:ASN:HD22	1.39	0.71
1:G:424:LEU:HD12	1:G:424:LEU:O	1.90	0.71
1:F:341:ASP:OD1	1:F:368:ASN:ND2	2.22	0.71
1:G:273:LEU:HD13	1:G:276:GLY:HA2	1.73	0.70
1:G:597:THR:O	2:G:641:HOH:O	2.11	0.69
1:E:302[B]:CYS:HG	1:F:507:HIS:CE1	2.05	0.69
1:F:391:PHE:C	1:F:391:PHE:CD1	2.68	0.68
1:C:460:ILE:HD11	1:C:566:LEU:HD11	1.74	0.68
1:E:527:GLU:H	1:E:527:GLU:CD	2.01	0.68
1:D:377:ASN:HD21	1:D:395:ALA:H	1.42	0.67
1:B:273:LEU:CD2	1:B:276:GLY:HA2	2.24	0.67
1:H:494:TYR:CE2	1:H:597:THR:CG2	2.78	0.67
1:B:508:GLY:N	1:B:509:PRO:HD2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:PHE:CZ	1:B:484:GLU:HG3	2.30	0.67
1:G:500:TYR:CE1	1:G:509:PRO:HG3	2.30	0.67
1:F:519:ILE:HG12	1:F:539:VAL:HG11	1.77	0.67
1:C:470:THR:HG23	1:C:495:ILE:HG21	1.77	0.66
1:H:374[A]:CYS:SG	1:H:376[A]:CYS:HB2	2.35	0.66
1:D:500:TYR:CE1	1:D:509:PRO:HG3	2.30	0.66
1:B:288:LYS:O	1:B:292:GLU:HG3	1.96	0.65
1:E:374[A]:CYS:SG	1:E:376[A]:CYS:HB2	2.37	0.65
1:E:515:LYS:HA	1:E:543:GLY:O	1.97	0.65
1:A:350:GLN:HE21	1:A:377:ASN:HD22	1.44	0.65
1:H:259:TYR:CD2	1:H:451:LEU:HD13	2.31	0.65
1:F:518:PRO:C	1:F:519:ILE:HD12	2.22	0.65
1:D:376[A]:CYS:SG	1:D:377:ASN:N	2.71	0.64
1:E:508:GLY:H	1:E:509:PRO:HD2	1.61	0.64
1:D:484:GLU:OE2	1:D:488:LYS:HE3	1.97	0.63
1:B:505:LEU:HD23	1:B:509:PRO:HB2	1.80	0.63
1:D:527:GLU:CD	1:D:527:GLU:H	2.05	0.63
1:A:469:HIS:CE1	1:B:469:HIS:CE1	2.86	0.63
1:F:257:GLU:HG2	1:F:405:LYS:HE2	1.79	0.63
1:A:391:PHE:CD1	1:A:391:PHE:C	2.76	0.63
1:A:523:VAL:HB	1:A:550:VAL:HG22	1.80	0.62
1:D:557:ARG:HD2	2:D:188:HOH:O	1.98	0.62
1:G:465:SER:HB3	1:G:594:ILE:HG21	1.82	0.62
1:A:352:GLY:HA2	1:A:383:LEU:HD12	1.81	0.61
1:E:391:PHE:CD1	1:E:391:PHE:C	2.78	0.61
1:A:288:LYS:O	1:A:292:GLU:HG3	2.01	0.60
1:E:246:SER:O	1:E:256:LYS:NZ	2.31	0.60
1:G:352:GLY:HA2	1:G:383:LEU:HD12	1.83	0.60
1:C:470:THR:CG2	1:C:495:ILE:HG21	2.31	0.60
1:G:551:ASP:O	1:G:554:VAL:HG22	2.01	0.60
1:C:469:HIS:O	1:C:470:THR:HG22	2.01	0.59
1:H:460:ILE:HD11	1:H:566:LEU:HD11	1.85	0.59
1:E:508:GLY:H	1:E:509:PRO:CD	2.15	0.59
1:A:273:LEU:HD13	1:A:276:GLY:HA2	1.84	0.59
1:A:391:PHE:C	1:A:391:PHE:HD1	2.11	0.59
1:F:310:MSE:HE1	1:F:483:ILE:HD12	1.84	0.58
1:H:402:ALA:HB1	1:H:488:LYS:HD2	1.86	0.58
1:H:304:THR:HG23	1:H:484:GLU:OE2	2.03	0.58
1:C:295:LYS:HG3	1:C:342:GLY:HA3	1.86	0.57
1:C:373:MSE:HE1	1:C:417:PHE:CD1	2.38	0.57
1:C:375:ILE:HD13	1:C:391:PHE:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ALA:HB1	1:C:488:LYS:HD3	1.85	0.57
1:F:519:ILE:HD12	1:F:519:ILE:N	2.19	0.57
1:E:391:PHE:C	1:E:391:PHE:HD1	2.11	0.57
1:B:505:LEU:HD13	1:B:539:VAL:HG23	1.84	0.57
1:B:505:LEU:HA	1:B:509:PRO:HG2	1.85	0.57
1:H:487:LEU:O	1:H:491:GLU:HB2	2.05	0.57
1:F:582:ILE:HB	1:F:583:PRO:HD3	1.87	0.57
1:C:338:VAL:HG11	1:D:323:PRO:HD3	1.87	0.56
1:C:566:LEU:N	1:C:566:LEU:HD12	2.19	0.56
1:F:333:ARG:NH1	1:F:356:ASP:OD1	2.36	0.56
1:C:469:HIS:CE1	1:D:469:HIS:CE1	2.93	0.56
1:C:518:PRO:C	1:C:519:ILE:HD12	2.30	0.56
1:G:257:GLU:HG2	1:G:405:LYS:HE2	1.86	0.56
1:B:515:LYS:HA	1:B:543:GLY:O	2.06	0.56
1:E:552:LYS:HG2	1:E:567:GLU:OE1	2.05	0.56
1:D:349:SER:HB3	1:D:383:LEU:HD23	1.88	0.56
1:C:494:TYR:CD1	1:D:511:ALA:HB1	2.41	0.56
1:C:511:ALA:HB1	1:D:494:TYR:CD1	2.40	0.56
1:D:484:GLU:OE2	1:D:488:LYS:CE	2.54	0.55
1:C:373:MSE:HE1	1:C:417:PHE:CE1	2.42	0.55
1:G:550:VAL:HG13	1:G:554:VAL:HG23	1.87	0.55
1:G:550:VAL:CG1	1:G:554:VAL:HG23	2.36	0.55
1:G:496:HIS:CD2	1:H:512:LEU:CD1	2.89	0.55
1:D:257:GLU:HG2	1:D:405:LYS:HE2	1.87	0.55
1:G:519:ILE:HG12	1:G:539:VAL:HG11	1.89	0.55
1:B:403:SER:OG	1:B:406:ALA:HB3	2.07	0.55
1:B:281:ASP:N	1:B:281:ASP:OD1	2.39	0.55
1:C:352:GLY:HA2	1:C:383:LEU:HD12	1.88	0.55
1:D:479:TYR:HB3	1:D:480:PRO:HD3	1.89	0.55
1:C:507:HIS:CD2	1:C:509:PRO:HD2	2.42	0.54
1:G:291:PHE:O	1:G:425:LYS:NZ	2.35	0.54
1:H:361:LEU:CD2	1:H:383:LEU:HD23	2.38	0.54
1:A:507[A]:HIS:ND1	1:A:508:GLY:N	2.55	0.54
1:H:475:ARG:HG3	1:H:502:SER:HB2	1.90	0.54
1:F:446:LEU:HB3	1:F:579:VAL:HG21	1.90	0.53
1:A:518:PRO:C	1:A:519:ILE:HD12	2.34	0.53
1:D:246:SER:O	1:D:256:LYS:HE3	2.09	0.53
1:B:245:ALA:O	1:B:253:TYR:OH	2.20	0.53
1:C:381:SER:OG	1:C:384:VAL:HG23	2.08	0.53
1:G:568:LEU:N	1:G:568:LEU:HD23	2.24	0.53
1:H:582:ILE:HB	1:H:583:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:424:LEU:O	1:G:424:LEU:CD1	2.56	0.53
1:E:400:GLY:O	1:E:601:GLN:NE2	2.39	0.53
1:F:568[A]:LEU:HD11	1:F:580:PHE:CE1	2.44	0.52
1:C:473:LEU:HD21	1:C:505:LEU:HD21	1.90	0.52
1:F:502:SER:OG	1:F:535:ASN:ND2	2.42	0.52
1:B:407:PHE:CE1	1:B:484:GLU:HG3	2.44	0.52
1:G:391:PHE:C	1:G:391:PHE:HD1	2.18	0.52
1:F:484:GLU:OE2	1:F:488:LYS:NZ	2.38	0.52
1:G:496:HIS:CD2	1:H:512:LEU:HD11	2.45	0.52
1:F:465:SER:HB3	1:F:594:ILE:HG21	1.92	0.52
1:D:352:GLY:HA2	1:D:383:LEU:CD2	2.39	0.51
1:F:312:ALA:HB2	1:F:414:LEU:HD13	1.92	0.51
1:E:302[B]:CYS:HG	1:F:507:HIS:CD2	2.12	0.51
1:G:465:SER:HB3	1:G:594:ILE:CG2	2.39	0.51
1:G:496:HIS:ND1	1:H:469:HIS:HD2	2.09	0.51
1:B:459:GLN:O	1:B:462:GLU:HB2	2.11	0.51
1:F:349:SER:O	1:F:376[B]:CYS:HA	2.11	0.51
1:G:349:SER:O	1:G:376[B]:CYS:HA	2.11	0.51
1:G:391:PHE:C	1:G:391:PHE:CD1	2.88	0.51
1:H:460:ILE:HD11	1:H:566:LEU:CD1	2.40	0.51
1:E:334:TYR:CZ	1:F:531:LYS:HE2	2.46	0.50
1:C:257:GLU:HG2	1:C:405:LYS:HE2	1.93	0.50
1:C:519:ILE:HG12	1:C:539:VAL:HG11	1.93	0.50
1:A:582:ILE:HB	1:A:583:PRO:HD3	1.92	0.50
1:F:492:ILE:HD11	1:F:588:SER:C	2.37	0.50
1:H:494:TYR:CE2	1:H:597:THR:HG21	2.45	0.50
1:A:492:ILE:HG13	1:A:592:ALA:HB2	1.94	0.50
1:G:469:HIS:NE2	1:H:469:HIS:NE2	2.59	0.50
1:D:377:ASN:ND2	1:D:393:THR:OG1	2.26	0.50
1:F:508:GLY:N	1:F:509:PRO:HD2	2.26	0.50
1:A:350:GLN:NE2	1:A:377:ASN:HD22	2.10	0.50
1:F:465:SER:HB3	1:F:594:ILE:CG2	2.42	0.50
1:A:515:LYS:HA	1:A:543:GLY:O	2.12	0.50
1:H:333:ARG:NH2	1:H:359:GLU:HG3	2.27	0.50
1:H:479:TYR:CZ	1:H:483:ILE:HD11	2.46	0.49
1:D:470:THR:O	1:D:497:ALA:HA	2.12	0.49
1:D:475:ARG:HG3	1:D:502:SER:HB2	1.93	0.49
1:F:505:LEU:HA	1:F:509:PRO:HG2	1.93	0.49
1:C:470:THR:HB	1:C:518:PRO:HB2	1.95	0.49
1:H:470:THR:HG23	1:H:518:PRO:HB2	1.94	0.49
1:A:295:LYS:HG3	1:A:342:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:ILE:HG13	1:C:592:ALA:HB2	1.95	0.49
1:C:519:ILE:HD12	1:C:519:ILE:N	2.28	0.49
1:G:475:ARG:HG3	1:G:502:SER:HB2	1.95	0.49
1:B:596:GLY:HA2	2:B:648:HOH:O	2.13	0.49
1:G:373:MSE:HG3	1:G:389:ILE:HG13	1.94	0.49
1:E:286:ARG:O	1:E:287:ALA:C	2.56	0.49
1:H:290:LEU:CD2	1:H:370:VAL:HG23	2.43	0.49
1:D:506:LYS:HA	1:D:510:LEU:HD12	1.95	0.48
1:E:334:TYR:OH	1:F:531:LYS:HE2	2.13	0.48
1:H:310:MSE:HE2	1:H:480:PRO:HG3	1.95	0.48
1:B:352:GLY:HA2	1:B:383:LEU:HD12	1.95	0.48
1:F:454:ASP:HA	1:F:586:LEU:HD13	1.95	0.48
1:G:460:ILE:HD11	1:G:564:ILE:HG21	1.96	0.48
1:A:280:LEU:HD13	1:A:420:VAL:HG13	1.94	0.48
1:C:529:LEU:HD22	1:C:554:VAL:HG22	1.96	0.48
1:E:508:GLY:N	1:E:509:PRO:CD	2.76	0.48
1:E:469:HIS:CE1	1:F:469:HIS:CE1	3.02	0.48
1:F:352:GLY:HA2	1:F:383:LEU:HD12	1.96	0.48
1:H:500:TYR:CG	1:H:509:PRO:HG3	2.48	0.48
1:B:274:ALA:O	1:B:275:ASP:HB2	2.14	0.47
1:C:527:GLU:CD	1:C:527:GLU:H	2.21	0.47
1:C:391:PHE:CD1	1:C:391:PHE:C	2.91	0.47
1:B:505:LEU:C	1:B:507:HIS:H	2.21	0.47
1:H:274:ALA:O	1:H:275:ASP:HB2	2.12	0.47
1:H:506:LYS:HE3	1:H:506:LYS:H	1.79	0.47
1:E:576:ALA:N	1:E:577:PRO:CD	2.77	0.47
1:A:379:PRO:O	1:A:380:ASN:HB3	2.14	0.47
1:D:557:ARG:CD	2:D:188:HOH:O	2.61	0.47
1:F:349:SER:O	1:F:376[A]:CYS:HA	2.14	0.47
1:B:508:GLY:N	1:B:509:PRO:CD	2.76	0.47
1:C:531:LYS:HE2	1:D:334:TYR:OH	2.15	0.47
1:D:284:ASP:O	1:D:285:LYS:C	2.56	0.47
1:E:424:LEU:HD23	1:E:424:LEU:O	2.15	0.47
1:D:352:GLY:HA2	1:D:383:LEU:HD22	1.97	0.47
1:E:292:GLU:HG3	1:E:424:LEU:HD21	1.95	0.47
1:G:349:SER:O	1:G:376[A]:CYS:HA	2.13	0.47
1:C:364:SER:HB2	1:C:369:TYR:CD2	2.49	0.47
1:H:256:LYS:HE3	1:H:260:GLU:OE1	2.14	0.47
1:G:529:LEU:HD11	1:G:533:LEU:HD11	1.97	0.47
1:A:494:TYR:CD1	1:B:511:ALA:HB1	2.49	0.47
1:E:284:ASP:OD1	1:E:285:LYS:HE3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:489:LEU:O	1:F:493:SER:OG	2.30	0.47
1:A:475:ARG:HG3	1:A:502:SER:HB2	1.96	0.46
1:F:265:VAL:HG13	1:F:412:VAL:HG21	1.97	0.46
1:F:492:ILE:HG13	1:F:592:ALA:HB2	1.97	0.46
1:E:479:TYR:HB3	1:E:480:PRO:HD3	1.96	0.46
1:H:513:VAL:HA	1:H:517:MSE:HG2	1.97	0.46
1:E:276:GLY:O	1:E:441:LYS:NZ	2.42	0.46
1:G:529:LEU:HD13	1:G:533:LEU:HD12	1.96	0.46
1:H:286:ARG:HD2	1:H:286:ARG:HA	1.72	0.46
1:H:310:MSE:HE2	1:H:310:MSE:HB3	1.69	0.46
1:H:568:LEU:HD23	1:H:568:LEU:N	2.30	0.46
1:B:291:PHE:HB2	1:B:424:LEU:CD1	2.45	0.46
1:G:288:LYS:O	1:G:292:GLU:HG3	2.14	0.46
1:G:529:LEU:CD1	1:G:533:LEU:CD1	2.94	0.46
1:E:402:ALA:HB1	1:E:488:LYS:HD3	1.98	0.46
1:H:344:LEU:HD12	1:H:371:GLY:O	2.16	0.46
1:B:373:MSE:HE1	1:B:417:PHE:CD1	2.50	0.46
1:C:391:PHE:C	1:C:391:PHE:HD1	2.23	0.46
1:G:519:ILE:N	1:G:519:ILE:HD12	2.31	0.46
1:G:424:LEU:HD12	1:G:424:LEU:C	2.40	0.46
1:D:278:ILE:HD12	1:D:437:THR:OG1	2.15	0.46
1:G:550:VAL:HG13	1:G:554:VAL:CG2	2.45	0.46
1:A:349:SER:O	1:A:376:CYS:HA	2.16	0.46
1:H:453:LEU:O	1:H:454:ASP:C	2.57	0.45
1:C:479:TYR:HB3	1:C:480:PRO:HD3	1.97	0.45
1:E:484:GLU:OE2	1:E:488:LYS:HE3	2.17	0.45
1:F:285:LYS:O	2:F:146:HOH:O	2.21	0.45
1:E:260:GLU:CD	1:E:405:LYS:HZ3	2.25	0.45
1:G:397:VAL:HG12	1:G:398:GLU:N	2.31	0.45
1:G:403:SER:OG	1:G:406:ALA:HB3	2.17	0.45
1:H:281:ASP:OD1	1:H:281:ASP:N	2.48	0.45
1:E:460:ILE:HG12	1:E:564:ILE:HG21	1.98	0.45
1:F:429:THR:O	1:F:433:ILE:HG12	2.17	0.45
1:G:500:TYR:CZ	1:G:509:PRO:HG3	2.52	0.45
1:D:479:TYR:CZ	1:D:501:PRO:HG3	2.51	0.45
1:G:338:VAL:HG11	1:H:323:PRO:HD3	1.99	0.45
1:H:265:VAL:HG13	1:H:412:VAL:HG21	1.99	0.45
1:H:509:PRO:O	1:H:511:ALA:N	2.50	0.45
1:C:349:SER:O	1:C:376[B]:CYS:HA	2.17	0.45
1:F:508:GLY:H	1:F:509:PRO:HD2	1.82	0.45
1:G:355:ALA:O	1:G:359:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:ASP:OD1	1:D:284:ASP:N	2.39	0.45
1:F:510:LEU:HD13	1:F:542:ARG:NE	2.32	0.45
1:H:488:LYS:HA	1:H:488:LYS:HD3	1.66	0.45
1:B:568:LEU:N	1:B:568:LEU:HD23	2.32	0.44
1:G:402:ALA:HB1	1:G:488:LYS:HE2	1.98	0.44
1:H:519:ILE:HD13	1:H:539:VAL:CG1	2.47	0.44
1:C:470:THR:O	1:C:497:ALA:HA	2.17	0.44
1:H:398:GLU:HG3	1:H:405:LYS:HE3	2.00	0.44
1:D:550:VAL:HG13	1:D:554:VAL:HG12	1.98	0.44
1:F:310:MSE:HE1	1:F:483:ILE:CD1	2.47	0.44
1:G:511:ALA:HB1	1:H:494:TYR:CD1	2.52	0.44
1:H:361:LEU:HD23	1:H:383:LEU:HD23	1.98	0.44
1:B:280:LEU:HD23	1:B:280:LEU:O	2.16	0.44
1:C:349:SER:O	1:C:376[A]:CYS:HA	2.17	0.44
1:A:505:LEU:HA	1:A:509:PRO:CG	2.43	0.44
1:E:304:THR:CG2	2:E:613:HOH:O	2.66	0.44
1:E:304:THR:HG22	2:E:613:HOH:O	2.18	0.44
1:G:487:LEU:O	1:G:491:GLU:HB2	2.18	0.44
1:C:515:LYS:HA	1:C:543:GLY:O	2.17	0.44
1:A:342:GLY:HA2	1:A:370:VAL:CG1	2.47	0.44
1:B:418:THR:O	1:B:421:ILE:HG22	2.18	0.44
1:F:302:CYS:SG	1:F:329:ALA:HB3	2.58	0.44
1:G:362:ARG:NH2	1:G:386:GLU:OE2	2.34	0.44
1:H:257:GLU:HG2	1:H:405:LYS:CE	2.41	0.44
1:H:594:ILE:O	1:H:594:ILE:CG2	2.63	0.44
1:H:492:ILE:HD12	1:H:592:ALA:HB2	2.00	0.44
1:B:526:ASP:HB2	2:B:655:HOH:O	2.19	0.43
1:E:510:LEU:HD23	1:E:510:LEU:HA	1.89	0.43
1:G:377:ASN:HD21	1:G:395:ALA:H	1.65	0.43
1:G:597:THR:HG22	1:G:598:ASP:H	1.82	0.43
1:H:314:TYR:HB2	1:H:477:LEU:HD23	1.99	0.43
1:E:303:GLY:O	1:E:306:TYR:HB3	2.18	0.43
1:F:523:VAL:HB	1:F:550:VAL:HG12	2.00	0.43
1:H:314:TYR:HB2	1:H:477:LEU:CD2	2.48	0.43
1:B:374:CYS:SG	1:B:376:CYS:CB	3.04	0.43
1:H:373:MSE:CE	1:H:417:PHE:CE1	2.98	0.43
1:B:576:ALA:N	1:B:577:PRO:CD	2.81	0.43
1:A:247:LYS:HE2	1:A:252:HIS:HA	2.01	0.43
1:B:523:VAL:HB	1:B:550:VAL:HG22	2.00	0.43
1:G:373:MSE:HG3	1:G:389:ILE:CG1	2.49	0.43
1:G:529:LEU:HD13	1:G:533:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:CYS:SG	1:C:354:THR:HG21	2.59	0.43
1:D:505:LEU:C	1:D:507:HIS:H	2.26	0.43
1:E:274:ALA:O	1:E:275:ASP:HB2	2.18	0.43
1:G:463:TYR:O	1:G:463:TYR:CG	2.72	0.43
1:B:312:ALA:HB2	1:B:414:LEU:HD13	2.00	0.43
1:E:265:VAL:HG13	1:E:412:VAL:HG21	2.00	0.43
1:F:304:THR:HG22	2:F:197:HOH:O	2.19	0.43
1:G:515:LYS:HA	1:G:543:GLY:O	2.18	0.43
1:B:269:ILE:HA	1:B:416:ILE:HD11	2.00	0.42
1:H:361:LEU:HD22	1:H:383:LEU:HD23	2.00	0.42
1:H:468:GLU:C	1:H:495:ILE:HG23	2.43	0.42
1:G:376[B]:CYS:SG	1:G:377:ASN:N	2.92	0.42
1:H:290:LEU:HD21	1:H:371:GLY:HA3	2.01	0.42
1:B:460:ILE:HD11	1:B:566:LEU:HD11	2.01	0.42
1:C:443:ILE:HG12	1:C:575:SER:CB	2.49	0.42
1:G:510:LEU:HD23	1:G:510:LEU:HA	1.86	0.42
1:A:395:ALA:O	1:A:405:LYS:CE	2.67	0.42
1:D:391:PHE:CD1	1:D:391:PHE:C	2.97	0.42
1:E:573:ASP:HB2	2:E:114:HOH:O	2.19	0.42
1:G:296:HIS:O	1:G:343:SER:HA	2.20	0.42
1:B:508:GLY:O	1:B:511:ALA:N	2.53	0.42
1:G:472:PHE:HA	1:G:520:VAL:O	2.19	0.42
1:A:519:ILE:HD12	1:A:519:ILE:N	2.35	0.42
1:B:505:LEU:CD2	1:B:509:PRO:HB2	2.49	0.42
1:B:287:ALA:C	1:B:289:GLU:N	2.77	0.42
1:F:519:ILE:N	1:F:519:ILE:CD1	2.83	0.42
1:F:568[B]:LEU:HD12	1:F:579:VAL:HG12	2.02	0.42
1:A:312:ALA:HB2	1:A:414:LEU:HD13	2.01	0.41
1:G:322:VAL:HG13	1:G:323:PRO:HD2	2.00	0.41
1:G:341:ASP:OD1	1:G:368:ASN:ND2	2.39	0.41
1:A:280:LEU:HD21	1:A:288:LYS:HB2	2.02	0.41
1:A:490:LYS:CD	1:B:512:LEU:HD11	2.51	0.41
1:B:489:LEU:O	1:B:493:SER:OG	2.36	0.41
1:A:262:PRO:HG3	1:A:447:VAL:HG12	2.03	0.41
1:A:558:VAL:O	1:A:558:VAL:HG12	2.19	0.41
1:B:508:GLY:O	1:B:509:PRO:C	2.63	0.41
1:D:515:LYS:HA	1:D:543:GLY:O	2.20	0.41
1:E:470:THR:O	1:E:497:ALA:HA	2.20	0.41
1:E:587:LEU:O	1:E:591:VAL:HG23	2.20	0.41
1:A:463:TYR:CZ	1:A:545:LYS:HG2	2.56	0.41
1:B:280:LEU:HD22	1:B:288:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:TYR:HD1	1:D:511:ALA:HB1	1.85	0.41
1:C:515:LYS:H	1:C:515:LYS:HG3	1.72	0.41
1:G:345:PHE:O	1:G:372:SER:HA	2.20	0.41
1:A:551:ASP:HA	1:A:568:LEU:O	2.20	0.41
1:H:269:ILE:HA	1:H:416:ILE:HD11	2.02	0.41
1:H:462:GLU:HA	1:H:594:ILE:HD13	2.02	0.41
1:A:395:ALA:O	1:A:405:LYS:NZ	2.54	0.41
1:D:479:TYR:CZ	1:D:483:ILE:HD11	2.56	0.41
1:E:376[A]:CYS:SG	1:E:377:ASN:N	2.93	0.41
1:G:523:VAL:HB	1:G:550:VAL:HG22	2.01	0.41
1:B:460:ILE:HG12	1:B:564:ILE:HG21	2.03	0.41
1:E:448:MSE:SE	2:E:641:HOH:O	2.87	0.41
1:G:292:GLU:HG2	1:G:424:LEU:HD11	2.03	0.41
1:H:494:TYR:CE2	1:H:597:THR:HG23	2.56	0.41
1:A:519:ILE:HG12	1:A:539:VAL:HG11	2.03	0.41
1:C:479:TYR:CZ	1:C:483:ILE:HD11	2.55	0.41
1:E:373:MSE:HE1	1:E:417:PHE:CD1	2.55	0.41
1:G:246:SER:O	1:G:256:LYS:HE2	2.20	0.41
1:H:509:PRO:O	1:H:510:LEU:C	2.63	0.41
1:A:576:ALA:N	1:A:577:PRO:CD	2.84	0.41
1:C:261:GLN:NE2	1:C:582:ILE:HD12	2.35	0.41
1:C:512:LEU:HD21	1:D:490:LYS:HG3	2.03	0.41
1:G:259:TYR:OH	1:G:454:ASP:OD2	2.34	0.41
1:G:470:THR:HG23	1:G:518:PRO:HB2	2.02	0.41
1:H:509:PRO:C	1:H:511:ALA:N	2.79	0.41
1:D:342:GLY:HA2	1:D:370:VAL:CG1	2.51	0.41
1:H:261:GLN:N	1:H:262:PRO:CD	2.84	0.41
1:A:460:ILE:HD13	1:A:460:ILE:HG21	1.86	0.40
1:H:454:ASP:C	1:H:454:ASP:OD1	2.64	0.40
1:A:402:ALA:HB1	1:A:488:LYS:HD3	2.03	0.40
1:B:251:LYS:HE3	1:B:251:LYS:HB2	1.88	0.40
1:B:376:CYS:SG	1:B:377:ASN:N	2.94	0.40
1:H:292:GLU:HG3	1:H:424:LEU:HD21	2.03	0.40
1:B:349:SER:O	1:B:376:CYS:HA	2.21	0.40
1:B:399:ILE:O	1:B:399:ILE:HG22	2.20	0.40
1:H:551:ASP:O	1:H:554:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	358/372 (96%)	348 (97%)	10 (3%)	0	100	100
1	B	351/372 (94%)	339 (97%)	11 (3%)	1 (0%)	36	44
1	C	360/372 (97%)	349 (97%)	8 (2%)	3 (1%)	16	18
1	D	359/372 (96%)	348 (97%)	11 (3%)	0	100	100
1	E	360/372 (97%)	350 (97%)	9 (2%)	1 (0%)	36	44
1	F	359/372 (96%)	348 (97%)	9 (2%)	2 (1%)	21	25
1	G	359/372 (96%)	343 (96%)	16 (4%)	0	100	100
1	H	359/372 (96%)	338 (94%)	19 (5%)	2 (1%)	21	25
All	All	2865/2976 (96%)	2763 (96%)	93 (3%)	9 (0%)	36	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	508	GLY
1	B	506	LYS
1	C	368	ASN
1	H	271	ALA
1	H	275	ASP
1	C	509	PRO
1	E	508	GLY
1	C	508	GLY
1	F	509	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	310/314 (99%)	293 (94%)	17 (6%)	19	26
1	B	304/314 (97%)	280 (92%)	24 (8%)	11	14
1	C	311/314 (99%)	290 (93%)	21 (7%)	14	18
1	D	310/314 (99%)	292 (94%)	18 (6%)	18	24
1	E	311/314 (99%)	299 (96%)	12 (4%)	28	41
1	F	310/314 (99%)	298 (96%)	12 (4%)	28	41
1	G	311/314 (99%)	290 (93%)	21 (7%)	14	18
1	H	312/314 (99%)	292 (94%)	20 (6%)	16	20
All	All	2479/2512 (99%)	2334 (94%)	145 (6%)	18	24

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	SER
1	A	270	LEU
1	A	285	LYS
1	A	290	LEU
1	A	295	LYS
1	A	298	CYS
1	A	343	SER
1	A	375	ILE
1	A	391	PHE
1	A	411	LEU
1	A	452	LYS
1	A	456	GLU
1	A	471	ILE
1	A	510	LEU
1	A	550	VAL
1	A	555	LYS
1	A	556	GLU
1	B	251	LYS
1	B	266	SER
1	B	270	LEU
1	B	273	LEU
1	B	278	ILE
1	B	280	LEU
1	B	281	ASP
1	B	288	LYS

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Mol	Chain	Res	Type
1	B	295	LYS
1	B	375	ILE
1	B	389	ILE
1	B	421	ILE
1	B	424	LEU
1	B	426	ASN
1	B	455	THR
1	B	456	GLU
1	B	462	GLU
1	B	488	LYS
1	B	519	ILE
1	B	522	VAL
1	B	531	LYS
1	B	539	VAL
1	B	557	ARG
1	B	597	THR
1	C	266	SER
1	C	270	LEU
1	C	285	LYS
1	C	295	LYS
1	C	332	ILE
1	C	340	VAL
1	C	358	LEU
1	C	363	LYS
1	C	365	LYS
1	C	403	SER
1	C	462	GLU
1	C	470	THR
1	C	490	LYS
1	C	506	LYS
1	C	515	LYS
1	C	536	LEU
1	C	546	LEU
1	C	550	VAL
1	C	554	VAL
1	C	557	ARG
1	C	561	ASP
1	D	256	LYS
1	D	266	SER
1	D	270	LEU
1	D	280	LEU
1	D	284	ASP

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Mol	Chain	Res	Type
1	D	290	LEU
1	D	332	ILE
1	D	375	ILE
1	D	383	LEU
1	D	389	ILE
1	D	399	ILE
1	D	403	SER
1	D	424	LEU
1	D	554	VAL
1	D	555	LYS
1	D	556	GLU
1	D	562	ASN
1	D	568	LEU
1	E	266	SER
1	E	288	LYS
1	E	389	ILE
1	E	391	PHE
1	E	403	SER
1	E	490	LYS
1	E	506	LYS
1	E	516	ASN
1	E	531	LYS
1	E	550	VAL
1	E	562	ASN
1	E	568	LEU
1	F	270	LEU
1	F	278	ILE
1	F	295	LYS
1	F	304	THR
1	F	391	PHE
1	F	403	SER
1	F	435	LYS
1	F	462	GLU
1	F	488	LYS
1	F	490	LYS
1	F	505	LEU
1	F	506	LYS
1	G	270	LEU
1	G	280	LEU
1	G	289[A]	GLU
1	G	289[B]	GLU
1	G	290	LEU

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Mol	Chain	Res	Type
1	G	295	LYS
1	G	298	CYS
1	G	304	THR
1	G	321	LYS
1	G	389	ILE
1	G	391	PHE
1	G	412	VAL
1	G	424	LEU
1	G	456	GLU
1	G	488	LYS
1	G	504	GLU
1	G	506	LYS
1	G	515	LYS
1	G	556	GLU
1	G	567	GLU
1	G	597	THR
1	H	244	SER
1	H	266	SER
1	H	281	ASP
1	H	325	SER
1	H	338	VAL
1	H	350	GLN
1	H	403	SER
1	H	411	LEU
1	H	427	SER
1	H	456	GLU
1	H	462	GLU
1	H	488	LYS
1	H	490	LYS
1	H	506	LYS
1	H	517	MSE
1	H	550	VAL
1	H	559	ASN
1	H	561	ASP
1	H	562	ASN
1	H	597	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	350	GLN

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Mol	Chain	Res	Type
1	A	367	GLN
1	A	559	ASN
1	A	562	ASN
1	A	572	HIS
1	A	585	GLN
1	B	261	GLN
1	B	525	ASN
1	B	537	GLN
1	B	559	ASN
1	B	585	GLN
1	C	525	ASN
1	C	572	HIS
1	D	377	ASN
1	D	410	GLN
1	D	525	ASN
1	D	562	ASN
1	E	261	GLN
1	E	525	ASN
1	E	537	GLN
1	E	585	GLN
1	F	350	GLN
1	F	426	ASN
1	F	535	ASN
1	F	572	HIS
1	G	261	GLN
1	G	377	ASN
1	G	469	HIS
1	G	525	ASN
1	G	535	ASN
1	G	537	GLN
1	G	585	GLN
1	H	261	GLN
1	H	380	ASN
1	H	469	HIS
1	H	585	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	351/372 (94%)	-0.46	0 100 100	9, 24, 48, 58	3 (0%)
1	B	348/372 (93%)	-0.35	5 (1%) 73 75	12, 29, 52, 74	1 (0%)
1	C	352/372 (94%)	-0.42	2 (0%) 85 86	13, 27, 48, 67	4 (1%)
1	D	351/372 (94%)	-0.34	1 (0%) 90 90	14, 30, 52, 65	4 (1%)
1	E	352/372 (94%)	-0.44	1 (0%) 90 90	13, 26, 50, 66	4 (1%)
1	F	352/372 (94%)	-0.34	2 (0%) 85 86	13, 29, 51, 62	3 (0%)
1	G	351/372 (94%)	-0.17	3 (0%) 81 82	17, 35, 62, 77	4 (1%)
1	H	351/372 (94%)	-0.16	7 (1%) 65 66	14, 33, 63, 76	6 (1%)
All	All	2808/2976 (94%)	-0.34	21 (0%) 84 85	9, 29, 54, 77	29 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	280	LEU	4.3
1	B	280	LEU	3.5
1	H	507	HIS	3.0
1	C	507	HIS	3.0
1	H	281	ASP	2.9
1	H	602	PRO	2.9
1	B	507	HIS	2.9
1	D	507	HIS	2.8
1	H	462	GLU	2.7
1	H	504[A]	GLU	2.5
1	F	602	PRO	2.4
1	B	245	ALA	2.4
1	E	507	HIS	2.4
1	F	507	HIS	2.3
1	B	282	SER	2.2
1	G	508	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	287	ALA	2.2
1	G	509	PRO	2.1
1	G	602	PRO	2.1
1	H	508	GLY	2.1
1	C	245	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.