



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:20 AM UTC

PDB ID : 3OQB / pdb_00003oqb
Title : CRYSTAL STRUCTURE OF putative oxidoreductase from Bradyrhizobium japonicum USDA 110
Authors : Malashkevich, V.N.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-09-02
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

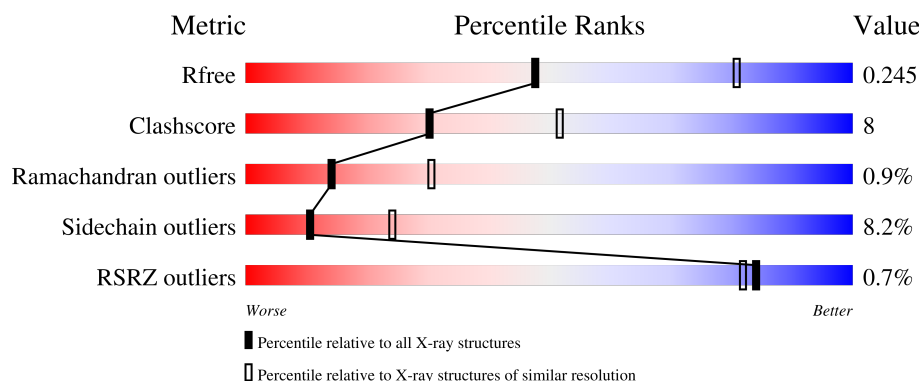
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	383	
1	B	383	
1	C	383	
1	D	383	
1	E	383	

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Mol	Chain	Length	Quality of chain
1	F	383	77% 18% • •
1	G	383	73% 23% • •
1	H	383	3% 73% 21% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24247 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 Oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	Se	0	0	0
			2989	1901	529	546	5	8			
1	B	377	Total	C	N	O	S	Se	0	0	0
			2998	1907	531	547	5	8			
1	C	377	Total	C	N	O	S	Se	0	0	0
			3000	1907	533	547	5	8			
1	D	378	Total	C	N	O	S	Se	0	0	0
			3005	1910	534	548	5	8			
1	E	377	Total	C	N	O	S	Se	0	0	0
			2994	1904	530	547	5	8			
1	F	379	Total	C	N	O	S	Se	0	0	0
			3014	1916	536	549	5	8			
1	G	378	Total	C	N	O	S	Se	0	0	0
			3005	1910	534	548	5	8			
1	H	375	Total	C	N	O	S	Se	0	0	0
			2977	1892	527	545	5	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q89RD2
A	2	LEU	-	expression tag	UNP Q89RD2
B	1	SER	-	expression tag	UNP Q89RD2
B	2	LEU	-	expression tag	UNP Q89RD2
C	1	SER	-	expression tag	UNP Q89RD2
C	2	LEU	-	expression tag	UNP Q89RD2
D	1	SER	-	expression tag	UNP Q89RD2
D	2	LEU	-	expression tag	UNP Q89RD2
E	1	SER	-	expression tag	UNP Q89RD2
E	2	LEU	-	expression tag	UNP Q89RD2
F	1	SER	-	expression tag	UNP Q89RD2
F	2	LEU	-	expression tag	UNP Q89RD2
G	1	SER	-	expression tag	UNP Q89RD2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	2	LEU	-	expression tag	UNP Q89RD2
H	1	SER	-	expression tag	UNP Q89RD2
H	2	LEU	-	expression tag	UNP Q89RD2

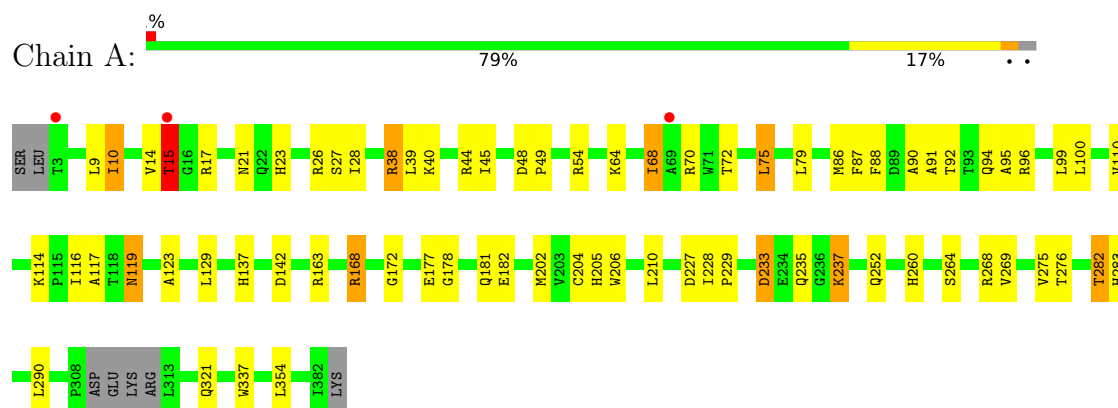
- Molecule 2 is water.

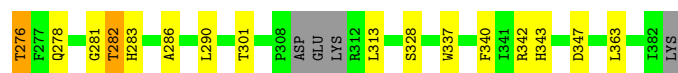
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total	O	0	0
			27	27		
2	B	45	Total	O	0	0
			45	45		
2	C	37	Total	O	0	0
			37	37		
2	D	36	Total	O	0	0
			36	36		
2	E	45	Total	O	0	0
			45	45		
2	F	24	Total	O	0	0
			24	24		
2	G	20	Total	O	0	0
			20	20		
2	H	31	Total	O	0	0
			31	31		

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.

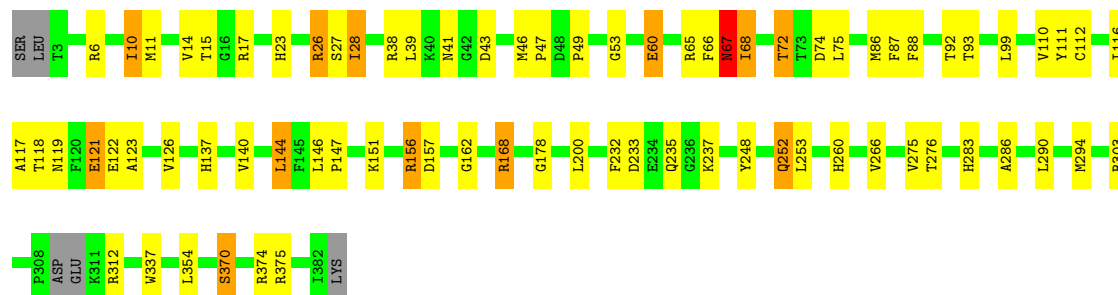
• Molecule 1: Oxidoreductase





• Molecule 1: Oxidoreductase

Chain D: 79% 17% ..



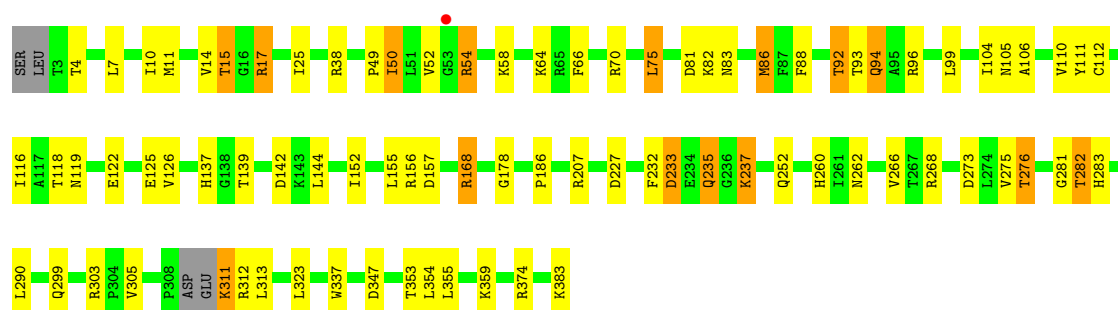
• Molecule 1: Oxidoreductase

Chain E: 78% 17% ..



• Molecule 1: Oxidoreductase

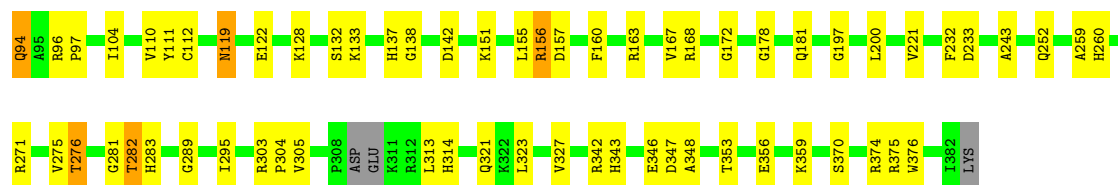
Chain F: 77% 18% ..



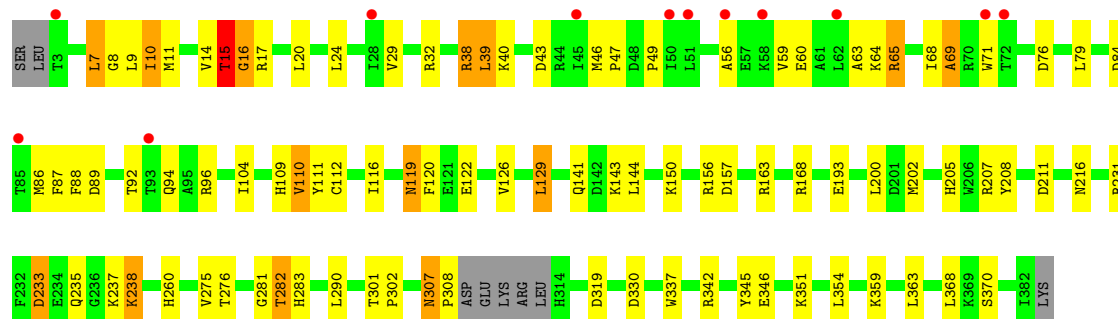
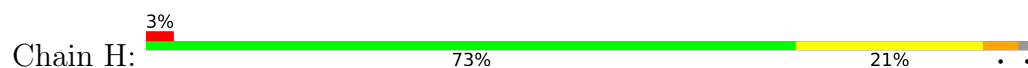
• Molecule 1: Oxidoreductase

Chain G: 73% 23% ..





• Molecule 1: Oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.70Å 163.85Å 117.73Å 90.00° 103.85° 90.00°	Depositor
Resolution (Å)	19.99 – 2.60 19.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-2.60) 99.6 (19.99-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.247 0.191 , 0.245	Depositor DCC
R_{free} test set	5257 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24247	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.58	0/3051	0.86	2/4117 (0.0%)
1	B	0.61	0/3060	0.85	0/4128
1	C	0.65	0/3062	0.92	5/4131 (0.1%)
1	D	0.68	0/3067	0.91	3/4138 (0.1%)
1	E	0.68	0/3056	0.92	1/4124 (0.0%)
1	F	0.61	0/3076	0.90	3/4149 (0.1%)
1	G	0.58	0/3067	0.88	2/4138 (0.0%)
1	H	0.64	0/3039	0.90	0/4102
All	All	0.63	0/24478	0.89	16/33027 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	142	ASP	N-CA-C	7.22	119.23	111.36
1	D	53	GLY	N-CA-C	6.71	124.24	114.10
1	C	212	ASN	N-CA-C	6.36	118.30	111.36
1	A	269	VAL	N-CA-C	6.19	116.30	106.88
1	G	314	HIS	N-CA-C	6.18	119.97	110.20
1	C	15	THR	N-CA-C	-5.92	107.29	114.75
1	A	142	ASP	N-CA-C	5.54	117.40	111.36
1	F	273	ASP	N-CA-C	5.47	116.46	108.14
1	D	28	ILE	N-CA-C	5.36	115.57	110.42
1	G	112	CYS	N-CA-C	5.30	116.58	108.42
1	C	120	PHE	N-CA-C	5.28	116.72	111.07
1	D	112	CYS	N-CA-C	5.18	116.95	108.76
1	F	142	ASP	N-CA-C	5.13	116.56	111.07
1	F	152	ILE	N-CA-C	-5.11	105.51	110.42
1	C	273	ASP	N-CA-C	5.10	115.27	108.38
1	C	264	SER	N-CA-C	5.01	116.67	108.55

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	2989	0	2929	46	0
1	B	2998	0	2942	49	0
1	C	3000	0	2942	54	0
1	D	3005	0	2944	57	0
1	E	2994	0	2931	48	0
1	F	3014	0	2957	52	0
1	G	3005	0	2944	49	0
1	H	2977	0	2907	64	0
2	A	27	0	0	3	0
2	B	45	0	0	4	0
2	C	37	0	0	4	0
2	D	36	0	0	5	0
2	E	45	0	0	1	0
2	F	24	0	0	2	0
2	G	20	0	0	3	0
2	H	31	0	0	2	0
All	All	24247	0	23496	400	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 (400) 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:H:65:ARG:HG3	1:H:65:ARG:HH11	1.12	1.13
1:D:119:ASN:ND2	1:D:121:GLU:HG2	1.63	1.12
1:G:282:THR:HG22	1:G:283:HIS:HD2	1.22	1.02
1:D:156:ARG:HG2	1:D:156:ARG:HH11	1.21	1.01
1:A:237:LYS:HE2	2:A:405:HOH:O	1.62	1.00
1:G:282:THR:HG22	1:G:283:HIS:CD2	1.96	1.00
1:E:9:LEU:HD13	1:E:86:MSE:HE3	1.41	0.98
1:G:156:ARG:HG2	1:G:156:ARG:HH11	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:THR:HG22	1:A:283:HIS:CD2	2.00	0.95
1:A:282:THR:HG22	1:A:283:HIS:HD2	1.36	0.88
1:C:282:THR:HG22	1:C:283:HIS:CD2	2.08	0.87
1:D:26:ARG:HG3	1:D:26:ARG:HH11	1.41	0.86
1:H:9:LEU:HD13	1:H:86:MSE:HE2	1.60	0.83
1:C:75:LEU:HD12	1:C:79:LEU:HD11	1.59	0.83
1:A:14:VAL:O	1:A:15:THR:HB	1.80	0.81
1:D:119:ASN:HD21	1:D:121:GLU:HG2	1.44	0.81
1:B:38:ARG:H	1:B:38:ARG:HD2	1.46	0.81
1:C:89:ASP:OD2	1:C:96:ARG:HG3	1.82	0.80
1:D:119:ASN:HD22	1:D:121:GLU:HG2	1.45	0.79
1:B:305:VAL:HA	2:B:391:HOH:O	1.81	0.79
1:E:276:THR:HG22	2:E:392:HOH:O	1.81	0.79
1:F:11:MSE:HE2	1:F:49:PRO:HB2	1.65	0.79
1:D:60:GLU:HG3	2:D:396:HOH:O	1.82	0.78
1:H:156:ARG:NH1	1:H:157:ASP:OD1	2.17	0.77
1:H:119:ASN:HB3	2:H:389:HOH:O	1.86	0.76
1:C:75:LEU:O	1:C:79:LEU:HD12	1.85	0.75
1:B:276:THR:HG22	2:B:410:HOH:O	1.86	0.75
1:G:9:LEU:HD13	1:G:86:MSE:HE3	1.68	0.75
1:A:92:THR:HG22	1:A:94:GLN:H	1.52	0.74
1:G:276:THR:HG22	2:G:391:HOH:O	1.87	0.74
1:G:15:THR:HA	1:G:20:LEU:HB2	1.70	0.74
1:H:122:GLU:HB2	2:H:389:HOH:O	1.88	0.73
1:G:172:GLY:O	1:G:271:ARG:NH2	2.22	0.73
1:H:122:GLU:O	1:H:126:VAL:HG23	1.90	0.72
1:A:38:ARG:HB3	1:A:44:ARG:HH11	1.54	0.72
1:C:156:ARG:NH1	1:C:157:ASP:OD1	2.22	0.72
1:A:119:ASN:HB3	2:A:390:HOH:O	1.90	0.71
1:H:65:ARG:HH11	1:H:65:ARG:CG	1.97	0.71
1:B:268:ARG:NH2	1:H:281:GLY:O	2.23	0.70
1:C:38:ARG:HD2	1:C:38:ARG:O	1.91	0.69
1:H:89:ASP:OD2	1:H:96:ARG:HG3	1.92	0.69
1:F:92:THR:HG22	1:F:94:GLN:HE21	1.56	0.68
1:D:86:MSE:HE1	1:D:337:TRP:CZ3	2.29	0.68
1:G:156:ARG:HG2	1:G:156:ARG:NH1	2.06	0.68
1:F:137:HIS:HD2	1:F:354:LEU:H	1.41	0.68
1:C:92:THR:HB	1:C:94:GLN:HE21	1.57	0.67
1:C:171:PHE:HB2	1:C:275:VAL:HG23	1.76	0.67
1:H:65:ARG:HG3	1:H:65:ARG:NH1	1.89	0.67
1:F:282:THR:HG22	1:F:283:HIS:CD2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:MSE:HE2	1:F:49:PRO:CB	2.25	0.67
1:D:370:SER:HB2	1:D:375:ARG:O	1.95	0.66
1:E:32:ARG:HG3	1:E:46:MSE:HE1	1.77	0.66
1:D:156:ARG:HH11	1:D:156:ARG:CG	2.04	0.66
1:H:56:ALA:HA	1:H:59:VAL:HG12	1.77	0.66
1:B:119:ASN:HB3	1:B:122:GLU:HB2	1.78	0.66
1:G:39:LEU:HD22	1:G:346:GLU:HB2	1.77	0.66
1:C:68:ILE:O	1:C:69:ALA:HB3	1.96	0.65
1:H:68:ILE:HG22	1:H:69:ALA:N	2.10	0.65
1:E:14:VAL:O	1:E:15:THR:HB	1.96	0.65
1:C:233:ASP:HB3	1:C:235:GLN:H	1.62	0.65
1:E:52:VAL:HG11	1:E:75:LEU:HD22	1.78	0.64
1:C:156:ARG:HH11	1:C:156:ARG:HG2	1.61	0.64
1:E:282:THR:HG22	1:E:283:HIS:ND1	2.11	0.64
1:F:17:ARG:H	1:F:17:ARG:HD3	1.63	0.64
1:H:205:HIS:HA	1:H:208:TYR:CE2	2.32	0.64
1:C:281:GLY:O	1:F:268:ARG:NH2	2.31	0.64
1:D:156:ARG:HG2	1:D:156:ARG:NH1	2.00	0.64
1:H:15:THR:HG23	1:H:15:THR:O	1.97	0.64
1:G:276:THR:CG2	2:G:391:HOH:O	2.45	0.63
1:B:32:ARG:HG3	1:B:46:MSE:HE1	1.79	0.63
1:F:156:ARG:NH1	1:F:157:ASP:OD1	2.31	0.63
1:H:233:ASP:HB3	1:H:235:GLN:H	1.62	0.63
1:H:86:MSE:HE1	1:H:337:TRP:HZ3	1.65	0.62
1:A:48:ASP:O	1:A:70:ARG:NH2	2.32	0.62
1:F:305:VAL:HA	2:F:399:HOH:O	2.00	0.62
1:G:65:ARG:CB	1:G:65:ARG:HH11	2.13	0.62
1:G:21:ASN:O	1:G:26:ARG:HG2	2.00	0.61
1:D:86:MSE:HE1	1:D:337:TRP:HZ3	1.64	0.61
1:E:14:VAL:HG21	1:E:24:LEU:HD22	1.81	0.61
1:H:233:ASP:HB2	1:H:237:LYS:H	1.65	0.61
1:D:233:ASP:HB3	1:D:235:GLN:H	1.65	0.61
1:D:11:MSE:HE2	1:D:14:VAL:HG11	1.82	0.61
1:F:92:THR:HG22	1:F:94:GLN:HG2	1.82	0.61
1:D:39:LEU:HD12	1:D:43:ASP:HB2	1.81	0.61
1:B:233:ASP:HB2	1:B:237:LYS:H	1.66	0.61
1:C:88:PHE:HA	1:C:111:TYR:O	2.00	0.60
1:B:233:ASP:HB3	1:B:235:GLN:H	1.67	0.60
1:H:307:ASN:C	1:H:307:ASN:HD22	2.10	0.60
1:A:275:VAL:HG12	1:A:290:LEU:HD12	1.84	0.59
1:B:14:VAL:HG22	1:B:14:VAL:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:ASP:HB3	1:E:235:GLN:H	1.66	0.59
1:F:233:ASP:HB2	1:F:237:LYS:H	1.67	0.59
1:D:23:HIS:O	1:D:27:SER:HB2	2.03	0.58
1:E:13:GLY:HA3	1:E:90:ALA:C	2.27	0.58
1:E:205:HIS:HA	1:E:208:TYR:CE2	2.38	0.58
1:D:260:HIS:CE1	1:E:260:HIS:CE1	2.92	0.58
1:G:156:ARG:NH1	1:G:157:ASP:OD1	2.34	0.58
1:D:303:ARG:NH2	1:E:182:GLU:O	2.33	0.58
1:D:156:ARG:NH1	1:D:157:ASP:OD1	2.37	0.58
1:G:96:ARG:N	1:G:97:PRO:HD2	2.19	0.58
1:E:88:PHE:HA	1:E:111:TYR:O	2.04	0.58
1:C:260:HIS:CE1	1:F:260:HIS:CE1	2.92	0.57
1:E:147:PRO:O	1:E:151:LYS:HG3	2.03	0.57
1:F:137:HIS:CD2	1:F:354:LEU:H	2.21	0.57
1:C:182:GLU:O	1:F:303:ARG:NH2	2.37	0.57
1:H:20:LEU:O	1:H:24:LEU:HB3	2.05	0.57
1:H:163:ARG:H	1:H:282:THR:HG22	1.68	0.57
1:H:63:ALA:HB2	1:H:71:TRP:HD1	1.68	0.57
1:A:23:HIS:O	1:A:27:SER:HB2	2.06	0.56
1:D:88:PHE:HA	1:D:111:TYR:O	2.04	0.56
1:E:136:LYS:HD2	1:E:343:HIS:NE2	2.20	0.56
1:H:282:THR:HG23	1:H:283:HIS:CD2	2.40	0.56
1:A:92:THR:HG22	1:A:95:ALA:H	1.70	0.56
1:A:116:ILE:HD11	1:A:123:ALA:HB1	1.87	0.56
1:B:47:PRO:O	1:B:49:PRO:HD3	2.06	0.56
1:E:10:ILE:HG13	1:E:87:PHE:HD1	1.69	0.56
1:D:66:PHE:C	1:D:67:ASN:HD22	2.15	0.55
1:F:54:ARG:CD	1:F:54:ARG:H	2.19	0.55
1:F:88:PHE:HA	1:F:111:TYR:O	2.06	0.55
1:E:14:VAL:O	1:E:15:THR:CB	2.54	0.55
1:E:9:LEU:HD13	1:E:86:MSE:CE	2.27	0.55
1:G:156:ARG:HH11	1:G:156:ARG:CG	2.11	0.55
1:E:68:ILE:O	1:E:69:ALA:CB	2.54	0.55
1:B:31:ILE:HG13	1:B:334:LYS:HE2	1.89	0.54
1:C:301:THR:OG1	1:F:268:ARG:HD3	2.07	0.54
1:C:68:ILE:O	1:C:69:ALA:CB	2.55	0.54
1:G:178:GLY:HA3	1:G:232:PHE:HB2	1.89	0.54
1:B:86:MSE:HG3	1:B:109:HIS:HB2	1.89	0.54
1:A:137:HIS:HD2	1:A:354:LEU:H	1.55	0.54
1:C:38:ARG:NH2	1:C:342:ARG:HD3	2.22	0.54
1:H:8:GLY:HA3	1:H:84:ASP:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASP:O	1:G:163:ARG:NH1	2.41	0.54
1:A:268:ARG:NH2	1:G:281:GLY:O	2.41	0.53
1:B:260:HIS:CE1	1:H:260:HIS:CE1	2.97	0.53
1:C:23:HIS:O	1:C:27:SER:HB2	2.08	0.53
1:H:32:ARG:HH21	1:H:49:PRO:HD3	1.72	0.53
1:B:14:VAL:HG21	1:B:24:LEU:HD13	1.91	0.53
1:F:54:ARG:H	1:F:54:ARG:HD2	1.72	0.53
1:B:299:GLN:HG2	1:F:155:LEU:HD23	1.91	0.53
1:A:168:ARG:NH2	2:A:409:HOH:O	2.41	0.53
1:D:26:ARG:HG3	1:D:26:ARG:NH1	2.17	0.53
1:D:168:ARG:NH1	2:D:407:HOH:O	2.40	0.53
1:A:182:GLU:O	1:G:303:ARG:NH2	2.42	0.53
1:D:66:PHE:HB2	1:D:68:ILE:HD12	1.90	0.52
1:E:68:ILE:O	1:E:69:ALA:HB3	2.08	0.52
1:H:56:ALA:HB1	1:H:71:TRP:HZ3	1.74	0.52
1:G:9:LEU:O	1:G:49:PRO:HA	2.10	0.52
1:D:86:MSE:CE	1:D:337:TRP:HZ3	2.22	0.52
1:F:275:VAL:HG22	1:F:276:THR:N	2.24	0.52
1:C:282:THR:CG2	1:C:283:HIS:CD2	2.88	0.52
1:B:230:GLU:HG2	1:B:238:LYS:HG2	1.90	0.52
1:C:233:ASP:HB2	1:C:237:LYS:H	1.73	0.52
1:G:304:PRO:HD2	2:G:384:HOH:O	2.09	0.52
1:E:81:ASP:O	1:E:82:LYS:HB2	2.09	0.52
1:H:15:THR:O	1:H:15:THR:CG2	2.57	0.52
1:D:11:MSE:HE2	1:D:14:VAL:CG1	2.39	0.51
1:E:14:VAL:HG23	1:E:20:LEU:HA	1.92	0.51
1:A:233:ASP:HB3	1:A:235:GLN:H	1.75	0.51
1:C:21:ASN:O	1:C:26:ARG:HG2	2.11	0.51
1:F:207:ARG:NH2	1:F:359:LYS:HE2	2.25	0.51
1:C:276:THR:CG2	2:C:413:HOH:O	2.58	0.51
1:G:61:ALA:O	1:G:65:ARG:HB2	2.10	0.51
1:D:86:MSE:CE	1:D:337:TRP:CZ3	2.94	0.51
1:H:24:LEU:O	1:H:29:VAL:HG23	2.11	0.51
1:G:59:VAL:HG13	1:G:71:TRP:HB2	1.93	0.51
1:B:79:LEU:HA	1:B:108:LYS:HE3	1.93	0.51
1:B:14:VAL:HG21	1:B:24:LEU:HD22	1.93	0.50
1:H:275:VAL:HG12	1:H:290:LEU:HD12	1.92	0.50
1:E:97:PRO:HG3	1:E:117:ALA:CB	2.41	0.50
1:A:110:VAL:O	1:A:137:HIS:HA	2.11	0.50
1:D:10:ILE:HG13	1:D:87:PHE:HD1	1.76	0.50
1:C:276:THR:HG23	2:C:413:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:343:HIS:HA	1:G:348:ALA:H	1.77	0.50
1:D:49:PRO:HG2	1:D:68:ILE:HG12	1.94	0.50
1:H:39:LEU:HB2	1:H:43:ASP:O	2.11	0.50
1:A:14:VAL:O	1:A:15:THR:CB	2.57	0.50
1:G:137:HIS:CE1	1:G:353:THR:HB	2.46	0.50
1:D:118:THR:O	1:D:118:THR:CG2	2.59	0.49
1:G:151:LYS:O	1:G:155:LEU:HG	2.13	0.49
1:G:221:VAL:HB	1:G:376:TRP:CD2	2.47	0.49
1:H:56:ALA:HB1	1:H:71:TRP:CZ3	2.47	0.49
1:H:193:GLU:H	1:H:193:GLU:CD	2.20	0.49
1:A:95:ALA:O	1:A:99:LEU:HD23	2.13	0.49
1:B:286:ALA:HA	1:B:294:MSE:O	2.12	0.49
1:D:23:HIS:HE1	1:D:140:VAL:HG21	1.78	0.49
1:B:9:LEU:HD13	1:B:86:MSE:HE2	1.94	0.49
1:D:118:THR:O	1:D:118:THR:HG22	2.09	0.49
1:E:303:ARG:O	1:E:303:ARG:HG2	2.13	0.49
1:C:268:ARG:NH2	1:F:281:GLY:O	2.46	0.49
1:D:15:THR:HG22	2:D:402:HOH:O	2.13	0.49
1:H:143:LYS:HE2	1:H:202:MSE:HE1	1.94	0.49
1:C:39:LEU:HD11	1:C:45:ILE:HD11	1.95	0.49
1:G:56:ALA:O	1:G:59:VAL:HG12	2.12	0.49
1:D:162:GLY:HA3	1:D:283:HIS:CD2	2.48	0.48
1:E:119:ASN:HB3	1:E:122:GLU:CB	2.43	0.48
1:E:100:LEU:HD22	1:E:110:VAL:HG11	1.95	0.48
1:G:119:ASN:HB3	1:G:122:GLU:HB3	1.95	0.48
1:B:137:HIS:HB2	1:B:354:LEU:HG	1.95	0.48
1:H:110:VAL:HG11	1:H:354:LEU:HD11	1.95	0.48
1:H:112:CYS:SG	1:H:116:ILE:HG22	2.54	0.48
1:B:122:GLU:O	1:B:126:VAL:HG23	2.13	0.48
1:D:248:TYR:CD2	1:D:248:TYR:N	2.82	0.48
1:A:38:ARG:H	1:A:38:ARG:HH21	1.62	0.48
1:C:3:THR:HG21	2:C:393:HOH:O	2.14	0.48
1:A:100:LEU:HD22	1:A:110:VAL:HG11	1.96	0.48
1:E:10:ILE:CG1	1:E:87:PHE:HD1	2.26	0.48
1:F:233:ASP:HB3	1:F:235:GLN:H	1.79	0.48
1:A:75:LEU:CD1	1:A:99:LEU:HD12	2.43	0.48
1:F:311:LYS:HE2	1:F:311:LYS:C	2.39	0.48
1:C:86:MSE:CE	1:C:337:TRP:HZ3	2.27	0.48
1:B:96:ARG:HD3	1:B:112:CYS:HB2	1.95	0.48
1:D:6:ARG:HG3	2:D:409:HOH:O	2.12	0.48
1:C:66:PHE:HB2	1:C:68:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:ARG:HD3	1:H:342:ARG:HD3	1.96	0.47
1:A:21:ASN:O	1:A:26:ARG:HG2	2.13	0.47
1:A:75:LEU:HD22	1:A:79:LEU:HG	1.95	0.47
1:G:343:HIS:O	1:G:347:ASP:HA	2.13	0.47
1:F:122:GLU:O	1:F:126:VAL:HG23	2.14	0.47
1:D:252:GLN:HG2	2:D:388:HOH:O	2.15	0.47
1:G:65:ARG:HH11	1:G:65:ARG:CG	2.27	0.47
1:B:233:ASP:OD1	1:B:237:LYS:HB2	2.14	0.47
1:D:122:GLU:O	1:D:126:VAL:HG23	2.15	0.47
1:B:200:LEU:HD23	2:B:417:HOH:O	2.14	0.47
1:E:79:LEU:O	1:E:108:LYS:HE2	2.15	0.47
1:F:355:LEU:O	1:F:359:LYS:HG3	2.15	0.47
1:B:114:LYS:HE3	1:B:205:HIS:CD2	2.49	0.47
1:A:86:MSE:CE	1:A:337:TRP:HZ3	2.27	0.47
1:C:16:GLY:C	1:C:17:ARG:HG3	2.39	0.47
1:B:50:ILE:HD12	1:B:70:ARG:HD2	1.96	0.47
1:C:30:ALA:O	1:C:34:GLN:HB2	2.15	0.47
1:D:26:ARG:HH11	1:D:26:ARG:CG	2.19	0.47
1:H:11:MSE:HE2	1:H:14:VAL:HG21	1.96	0.47
1:H:15:THR:HA	1:H:20:LEU:HB2	1.97	0.47
1:E:278:GLN:HG3	1:E:287:VAL:HG22	1.97	0.46
1:E:75:LEU:HD12	1:E:79:LEU:HG	1.97	0.46
1:F:7:LEU:HD11	1:F:86:MSE:HB2	1.97	0.46
1:B:66:PHE:O	1:B:67:ASN:HB2	2.15	0.46
1:C:114:LYS:NZ	1:C:201:ASP:OD1	2.49	0.46
1:C:170:GLU:HB2	1:C:276:THR:HG22	1.97	0.46
1:E:97:PRO:HG3	1:E:117:ALA:HB2	1.98	0.46
1:F:14:VAL:O	1:F:15:THR:HB	2.15	0.46
1:F:86:MSE:HE1	1:F:337:TRP:CZ3	2.51	0.46
1:H:9:LEU:HD13	1:H:86:MSE:CE	2.38	0.46
1:B:233:ASP:HB2	1:B:237:LYS:N	2.29	0.46
1:C:104:ILE:HG22	1:C:133:LYS:HG3	1.98	0.46
1:G:10:ILE:HG13	1:G:87:PHE:HD1	1.81	0.46
1:G:55:SER:HB2	1:G:58:LYS:HG3	1.97	0.46
1:E:68:ILE:HG22	1:E:69:ALA:N	2.30	0.46
1:H:207:ARG:CZ	1:H:359:LYS:HB3	2.46	0.46
1:F:112:CYS:SG	1:F:116:ILE:HG22	2.55	0.46
1:G:370:SER:HB2	1:G:375:ARG:O	2.16	0.46
1:H:39:LEU:HB3	1:H:40:LYS:H	1.58	0.46
1:C:156:ARG:NH1	1:C:156:ARG:HG2	2.29	0.46
1:E:121:GLU:CD	1:E:121:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HB3	1:A:123:ALA:HB2	1.96	0.45
1:H:68:ILE:CG2	1:H:69:ALA:N	2.79	0.45
1:E:68:ILE:CG2	1:E:69:ALA:N	2.79	0.45
1:D:162:GLY:HA3	1:D:283:HIS:HD2	1.81	0.45
1:F:50:ILE:HD12	1:F:70:ARG:HB3	1.98	0.45
1:A:206:TRP:O	1:A:210:LEU:HG	2.15	0.45
1:G:155:LEU:HD21	1:G:323:LEU:HD11	1.98	0.45
1:H:342:ARG:O	1:H:346:GLU:HB3	2.16	0.45
1:E:199:ILE:O	1:E:203:VAL:HB	2.17	0.45
1:F:104:ILE:C	1:F:106:ALA:H	2.24	0.45
1:B:114:LYS:HE2	1:B:204:CYS:SG	2.57	0.45
1:B:268:ARG:HD3	1:H:301:THR:OG1	2.17	0.45
1:C:136:LYS:HE3	1:C:343:HIS:O	2.16	0.45
1:H:200:LEU:HD23	1:H:368:LEU:HD11	1.99	0.45
1:H:211:ASP:OD1	1:H:216:ASN:HA	2.16	0.45
1:C:7:LEU:O	1:C:7:LEU:HG	2.16	0.45
1:B:14:VAL:CG2	1:B:24:LEU:HD22	2.46	0.45
1:B:96:ARG:N	1:B:97:PRO:HD2	2.32	0.45
1:D:275:VAL:HG12	1:D:290:LEU:HD12	1.98	0.45
1:H:16:GLY:HA3	1:H:17:ARG:C	2.41	0.45
1:B:21:ASN:HA	1:B:25:ILE:HD12	1.98	0.44
1:B:178:GLY:HA2	1:B:181:GLN:O	2.18	0.44
1:F:119:ASN:HD21	1:F:122:GLU:HB2	1.81	0.44
1:D:117:ALA:HB3	1:D:123:ALA:HB2	1.99	0.44
1:G:356:GLU:HA	1:G:359:LYS:HD2	1.99	0.44
1:A:96:ARG:O	1:A:100:LEU:HG	2.18	0.44
1:A:233:ASP:HB2	1:A:237:LYS:H	1.83	0.44
1:B:14:VAL:HG11	1:B:51:LEU:HD22	1.99	0.44
1:C:172:GLY:HA3	1:C:264:SER:O	2.18	0.44
1:E:38:ARG:H	1:E:38:ARG:HD3	1.82	0.44
1:H:32:ARG:HH21	1:H:49:PRO:CD	2.31	0.44
1:A:260:HIS:CE1	1:G:260:HIS:CE1	3.06	0.44
1:C:119:ASN:ND2	2:C:390:HOH:O	2.49	0.44
1:E:10:ILE:HA	1:E:50:ILE:HG23	1.99	0.44
1:H:231:ARG:O	1:H:238:LYS:HA	2.18	0.44
1:G:51:LEU:HD11	1:G:68:ILE:HG13	1.99	0.44
1:H:10:ILE:HG13	1:H:87:PHE:HD1	1.83	0.44
1:H:63:ALA:HB2	1:H:71:TRP:CD1	2.50	0.44
1:F:96:ARG:HD2	1:F:112:CYS:HB2	1.99	0.44
1:G:197:GLY:HA2	1:G:243:ALA:HB1	1.98	0.44
1:B:299:GLN:O	1:F:323:LEU:HD22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:MSE:HE1	1:C:337:TRP:CZ3	2.53	0.44
1:D:26:ARG:NH1	1:D:26:ARG:CG	2.80	0.44
1:F:139:THR:HG22	1:F:353:THR:O	2.17	0.44
1:A:10:ILE:HG13	1:A:87:PHE:HD1	1.83	0.44
1:D:147:PRO:O	1:D:151:LYS:HG3	2.18	0.44
1:H:104:ILE:HG21	1:H:129:LEU:HB3	1.99	0.44
1:C:143:LYS:HD2	1:C:205:HIS:ND1	2.33	0.44
1:D:137:HIS:HB2	1:D:354:LEU:HG	1.99	0.44
1:H:76:ASP:HA	1:H:79:LEU:HB2	2.00	0.44
1:A:114:LYS:HE2	1:A:204:CYS:HB3	2.00	0.43
1:D:156:ARG:CG	1:D:156:ARG:NH1	2.70	0.43
1:G:160:PHE:CZ	1:G:295:ILE:HB	2.53	0.43
1:G:342:ARG:O	1:G:346:GLU:HB3	2.18	0.43
1:D:374:ARG:HH22	1:E:378:ASP:CG	2.25	0.43
1:A:68:ILE:HG22	1:A:70:ARG:H	1.82	0.43
1:B:168:ARG:NH2	2:B:390:HOH:O	2.28	0.43
1:F:17:ARG:HH12	1:F:186:PRO:HG3	1.83	0.43
1:F:119:ASN:ND2	1:F:122:GLU:HB2	2.34	0.43
1:F:275:VAL:HG22	1:F:276:THR:H	1.83	0.43
1:G:178:GLY:HA2	1:G:181:GLN:O	2.17	0.43
1:H:46:MSE:HA	1:H:47:PRO:HD3	1.83	0.43
1:B:92:THR:HG22	1:B:94:GLN:HG2	2.00	0.43
1:E:119:ASN:OD1	1:E:121:GLU:HG2	2.19	0.43
1:F:168:ARG:NH1	2:F:391:HOH:O	2.43	0.43
1:A:9:LEU:O	1:A:49:PRO:HA	2.19	0.43
1:D:233:ASP:HB2	1:D:237:LYS:H	1.83	0.43
1:H:207:ARG:HD3	1:H:363:LEU:HB2	1.99	0.43
1:H:346:GLU:O	1:H:346:GLU:HG2	2.19	0.43
1:A:163:ARG:H	1:A:282:THR:HB	1.83	0.43
1:B:230:GLU:CD	1:B:238:LYS:HD3	2.43	0.43
1:E:119:ASN:HB3	1:E:122:GLU:HB3	2.00	0.43
1:H:7:LEU:HD13	1:H:345:TYR:OH	2.19	0.43
1:C:340:PHE:O	1:C:343:HIS:HB3	2.19	0.43
1:B:313:LEU:O	1:B:313:LEU:HG	2.19	0.43
1:D:144:LEU:HD12	1:D:144:LEU:HA	1.92	0.43
1:D:178:GLY:HA3	1:D:232:PHE:HB2	2.01	0.43
1:F:64:LYS:HB2	1:F:64:LYS:HE3	1.86	0.43
1:F:81:ASP:HB3	1:F:83:ASN:OD1	2.19	0.43
1:A:172:GLY:HA3	1:A:264:SER:O	2.19	0.42
1:E:97:PRO:HG2	1:E:122:GLU:OE2	2.19	0.42
1:A:86:MSE:CE	1:A:337:TRP:CZ3	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:THR:HA	1:E:288:ALA:O	2.19	0.42
1:B:39:LEU:HD22	1:B:346:GLU:HB2	2.00	0.42
1:B:116:ILE:HD11	1:B:123:ALA:HB1	2.01	0.42
1:F:178:GLY:HA3	1:F:232:PHE:HB2	2.02	0.42
1:G:94:GLN:CD	1:G:94:GLN:H	2.28	0.42
1:C:35:GLY:O	1:C:44:ARG:HD3	2.19	0.42
1:E:100:LEU:HD22	1:E:110:VAL:CG1	2.49	0.42
1:H:68:ILE:HG22	1:H:69:ALA:H	1.84	0.42
1:C:207:ARG:HD3	1:C:363:LEU:HB2	2.00	0.42
1:C:278:GLN:HA	1:C:286:ALA:O	2.19	0.42
1:G:89:ASP:OD2	1:G:96:ARG:HG3	2.19	0.42
1:H:86:MSE:HG3	1:H:109:HIS:HB2	2.01	0.42
1:B:17:ARG:C	1:B:19:GLY:H	2.27	0.42
1:D:119:ASN:HD22	1:D:121:GLU:CG	2.24	0.42
1:E:14:VAL:HG22	1:E:15:THR:N	2.34	0.42
1:F:10:ILE:HA	1:F:50:ILE:HG23	2.02	0.42
1:F:52:VAL:HG21	1:F:75:LEU:HD23	2.02	0.42
1:H:302:PRO:HG3	1:H:319:ASP:OD1	2.19	0.42
1:A:177:GLU:HG2	1:A:228:ILE:HG21	2.02	0.42
1:F:260:HIS:NE2	1:F:262:ASN:OD1	2.47	0.42
1:H:307:ASN:HA	1:H:308:PRO:HD3	1.84	0.42
1:A:86:MSE:HE2	1:A:337:TRP:HZ3	1.85	0.41
1:C:171:PHE:CD2	1:C:171:PHE:C	2.98	0.41
1:D:116:ILE:HD11	1:D:123:ALA:HB1	2.03	0.41
1:E:248:TYR:CD2	1:E:248:TYR:N	2.87	0.41
1:F:156:ARG:HG2	1:F:156:ARG:HH11	1.85	0.41
1:G:7:LEU:HB3	1:G:47:PRO:HA	2.02	0.41
1:B:111:TYR:HA	1:B:138:GLY:O	2.20	0.41
1:C:117:ALA:HB3	1:C:123:ALA:HB2	2.01	0.41
1:C:163:ARG:NH1	1:F:227:ASP:O	2.53	0.41
1:D:23:HIS:CE1	1:D:140:VAL:HG21	2.55	0.41
1:E:334:LYS:O	1:E:338:GLU:HG3	2.19	0.41
1:G:111:TYR:HA	1:G:138:GLY:O	2.20	0.41
1:A:39:LEU:HD11	1:A:45:ILE:HG12	2.01	0.41
1:C:38:ARG:HD2	1:C:38:ARG:C	2.44	0.41
1:C:275:VAL:HG12	1:C:290:LEU:CD1	2.51	0.41
1:D:72:THR:HB	1:D:74:ASP:H	1.84	0.41
1:G:104:ILE:HG22	1:G:133:LYS:HG3	2.01	0.41
1:G:167:VAL:O	1:G:259:ALA:HA	2.19	0.41
1:A:202:MSE:O	1:A:205:HIS:HB2	2.21	0.41
1:B:92:THR:HB	1:B:95:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:VAL:O	1:G:289:GLY:HA2	2.21	0.41
1:H:88:PHE:HA	1:H:111:TYR:O	2.20	0.41
1:B:155:LEU:HD23	1:F:299:GLN:HG2	2.03	0.41
1:C:17:ARG:HB2	1:C:18:MSE:H	1.73	0.41
1:C:143:LYS:HE2	1:C:202:MSE:HE1	2.02	0.41
1:D:286:ALA:HA	1:D:294:MSE:O	2.21	0.41
1:F:25:ILE:HG12	1:F:66:PHE:CZ	2.56	0.41
1:H:119:ASN:ND2	1:H:120:PHE:N	2.68	0.41
1:A:178:GLY:HA2	1:A:181:GLN:O	2.20	0.41
1:F:275:VAL:HG12	1:F:290:LEU:HD12	2.02	0.41
1:C:203:VAL:HA	1:C:206:TRP:CD1	2.55	0.40
1:D:46:MSE:HA	1:D:47:PRO:HD3	1.98	0.40
1:E:23:HIS:O	1:E:27:SER:HB2	2.21	0.40
1:E:234:GLU:H	1:E:234:GLU:CD	2.29	0.40
1:A:228:ILE:HA	1:A:229:PRO:HD3	1.99	0.40
1:B:197:GLY:HA2	1:B:243:ALA:HB1	2.03	0.40
1:C:86:MSE:HE1	1:C:337:TRP:HZ3	1.86	0.40
1:D:146:LEU:O	1:D:147:PRO:C	2.62	0.40
1:F:86:MSE:HE1	1:F:337:TRP:HZ3	1.86	0.40
1:A:88:PHE:CZ	1:A:90:ALA:HB2	2.57	0.40
1:D:252:GLN:HE21	1:D:252:GLN:HB2	1.66	0.40
1:H:275:VAL:HG12	1:H:290:LEU:CD1	2.51	0.40
1:B:88:PHE:HA	1:B:111:TYR:O	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	372/383 (97%)	353 (95%)	15 (4%)	4 (1%)	11	25
1	B	373/383 (97%)	352 (94%)	19 (5%)	2 (0%)	24	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	373/383 (97%)	358 (96%)	11 (3%)	4 (1%)	11	25
1	D	374/383 (98%)	352 (94%)	21 (6%)	1 (0%)	36	58
1	E	373/383 (97%)	355 (95%)	15 (4%)	3 (1%)	16	34
1	F	375/383 (98%)	355 (95%)	17 (4%)	3 (1%)	16	34
1	G	374/383 (98%)	350 (94%)	19 (5%)	5 (1%)	9	21
1	H	371/383 (97%)	339 (91%)	28 (8%)	4 (1%)	11	25
All	All	2985/3064 (97%)	2814 (94%)	145 (5%)	26 (1%)	14	30

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	15	THR
1	E	69	ALA
1	G	313	LEU
1	H	15	THR
1	H	233	ASP
1	A	15	THR
1	A	91	ALA
1	B	16	GLY
1	B	233	ASP
1	C	69	ALA
1	E	233	ASP
1	F	105	ASN
1	G	67	ASN
1	H	16	GLY
1	H	69	ALA
1	A	17	ARG
1	D	67	ASN
1	G	16	GLY
1	G	91	ALA
1	C	17	ARG
1	C	233	ASP
1	F	15	THR
1	G	233	ASP
1	A	233	ASP
1	C	91	ALA
1	F	233	ASP

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	310/309 (100%)	292 (94%)	18 (6%)	18	39
1	B	311/309 (101%)	285 (92%)	26 (8%)	10	23
1	C	311/309 (101%)	287 (92%)	24 (8%)	12	27
1	D	311/309 (101%)	284 (91%)	27 (9%)	9	21
1	E	310/309 (100%)	283 (91%)	27 (9%)	9	21
1	F	312/309 (101%)	282 (90%)	30 (10%)	8	17
1	G	311/309 (101%)	283 (91%)	28 (9%)	9	20
1	H	308/309 (100%)	284 (92%)	24 (8%)	11	26
All	All	2484/2472 (100%)	2280 (92%)	204 (8%)	10	24

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	15	THR
1	A	28	ILE
1	A	38	ARG
1	A	40	LYS
1	A	54	ARG
1	A	64	LYS
1	A	68	ILE
1	A	72	THR
1	A	75	LEU
1	A	119	ASN
1	A	129	LEU
1	A	168	ARG
1	A	237	LYS
1	A	252	GLN
1	A	276	THR
1	A	282	THR
1	A	321	GLN
1	B	4	THR

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Mol	Chain	Res	Type
1	B	10	ILE
1	B	20	LEU
1	B	28	ILE
1	B	38	ARG
1	B	40	LYS
1	B	43	ASP
1	B	68	ILE
1	B	70	ARG
1	B	72	THR
1	B	74	ASP
1	B	75	LEU
1	B	82	LYS
1	B	94	GLN
1	B	101	THR
1	B	110	VAL
1	B	118	THR
1	B	141	GLN
1	B	143	LYS
1	B	168	ARG
1	B	200	LEU
1	B	230	GLU
1	B	233	ASP
1	B	276	THR
1	B	307	ASN
1	B	321	GLN
1	C	17	ARG
1	C	21	ASN
1	C	38	ARG
1	C	68	ILE
1	C	72	THR
1	C	75	LEU
1	C	76	ASP
1	C	85	THR
1	C	93	THR
1	C	94	GLN
1	C	110	VAL
1	C	114	LYS
1	C	119	ASN
1	C	144	LEU
1	C	168	ARG
1	C	200	LEU
1	C	204	CYS

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Mol	Chain	Res	Type
1	C	230	GLU
1	C	266	VAL
1	C	276	THR
1	C	282	THR
1	C	313	LEU
1	C	328	SER
1	C	347	ASP
1	D	10	ILE
1	D	17	ARG
1	D	26	ARG
1	D	28	ILE
1	D	38	ARG
1	D	41	ASN
1	D	60	GLU
1	D	65	ARG
1	D	67	ASN
1	D	68	ILE
1	D	72	THR
1	D	75	LEU
1	D	92	THR
1	D	93	THR
1	D	99	LEU
1	D	110	VAL
1	D	121	GLU
1	D	144	LEU
1	D	156	ARG
1	D	168	ARG
1	D	200	LEU
1	D	252	GLN
1	D	253	LEU
1	D	266	VAL
1	D	276	THR
1	D	312	ARG
1	D	370	SER
1	E	10	ILE
1	E	11	MSE
1	E	32	ARG
1	E	68	ILE
1	E	72	THR
1	E	75	LEU
1	E	83	ASN
1	E	85	THR

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Mol	Chain	Res	Type
1	E	92	THR
1	E	93	THR
1	E	99	LEU
1	E	110	VAL
1	E	118	THR
1	E	121	GLU
1	E	124	LEU
1	E	135	VAL
1	E	144	LEU
1	E	168	ARG
1	E	200	LEU
1	E	266	VAL
1	E	276	THR
1	E	282	THR
1	E	305	VAL
1	E	313	LEU
1	E	330	ASP
1	E	347	ASP
1	E	383	LYS
1	F	4	THR
1	F	17	ARG
1	F	38	ARG
1	F	50	ILE
1	F	54	ARG
1	F	58	LYS
1	F	75	LEU
1	F	82	LYS
1	F	86	MSE
1	F	92	THR
1	F	93	THR
1	F	94	GLN
1	F	99	LEU
1	F	110	VAL
1	F	118	THR
1	F	125	GLU
1	F	144	LEU
1	F	168	ARG
1	F	235	GLN
1	F	237	LYS
1	F	252	GLN
1	F	266	VAL
1	F	276	THR

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Mol	Chain	Res	Type
1	F	282	THR
1	F	311	LYS
1	F	312	ARG
1	F	313	LEU
1	F	347	ASP
1	F	374	ARG
1	F	383	LYS
1	G	10	ILE
1	G	11	MSE
1	G	15	THR
1	G	28	ILE
1	G	40	LYS
1	G	43	ASP
1	G	54	ARG
1	G	65	ARG
1	G	73	THR
1	G	75	LEU
1	G	76	ASP
1	G	93	THR
1	G	94	GLN
1	G	110	VAL
1	G	119	ASN
1	G	128	LYS
1	G	132	SER
1	G	142	ASP
1	G	156	ARG
1	G	168	ARG
1	G	200	LEU
1	G	252	GLN
1	G	276	THR
1	G	282	THR
1	G	305	VAL
1	G	321	GLN
1	G	327	VAL
1	G	374	ARG
1	H	7	LEU
1	H	10	ILE
1	H	15	THR
1	H	38	ARG
1	H	39	LEU
1	H	60	GLU
1	H	64	LYS

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Mol	Chain	Res	Type
1	H	65	ARG
1	H	92	THR
1	H	94	GLN
1	H	110	VAL
1	H	119	ASN
1	H	129	LEU
1	H	141	GLN
1	H	144	LEU
1	H	150	LYS
1	H	168	ARG
1	H	238	LYS
1	H	276	THR
1	H	282	THR
1	H	307	ASN
1	H	330	ASP
1	H	351	LYS
1	H	370	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	21	ASN
1	A	137	HIS
1	A	235	GLN
1	A	252	GLN
1	A	283	HIS
1	A	296	GLN
1	B	41	ASN
1	B	189	ASN
1	B	235	GLN
1	B	283	HIS
1	C	22	GLN
1	C	94	GLN
1	C	141	GLN
1	C	235	GLN
1	C	283	HIS
1	C	321	GLN
1	D	67	ASN
1	D	216	ASN
1	D	235	GLN
1	D	252	GLN

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Mol	Chain	Res	Type
1	D	283	HIS
1	E	102	GLN
1	E	141	GLN
1	E	212	ASN
1	E	216	ASN
1	E	235	GLN
1	F	34	GLN
1	F	94	GLN
1	F	137	HIS
1	F	141	GLN
1	F	216	ASN
1	F	235	GLN
1	F	252	GLN
1	F	283	HIS
1	G	119	ASN
1	G	189	ASN
1	G	218	GLN
1	G	283	HIS
1	G	296	GLN
1	H	21	ASN
1	H	22	GLN
1	H	102	GLN
1	H	141	GLN
1	H	216	ASN
1	H	283	HIS
1	H	307	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	368/383 (96%)	-0.44	3 (0%) 82 80	26, 53, 101, 116	0
1	B	369/383 (96%)	-0.40	0 100 100	22, 50, 107, 115	0
1	C	369/383 (96%)	-0.60	2 (0%) 87 85	25, 43, 83, 110	0
1	D	370/383 (96%)	-0.54	0 100 100	20, 46, 90, 106	0
1	E	369/383 (96%)	-0.65	1 (0%) 90 88	22, 41, 76, 92	0
1	F	371/383 (96%)	-0.42	1 (0%) 90 88	26, 53, 88, 98	0
1	G	370/383 (96%)	-0.26	1 (0%) 90 88	26, 60, 125, 137	0
1	H	367/383 (95%)	-0.25	12 (3%) 49 43	24, 46, 132, 144	0
All	All	2953/3064 (96%)	-0.44	20 (0%) 84 82	20, 49, 108, 144	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	180	TRP	3.0
1	A	3	THR	2.8
1	H	71	TRP	2.8
1	H	50	ILE	2.7
1	A	15	THR	2.5
1	F	53	GLY	2.4
1	H	56	ALA	2.4
1	A	69	ALA	2.4
1	H	72	THR	2.3
1	H	51	LEU	2.3
1	H	93	THR	2.2
1	H	45	ILE	2.2
1	G	75	LEU	2.2
1	E	313	LEU	2.1
1	C	38	ARG	2.1
1	H	62	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	3	THR	2.0
1	H	85	THR	2.0
1	H	28	ILE	2.0
1	H	58	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.