



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:40 AM GMT

PDB ID : 3V5N  
Title : The crystal structure of oxidoreductase from Sinorhizobium meliloti  
Authors : Zhang, Z.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2011-12-16  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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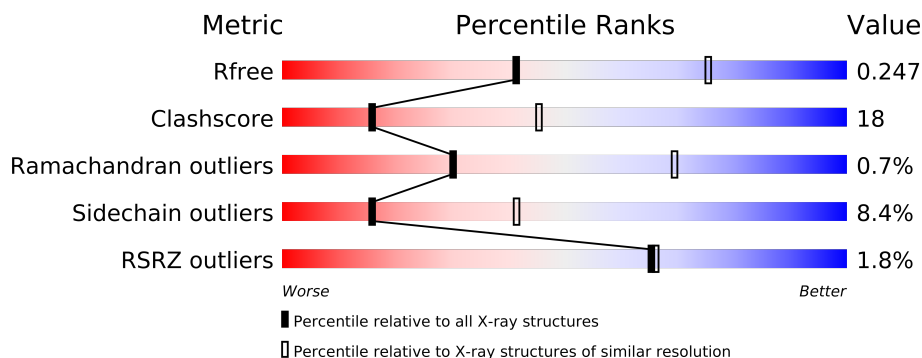
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	417	
1	B	417	
1	C	417	
1	D	417	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10952 atoms, of which 0 are hydrogen and 0 are deuterium.

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	356	Total	C	N	O	S	Se	0	0	0
			2738	1719	493	512	4	10			
1	B	355	Total	C	N	O	S	Se	0	0	0
			2730	1715	491	510	4	10			
1	C	352	Total	C	N	O	S	Se	0	0	0
			2706	1701	484	507	4	10			
1	D	350	Total	C	N	O	S	Se	0	0	0
			2696	1693	486	503	4	10			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	EXPRESSION TAG	UNP Q92LX1
A	-21	HIS	-	EXPRESSION TAG	UNP Q92LX1
A	-20	HIS	-	EXPRESSION TAG	UNP Q92LX1
A	-19	HIS	-	EXPRESSION TAG	UNP Q92LX1
A	-18	HIS	-	EXPRESSION TAG	UNP Q92LX1
A	-17	HIS	-	EXPRESSION TAG	UNP Q92LX1
A	-16	HIS	-	EXPRESSION TAG	UNP Q92LX1
A	-15	SER	-	EXPRESSION TAG	UNP Q92LX1
A	-14	SER	-	EXPRESSION TAG	UNP Q92LX1
A	-13	GLY	-	EXPRESSION TAG	UNP Q92LX1
A	-12	VAL	-	EXPRESSION TAG	UNP Q92LX1
A	-11	ASP	-	EXPRESSION TAG	UNP Q92LX1
A	-10	LEU	-	EXPRESSION TAG	UNP Q92LX1
A	-9	GLY	-	EXPRESSION TAG	UNP Q92LX1
A	-8	THR	-	EXPRESSION TAG	UNP Q92LX1
A	-7	GLU	-	EXPRESSION TAG	UNP Q92LX1
A	-6	ASN	-	EXPRESSION TAG	UNP Q92LX1
A	-5	LEU	-	EXPRESSION TAG	UNP Q92LX1
A	-4	TYR	-	EXPRESSION TAG	UNP Q92LX1
A	-3	PHE	-	EXPRESSION TAG	UNP Q92LX1
A	-2	GLN	-	EXPRESSION TAG	UNP Q92LX1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q92LX1
A	0	MSE	-	EXPRESSION TAG	UNP Q92LX1
B	-22	MSE	-	EXPRESSION TAG	UNP Q92LX1
B	-21	HIS	-	EXPRESSION TAG	UNP Q92LX1
B	-20	HIS	-	EXPRESSION TAG	UNP Q92LX1
B	-19	HIS	-	EXPRESSION TAG	UNP Q92LX1
B	-18	HIS	-	EXPRESSION TAG	UNP Q92LX1
B	-17	HIS	-	EXPRESSION TAG	UNP Q92LX1
B	-16	HIS	-	EXPRESSION TAG	UNP Q92LX1
B	-15	SER	-	EXPRESSION TAG	UNP Q92LX1
B	-14	SER	-	EXPRESSION TAG	UNP Q92LX1
B	-13	GLY	-	EXPRESSION TAG	UNP Q92LX1
B	-12	VAL	-	EXPRESSION TAG	UNP Q92LX1
B	-11	ASP	-	EXPRESSION TAG	UNP Q92LX1
B	-10	LEU	-	EXPRESSION TAG	UNP Q92LX1
B	-9	GLY	-	EXPRESSION TAG	UNP Q92LX1
B	-8	THR	-	EXPRESSION TAG	UNP Q92LX1
B	-7	GLU	-	EXPRESSION TAG	UNP Q92LX1
B	-6	ASN	-	EXPRESSION TAG	UNP Q92LX1
B	-5	LEU	-	EXPRESSION TAG	UNP Q92LX1
B	-4	TYR	-	EXPRESSION TAG	UNP Q92LX1
B	-3	PHE	-	EXPRESSION TAG	UNP Q92LX1
B	-2	GLN	-	EXPRESSION TAG	UNP Q92LX1
B	-1	SER	-	EXPRESSION TAG	UNP Q92LX1
B	0	MSE	-	EXPRESSION TAG	UNP Q92LX1
C	-22	MSE	-	EXPRESSION TAG	UNP Q92LX1
C	-21	HIS	-	EXPRESSION TAG	UNP Q92LX1
C	-20	HIS	-	EXPRESSION TAG	UNP Q92LX1
C	-19	HIS	-	EXPRESSION TAG	UNP Q92LX1
C	-18	HIS	-	EXPRESSION TAG	UNP Q92LX1
C	-17	HIS	-	EXPRESSION TAG	UNP Q92LX1
C	-16	HIS	-	EXPRESSION TAG	UNP Q92LX1
C	-15	SER	-	EXPRESSION TAG	UNP Q92LX1
C	-14	SER	-	EXPRESSION TAG	UNP Q92LX1
C	-13	GLY	-	EXPRESSION TAG	UNP Q92LX1
C	-12	VAL	-	EXPRESSION TAG	UNP Q92LX1
C	-11	ASP	-	EXPRESSION TAG	UNP Q92LX1
C	-10	LEU	-	EXPRESSION TAG	UNP Q92LX1
C	-9	GLY	-	EXPRESSION TAG	UNP Q92LX1
C	-8	THR	-	EXPRESSION TAG	UNP Q92LX1
C	-7	GLU	-	EXPRESSION TAG	UNP Q92LX1
C	-6	ASN	-	EXPRESSION TAG	UNP Q92LX1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	LEU	-	EXPRESSION TAG	UNP Q92LX1
C	-4	TYR	-	EXPRESSION TAG	UNP Q92LX1
C	-3	PHE	-	EXPRESSION TAG	UNP Q92LX1
C	-2	GLN	-	EXPRESSION TAG	UNP Q92LX1
C	-1	SER	-	EXPRESSION TAG	UNP Q92LX1
C	0	MSE	-	EXPRESSION TAG	UNP Q92LX1
D	-22	MSE	-	EXPRESSION TAG	UNP Q92LX1
D	-21	HIS	-	EXPRESSION TAG	UNP Q92LX1
D	-20	HIS	-	EXPRESSION TAG	UNP Q92LX1
D	-19	HIS	-	EXPRESSION TAG	UNP Q92LX1
D	-18	HIS	-	EXPRESSION TAG	UNP Q92LX1
D	-17	HIS	-	EXPRESSION TAG	UNP Q92LX1
D	-16	HIS	-	EXPRESSION TAG	UNP Q92LX1
D	-15	SER	-	EXPRESSION TAG	UNP Q92LX1
D	-14	SER	-	EXPRESSION TAG	UNP Q92LX1
D	-13	GLY	-	EXPRESSION TAG	UNP Q92LX1
D	-12	VAL	-	EXPRESSION TAG	UNP Q92LX1
D	-11	ASP	-	EXPRESSION TAG	UNP Q92LX1
D	-10	LEU	-	EXPRESSION TAG	UNP Q92LX1
D	-9	GLY	-	EXPRESSION TAG	UNP Q92LX1
D	-8	THR	-	EXPRESSION TAG	UNP Q92LX1
D	-7	GLU	-	EXPRESSION TAG	UNP Q92LX1
D	-6	ASN	-	EXPRESSION TAG	UNP Q92LX1
D	-5	LEU	-	EXPRESSION TAG	UNP Q92LX1
D	-4	TYR	-	EXPRESSION TAG	UNP Q92LX1
D	-3	PHE	-	EXPRESSION TAG	UNP Q92LX1
D	-2	GLN	-	EXPRESSION TAG	UNP Q92LX1
D	-1	SER	-	EXPRESSION TAG	UNP Q92LX1
D	0	MSE	-	EXPRESSION TAG	UNP Q92LX1

- Molecule 2 is water.

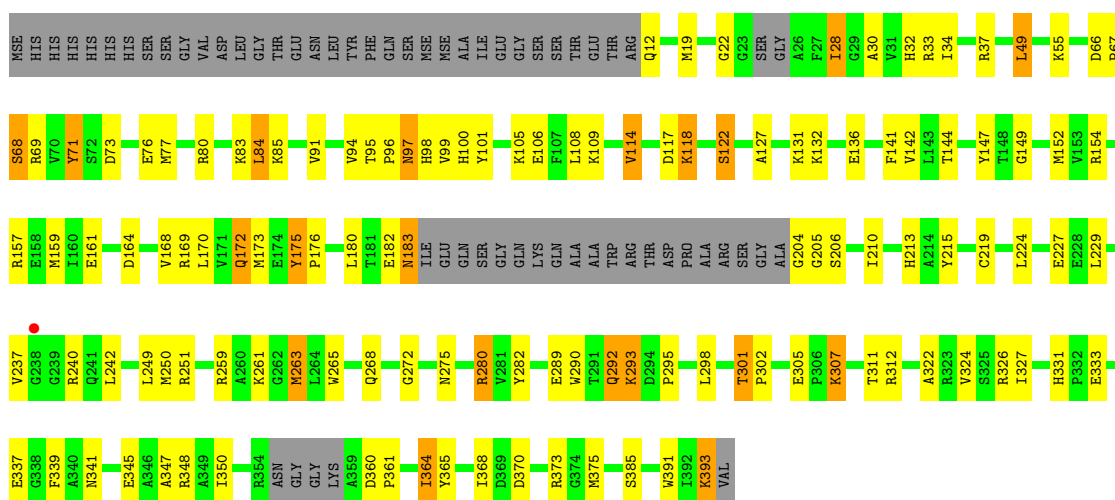
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	28	Total O 28 28	0	0
2	C	12	Total O 12 12	0	0
2	D	15	Total O 15 15	0	0

### 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 errors 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.

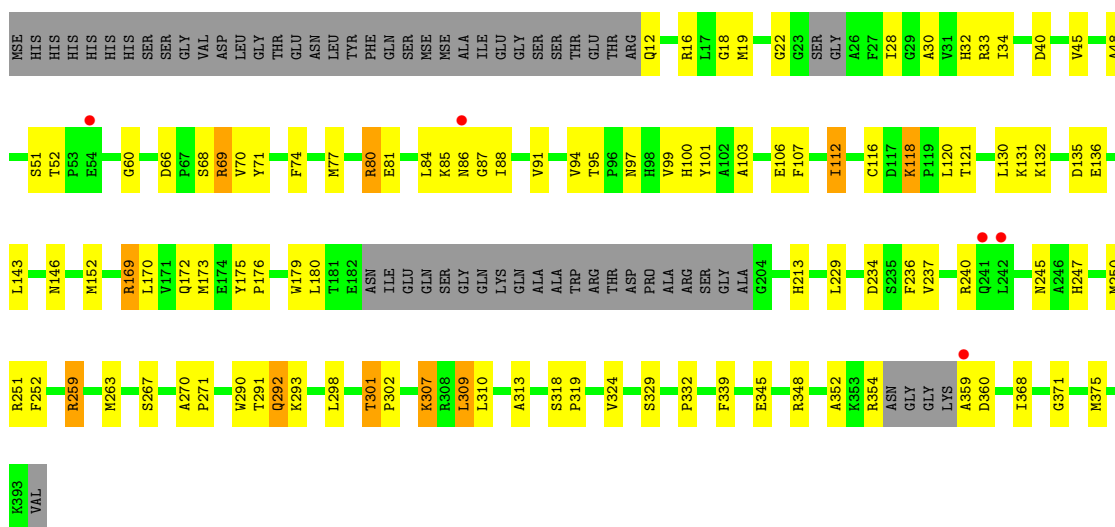
#### • Molecule 1: Oxidoreductase

Chain A:



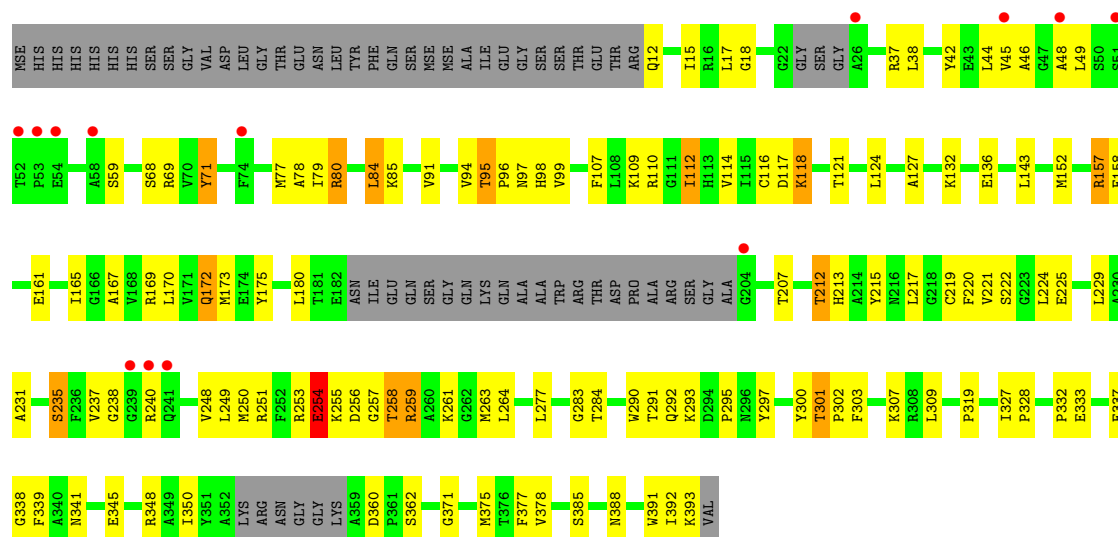
#### • Molecule 1: Oxidoreductase

Chain B:



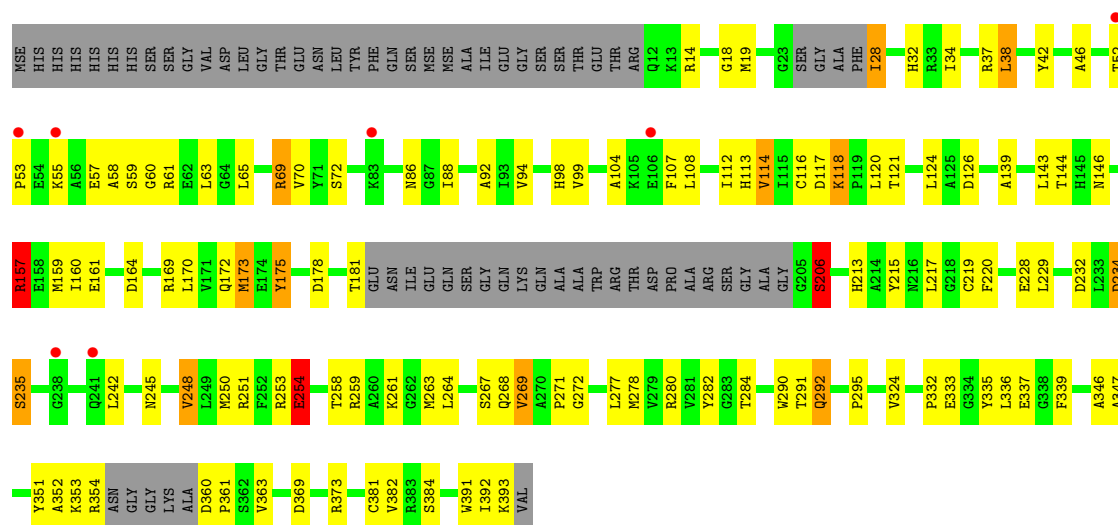
#### • Molecule 1: Oxidoreductase

## Chain C:



## • Molecule 1: Oxidoreductase

## Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.20Å 77.72Å 107.73Å 90.00° 113.83° 90.00°	Depositor
Resolution (Å)	49.27 – 2.80 49.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.27-2.80) 99.7 (49.27-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.185 , 0.252 0.184 , 0.247	Depositor DCC
$R_{free}$ test set	2009 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 29.0	EDS
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 40048 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 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	0.68	0/2783	0.75	0/3739
1	B	0.67	0/2775	0.75	1/3728 (0.0%)
1	C	0.57	0/2751	0.72	0/3698
1	D	0.61	0/2740	0.74	2/3681 (0.1%)
All	All	0.64	0/11049	0.74	3/14846 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	D	38	LEU	CA-CB-CG	-5.29	103.13	115.30
1	B	169	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2738	0	2696	118	0
1	B	2730	0	2690	94	0
1	C	2706	0	2661	117	0
1	D	2696	0	2662	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	0	1	0
2	B	28	0	0	3	0
2	C	12	0	0	0	0
2	D	15	0	0	0	0
All	All	10952	0	10709	396	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (396) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:173:MSE:HE1	1:A:250:MSE:HE2	1.15	1.08
1:C:333:GLU:HG2	1:C:337:GLU:HG2	1.46	0.95
1:C:118:LYS:HD3	1:C:118:LYS:H	1.33	0.94
1:D:172:GLN:HE21	1:D:263:MSE:HE2	1.37	0.89
1:C:118:LYS:HE3	1:C:213:HIS:CE1	2.08	0.89
1:B:173:MSE:HE1	1:B:250:MSE:HE2	1.55	0.87
1:B:180:LEU:HB3	1:B:240:ARG:NH1	1.88	0.87
1:A:333:GLU:HG2	1:A:337:GLU:HG2	1.57	0.85
1:B:180:LEU:HB3	1:B:240:ARG:HH12	1.42	0.84
1:A:173:MSE:HE1	1:A:250:MSE:CE	2.06	0.82
1:B:301:THR:HB	1:B:307:LYS:HB2	1.60	0.81
1:A:172:GLN:NE2	1:A:263:MSE:H	1.77	0.81
1:A:73:ASP:HB3	1:A:76:GLU:HB2	1.63	0.81
1:C:109:LYS:HD3	1:C:110:ARG:HH12	1.46	0.81
1:D:60:GLY:HA2	1:D:65:LEU:HD12	1.63	0.80
1:C:107:PHE:CD1	1:C:112:ILE:HD11	2.17	0.79
1:C:251:ARG:NH1	1:C:391:TRP:CE2	2.51	0.78
1:D:118:LYS:HE3	1:D:213:HIS:NE2	1.97	0.78
1:B:252:PHE:O	1:B:259:ARG:HD3	1.86	0.75
1:A:105:LYS:O	1:A:109:LYS:HB2	1.86	0.74
1:B:245:ASN:OD1	1:B:267:SER:HB2	1.87	0.74
1:C:157:ARG:HG3	1:C:220:PHE:O	1.87	0.74
1:B:301:THR:HG22	2:B:405:HOH:O	1.88	0.74
1:A:170:LEU:HB2	1:A:282:TYR:HB2	1.71	0.72
1:C:169:ARG:CZ	1:C:284:THR:HG22	2.20	0.72
1:A:173:MSE:CE	1:A:250:MSE:HE2	2.08	0.71
1:D:172:GLN:NE2	1:D:263:MSE:HB2	2.06	0.70
1:A:172:GLN:NE2	1:A:263:MSE:HG2	2.07	0.70
1:D:215:TYR:CE1	1:D:219:CYS:SG	2.85	0.69
1:D:118:LYS:HE3	1:D:213:HIS:CE1	2.28	0.69
1:B:94:VAL:O	1:B:94:VAL:HG12	1.93	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:19:MSE:HE1	1:B:33:ARG:NH1	2.08	0.68
1:C:255:LYS:O	1:C:257:GLY:N	2.25	0.68
1:B:107:PHE:HB3	1:B:112:ILE:HG12	1.76	0.68
1:B:131:LYS:HG2	1:B:135:ASP:OD2	1.92	0.68
1:D:117:ASP:HA	1:D:144:THR:OG1	1.93	0.68
1:D:98:HIS:CD2	1:D:99:VAL:HG23	2.29	0.67
1:D:360:ASP:HB3	1:D:363:VAL:HG23	1.75	0.67
1:C:109:LYS:HD3	1:C:110:ARG:NH1	2.07	0.67
1:D:69:ARG:NH2	1:D:86:ASN:HB3	2.08	0.67
1:D:251:ARG:HB3	1:D:259:ARG:NH2	2.10	0.67
1:D:369:ASP:HB3	1:D:373:ARG:HH12	1.59	0.67
1:A:55:LYS:HA	1:A:55:LYS:HE2	1.77	0.66
1:B:118:LYS:HE3	1:B:213:HIS:NE2	2.10	0.66
1:D:181:THR:HA	1:D:269:VAL:HG12	1.76	0.66
1:C:169:ARG:NH2	1:C:284:THR:HG22	2.11	0.66
1:A:249:LEU:HD23	1:A:263:MSE:HE3	1.78	0.65
1:B:69:ARG:HH12	1:B:87:GLY:HA2	1.61	0.65
1:D:251:ARG:HG3	1:D:391:TRP:CZ3	2.31	0.65
1:D:333:GLU:HG2	1:D:337:GLU:HG2	1.78	0.65
1:B:292:GLN:HE22	1:C:332:PRO:HD3	1.59	0.65
1:C:71:TYR:CE1	1:C:77:MSE:HA	2.31	0.65
1:B:360:ASP:HB2	2:B:409:HOH:O	1.95	0.65
1:D:392:ILE:HG22	1:D:393:LYS:N	2.11	0.65
1:C:80:ARG:NH1	1:C:84:LEU:HD21	2.11	0.65
1:C:118:LYS:HE3	1:C:213:HIS:HE1	1.59	0.64
1:C:173:MSE:CE	1:C:264:LEU:HD12	2.27	0.64
1:A:152:MSE:HE3	1:A:312:ARG:HA	1.79	0.64
1:A:172:GLN:NE2	1:A:263:MSE:N	2.47	0.63
1:D:173:MSE:O	1:D:264:LEU:HA	1.99	0.63
1:A:172:GLN:HE22	1:A:263:MSE:N	1.95	0.63
1:D:121:THR:HG21	1:D:126:ASP:HB3	1.81	0.63
1:D:169:ARG:HG2	1:D:258:THR:HG21	1.81	0.62
1:C:49:LEU:HD12	1:C:59:SER:HB2	1.80	0.62
1:A:168:VAL:HG11	1:A:224:LEU:HD11	1.81	0.62
1:A:172:GLN:HE22	1:A:263:MSE:H	1.47	0.62
1:A:19:MSE:HE3	1:A:22:GLY:HA3	1.81	0.62
1:D:116:CYS:O	1:D:143:LEU:HD12	2.00	0.62
1:A:94:VAL:HG12	1:A:94:VAL:O	1.98	0.62
1:B:173:MSE:CE	1:B:250:MSE:HE2	2.29	0.62
1:D:251:ARG:HB3	1:D:259:ARG:HH22	1.65	0.61
1:C:231:ALA:CB	1:C:248:VAL:HG22	2.30	0.61
1:A:292:GLN:HE22	1:D:332:PRO:HD3	1.64	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:60:GLY:HA3	1:B:70:VAL:HG21	1.81	0.61
1:A:19:MSE:HE1	1:A:33:ARG:NH1	2.15	0.61
1:A:94:VAL:CG1	1:A:94:VAL:O	2.48	0.61
1:B:179:TRP:CZ3	1:B:180:LEU:HD21	2.36	0.61
1:D:113:HIS:HA	1:D:139:ALA:HB1	1.83	0.61
1:C:79:ILE:HG12	1:C:110:ARG:HE	1.66	0.60
1:C:107:PHE:CD1	1:C:112:ILE:CD1	2.84	0.60
1:C:264:LEU:C	1:C:264:LEU:HD23	2.22	0.60
1:B:132:LYS:HE2	1:B:136:GLU:OE2	2.02	0.60
1:D:104:ALA:O	1:D:108:LEU:HD12	2.02	0.59
1:B:120:LEU:HD13	1:B:371:GLY:HA3	1.84	0.59
1:A:175:TYR:CE1	1:A:210:ILE:HG22	2.37	0.59
1:A:327:ILE:HD12	1:A:331:HIS:HB3	1.82	0.59
1:A:180:LEU:HB3	1:A:240:ARG:NH1	2.18	0.59
1:A:301:THR:HG21	1:A:307:LYS:HE2	1.84	0.59
1:A:117:ASP:HA	1:A:144:THR:OG1	2.03	0.59
1:A:95:THR:HB	1:A:96:PRO:HD2	1.83	0.59
1:C:107:PHE:HD1	1:C:112:ILE:CD1	2.15	0.59
1:D:19:MSE:HG3	1:D:92:ALA:HB3	1.84	0.59
1:C:229:LEU:O	1:C:391:TRP:HA	2.03	0.59
1:C:116:CYS:O	1:C:143:LEU:HD12	2.02	0.58
1:A:66:ASP:OD1	1:A:68:SER:HB3	2.03	0.58
1:D:360:ASP:OD1	1:D:361:PRO:HD2	2.04	0.58
1:D:251:ARG:CD	1:D:259:ARG:HH22	2.17	0.58
1:B:345:GLU:OE1	1:B:348:ARG:NH1	2.37	0.58
1:B:107:PHE:CD1	1:B:112:ILE:HD11	2.39	0.57
1:C:107:PHE:HB3	1:C:112:ILE:HG12	1.84	0.57
1:D:228:GLU:OE1	1:D:391:TRP:HB3	2.03	0.57
1:A:100:HIS:CE1	1:A:117:ASP:O	2.57	0.57
1:A:154:ARG:NH1	1:A:364:ILE:HG13	2.19	0.57
1:B:19:MSE:HE1	1:B:33:ARG:HH11	1.68	0.57
1:C:173:MSE:CE	1:C:215:TYR:HA	2.33	0.57
1:B:118:LYS:HE3	1:B:213:HIS:CE1	2.40	0.57
1:A:360:ASP:OD1	1:A:361:PRO:HD2	2.05	0.57
1:B:173:MSE:HE1	1:B:250:MSE:CE	2.30	0.57
1:B:19:MSE:HE3	1:B:22:GLY:HA3	1.87	0.56
1:C:107:PHE:HB3	1:C:112:ILE:CG1	2.35	0.56
1:C:99:VAL:O	1:C:99:VAL:HG12	2.05	0.56
1:D:28:ILE:O	1:D:28:ILE:HG12	2.00	0.56
1:B:313:ALA:O	1:B:329:SER:HB3	2.05	0.56
1:D:175:TYR:CD1	1:D:277:LEU:HD13	2.40	0.56
1:A:213:HIS:ND1	2:A:411:HOH:O	2.32	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:301:THR:HB	1:A:307:LYS:HA	1.86	0.56
1:B:116:CYS:O	1:B:143:LEU:HD12	2.05	0.56
1:B:180:LEU:CB	1:B:240:ARG:HH12	2.17	0.56
1:A:180:LEU:HB3	1:A:240:ARG:NH2	2.20	0.56
1:A:176:PRO:HG3	1:A:265:TRP:CZ3	2.40	0.56
1:C:180:LEU:HB3	1:C:240:ARG:NH2	2.21	0.56
1:A:172:GLN:NE2	1:A:172:GLN:HA	2.21	0.56
1:A:237:VAL:O	1:A:240:ARG:HB3	2.07	0.55
1:B:66:ASP:OD1	1:B:68:SER:HB3	2.05	0.55
1:D:245:ASN:OD1	1:D:267:SER:HB2	2.06	0.55
1:D:157:ARG:HD2	1:D:220:PHE:CZ	2.41	0.55
1:D:229:LEU:O	1:D:229:LEU:HD12	2.06	0.55
1:C:95:THR:HB	1:C:96:PRO:HD2	1.88	0.55
1:B:18:GLY:C	1:B:91:VAL:HG23	2.26	0.55
1:C:152:MSE:HE2	1:C:152:MSE:HA	1.87	0.55
1:C:173:MSE:HE3	1:C:215:TYR:HA	1.88	0.55
1:A:37:ARG:O	1:D:37:ARG:HD2	2.07	0.55
1:C:263:MSE:CE	1:D:263:MSE:HG2	2.36	0.54
1:C:95:THR:HB	1:C:96:PRO:CD	2.37	0.54
1:C:392:ILE:HG22	1:C:393:LYS:N	2.22	0.54
1:D:229:LEU:C	1:D:229:LEU:HD12	2.27	0.54
1:C:255:LYS:C	1:C:257:GLY:H	2.11	0.54
1:C:392:ILE:HG22	1:C:393:LYS:H	1.72	0.54
1:C:388:ASN:ND2	1:D:391:TRP:CD1	2.76	0.54
1:C:300:TYR:CE2	1:C:302:PRO:HG3	2.43	0.54
1:D:46:ALA:HB2	1:D:69:ARG:HG2	1.89	0.54
1:D:18:GLY:HA3	1:D:88:ILE:HD12	1.90	0.53
1:A:345:GLU:OE1	1:A:348:ARG:NH1	2.42	0.53
1:A:131:LYS:HA	1:A:368:ILE:HG12	1.91	0.53
1:D:253:ARG:O	1:D:254:GLU:C	2.45	0.53
1:D:172:GLN:NE2	1:D:263:MSE:HE2	2.17	0.53
1:C:263:MSE:HE1	1:D:263:MSE:HG2	1.90	0.52
1:B:95:THR:OG1	1:B:99:VAL:HB	2.09	0.52
1:D:172:GLN:NE2	1:D:263:MSE:CB	2.73	0.52
1:A:95:THR:HB	1:A:96:PRO:CD	2.40	0.52
1:A:49:LEU:HD12	1:A:49:LEU:H	1.73	0.52
1:A:106:GLU:OE1	1:A:106:GLU:HA	2.10	0.52
1:C:71:TYR:CD2	1:C:71:TYR:N	2.76	0.52
1:A:30:ALA:O	1:A:34:ILE:HG13	2.10	0.52
1:B:309:LEU:C	1:B:309:LEU:HD12	2.30	0.52
1:C:297:TYR:HB3	1:C:309:LEU:HD11	1.92	0.52
1:C:117:ASP:OD1	1:C:118:LYS:HD3	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:118:LYS:CE	1:B:213:HIS:NE2	2.73	0.52
1:D:352:ALA:O	1:D:354:ARG:N	2.43	0.52
1:D:206:SER:HA	1:D:268:GLN:NE2	2.25	0.52
1:C:303:PHE:CE1	1:D:181:THR:HB	2.44	0.52
1:A:127:ALA:HB2	1:A:375:MSE:HG3	1.92	0.52
1:A:172:GLN:HE21	1:A:172:GLN:HA	1.75	0.51
1:C:96:PRO:HB2	1:C:98:HIS:CE1	2.45	0.51
1:D:34:ILE:HG21	1:D:336:LEU:HD13	1.92	0.51
1:D:280:ARG:HD2	1:D:282:TYR:OH	2.10	0.51
1:C:292:GLN:O	1:C:295:PRO:HD3	2.10	0.51
1:A:118:LYS:H	1:A:118:LYS:HD3	1.75	0.51
1:B:66:ASP:CG	1:B:68:SER:HB3	2.31	0.51
1:B:71:TYR:CD1	1:B:77:MSE:HA	2.46	0.51
1:B:118:LYS:H	1:B:118:LYS:HD3	1.75	0.51
1:A:180:LEU:HB3	1:A:240:ARG:CZ	2.40	0.51
1:A:98:HIS:HA	1:A:122:SER:HB3	1.92	0.51
1:B:169:ARG:O	1:B:170:LEU:HD23	2.11	0.51
1:C:249:LEU:C	1:C:250:MSE:HG2	2.31	0.51
1:C:15:ILE:HD13	1:C:350:ILE:HG21	1.93	0.51
1:C:224:LEU:CD2	1:C:255:LYS:HD3	2.41	0.51
1:B:107:PHE:HD1	1:B:112:ILE:CD1	2.23	0.51
1:B:107:PHE:HB3	1:B:112:ILE:CG1	2.40	0.51
1:B:71:TYR:CG	1:B:77:MSE:HB2	2.46	0.51
1:A:141:PHE:CD2	1:A:141:PHE:C	2.84	0.50
1:A:272:GLY:HA2	1:B:301:THR:HG21	1.92	0.50
1:B:69:ARG:HD2	1:B:81:GLU:OE2	2.12	0.50
1:B:77:MSE:HE2	1:B:88:ILE:HD13	1.94	0.50
1:D:235:SER:HB2	1:D:242:LEU:O	2.10	0.50
1:A:272:GLY:CA	1:B:301:THR:HG21	2.42	0.50
1:C:338:GLY:O	1:C:341:ASN:HB2	2.12	0.50
1:B:30:ALA:O	1:B:34:ILE:HG13	2.10	0.50
1:A:180:LEU:HB3	1:A:240:ARG:HH12	1.76	0.50
1:D:159:MSE:HG2	1:D:164:ASP:OD2	2.12	0.50
1:A:205:GLY:N	1:A:242:LEU:HD13	2.26	0.50
1:C:301:THR:HG21	1:C:307:LYS:HE2	1.93	0.50
1:A:98:HIS:CD2	1:A:99:VAL:HG23	2.47	0.50
1:B:40:ASP:HB2	1:C:37:ARG:CZ	2.41	0.50
1:D:58:ALA:O	1:D:61:ARG:HB3	2.12	0.49
1:B:237:VAL:HG21	1:B:240:ARG:NH2	2.27	0.49
1:A:33:ARG:O	1:A:37:ARG:HG3	2.12	0.49
1:C:290:TRP:CH2	1:C:292:GLN:CB	2.95	0.49
1:D:352:ALA:C	1:D:354:ARG:H	2.16	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:309:LEU:HD12	1:B:310:LEU:N	2.28	0.49
1:A:360:ASP:OD1	1:A:361:PRO:CD	2.60	0.49
1:A:263:MSE:HE2	1:B:263:MSE:SE	2.63	0.49
1:C:251:ARG:NH1	1:C:391:TRP:CZ2	2.80	0.49
1:A:261:LYS:HG3	1:B:234:ASP:OD1	2.13	0.49
1:C:71:TYR:CD1	1:C:77:MSE:HA	2.48	0.49
1:C:112:ILE:HG13	1:C:112:ILE:O	2.10	0.49
1:C:231:ALA:HB2	1:C:248:VAL:HG22	1.95	0.48
1:C:118:LYS:HE3	1:C:213:HIS:NE2	2.27	0.48
1:B:69:ARG:NH1	1:B:87:GLY:HA2	2.26	0.48
1:B:40:ASP:HB2	1:C:37:ARG:NE	2.28	0.48
1:A:182:GLU:O	1:A:183:ASN:HB2	2.11	0.48
1:C:170:LEU:HA	1:C:261:LYS:O	2.13	0.48
1:C:301:THR:CG2	1:C:307:LYS:HE2	2.44	0.48
1:C:121:THR:OG1	1:C:127:ALA:HB2	2.13	0.48
1:D:392:ILE:CG2	1:D:393:LYS:N	2.75	0.48
1:C:173:MSE:HE2	1:C:264:LEU:HD12	1.93	0.48
1:B:120:LEU:HG	1:B:130:LEU:HD23	1.94	0.48
1:D:251:ARG:HG3	1:D:391:TRP:CH2	2.47	0.48
1:B:107:PHE:CD1	1:B:112:ILE:CD1	2.97	0.48
1:C:80:ARG:HH11	1:C:80:ARG:CG	2.27	0.48
1:A:180:LEU:HB3	1:A:240:ARG:HH22	1.79	0.48
1:A:263:MSE:CE	1:B:263:MSE:HG2	2.44	0.47
1:B:332:PRO:HD3	1:C:292:GLN:HE22	1.79	0.47
1:A:71:TYR:N	1:A:71:TYR:CD2	2.82	0.47
1:B:121:THR:OG1	1:B:375:MSE:HE2	2.14	0.47
1:D:18:GLY:HA3	1:D:88:ILE:CD1	2.45	0.47
1:C:45:VAL:HG23	1:C:46:ALA:N	2.29	0.47
1:A:142:VAL:HG22	1:A:365:TYR:CE1	2.50	0.47
1:A:172:GLN:HE21	1:A:263:MSE:H	1.61	0.47
1:A:249:LEU:HD22	1:B:247:HIS:HB3	1.97	0.47
1:A:180:LEU:O	1:A:237:VAL:HG21	2.13	0.47
1:A:108:LEU:HG	1:A:114:VAL:CG1	2.44	0.47
1:D:251:ARG:HD3	1:D:259:ARG:HH22	1.79	0.47
1:A:175:TYR:CZ	1:A:210:ILE:HG22	2.48	0.47
1:A:215:TYR:CE1	1:A:219:CYS:SG	3.07	0.47
1:C:207:THR:HG22	1:C:378:VAL:HG22	1.96	0.47
1:A:168:VAL:CG1	1:A:224:LEU:HD11	2.44	0.47
1:D:52:THR:OG1	1:D:55:LYS:HB2	2.15	0.47
1:B:290:TRP:CH2	1:B:292:GLN:HB2	2.49	0.47
1:D:120:LEU:HD12	1:D:120:LEU:HA	1.54	0.47
1:A:100:HIS:HE1	1:A:117:ASP:O	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:251:ARG:HD2	1:A:391:TRP:CZ3	2.50	0.47
1:A:206:SER:HB3	1:A:268:GLN:HG3	1.95	0.47
1:B:352:ALA:CB	1:B:359:ALA:HB2	2.44	0.47
1:B:94:VAL:O	1:B:94:VAL:CG1	2.62	0.47
1:C:80:ARG:O	1:C:84:LEU:HD13	2.14	0.47
1:A:147:TYR:C	1:A:149:GLY:H	2.17	0.47
1:D:292:GLN:O	1:D:295:PRO:HG3	2.14	0.47
1:C:231:ALA:HB1	1:C:248:VAL:HG22	1.97	0.47
1:C:300:TYR:CZ	1:C:302:PRO:HG3	2.50	0.47
1:B:298:LEU:O	1:B:310:LEU:HB2	2.14	0.47
1:B:69:ARG:NH1	1:B:81:GLU:OE1	2.48	0.46
1:D:384:SER:HB2	1:D:392:ILE:HG12	1.97	0.46
1:A:312:ARG:NH2	1:A:331:HIS:O	2.48	0.46
1:C:301:THR:HG21	1:D:272:GLY:HA2	1.97	0.46
1:C:80:ARG:HH12	1:C:84:LEU:HD21	1.79	0.46
1:A:229:LEU:C	1:A:229:LEU:HD12	2.36	0.46
1:C:217:LEU:O	1:C:221:VAL:HG23	2.14	0.46
1:B:152:MSE:HE3	1:B:298:LEU:CB	2.45	0.46
1:B:318:SER:HB2	1:B:319:PRO:HD2	1.98	0.46
1:C:169:ARG:NE	1:C:284:THR:HG22	2.29	0.46
1:B:71:TYR:CE1	1:B:77:MSE:HA	2.50	0.46
1:B:28:ILE:O	1:B:32:HIS:HD2	1.98	0.46
1:B:74:PHE:CD1	1:B:103:ALA:HA	2.51	0.46
1:C:388:ASN:ND2	1:C:388:ASN:O	2.49	0.46
1:C:49:LEU:HD12	1:C:59:SER:CB	2.46	0.46
1:C:17:LEU:O	1:C:44:LEU:HD12	2.16	0.46
1:C:251:ARG:HD2	1:C:391:TRP:CZ3	2.51	0.46
1:A:292:GLN:O	1:A:295:PRO:HG3	2.16	0.46
1:A:28:ILE:O	1:A:32:HIS:HD2	1.99	0.46
1:C:290:TRP:CH2	1:C:292:GLN:HB3	2.51	0.46
1:C:229:LEU:C	1:C:229:LEU:HD12	2.37	0.45
1:D:381:CYS:O	1:D:382:VAL:C	2.53	0.45
1:C:237:VAL:HG12	1:C:238:GLY:O	2.15	0.45
1:A:118:LYS:HG3	1:A:213:HIS:NE2	2.31	0.45
1:C:261:LYS:NZ	1:D:234:ASP:OD1	2.42	0.45
1:A:152:MSE:CE	1:A:312:ARG:HA	2.45	0.45
1:B:251:ARG:HD3	1:B:259:ARG:NH1	2.32	0.45
1:D:369:ASP:CB	1:D:373:ARG:HH12	2.30	0.45
1:C:264:LEU:HD13	1:C:377:PHE:HZ	1.82	0.45
1:D:290:TRP:CH2	1:D:292:GLN:CB	3.00	0.45
1:D:178:ASP:HB2	1:D:271:PRO:HA	1.99	0.45
1:C:225:GLU:HB2	1:C:253:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:346:ALA:O	1:D:347:ALA:C	2.53	0.45
1:A:227:GLU:O	1:A:393:LYS:HB3	2.16	0.45
1:A:83:LYS:O	1:A:84:LEU:C	2.55	0.45
1:A:169:ARG:HG2	1:B:236:PHE:CD1	2.52	0.45
1:C:215:TYR:CE1	1:C:219:CYS:SG	3.10	0.44
1:A:301:THR:CG2	1:A:307:LYS:HE2	2.47	0.44
1:D:53:PRO:HA	1:D:72:SER:HB2	1.98	0.44
1:D:57:GLU:HA	1:D:70:VAL:HG11	1.99	0.44
1:B:19:MSE:CE	1:B:33:ARG:HH11	2.31	0.44
1:D:170:LEU:HA	1:D:261:LYS:O	2.18	0.44
1:A:97:ASN:HD22	1:A:98:HIS:N	2.15	0.44
1:C:222:SER:HB2	1:C:224:LEU:HG	1.99	0.44
1:C:158:GLU:OE2	1:C:319:PRO:HB2	2.17	0.44
1:C:391:TRP:O	1:C:392:ILE:HD13	2.17	0.44
1:C:217:LEU:HD23	1:C:277:LEU:HD11	2.00	0.44
1:D:217:LEU:O	1:D:217:LEU:HD12	2.16	0.44
1:C:132:LYS:O	1:C:136:GLU:HG3	2.17	0.44
1:D:264:LEU:HD23	1:D:264:LEU:C	2.38	0.44
1:B:301:THR:HA	1:B:302:PRO:HD3	1.84	0.44
1:C:44:LEU:HA	1:C:44:LEU:HD12	1.68	0.44
1:B:80:ARG:O	1:B:84:LEU:HB2	2.18	0.44
1:B:88:ILE:HD12	1:B:91:VAL:HB	2.00	0.44
1:C:78:ALA:HB1	1:C:110:ARG:HD2	2.00	0.43
1:A:327:ILE:HD11	1:A:331:HIS:O	2.18	0.43
1:C:261:LYS:HD2	1:D:232:ASP:OD2	2.18	0.43
1:A:101:TYR:O	1:A:105:LYS:HG2	2.18	0.43
1:B:40:ASP:HB2	1:C:37:ARG:CD	2.49	0.43
1:B:270:ALA:O	1:B:271:PRO:C	2.56	0.43
1:B:301:THR:HB	1:B:307:LYS:CB	2.41	0.43
1:B:152:MSE:HE3	1:B:298:LEU:HB3	1.98	0.43
1:A:331:HIS:HD2	1:D:335:TYR:CZ	2.37	0.43
1:A:84:LEU:HD12	1:A:84:LEU:HA	1.67	0.43
1:C:371:GLY:O	1:C:375:MSE:HG2	2.19	0.43
1:C:48:ALA:HB2	1:C:71:TYR:HB2	2.00	0.43
1:B:120:LEU:HD11	1:B:368:ILE:HD12	2.01	0.43
1:C:124:LEU:HD13	1:C:375:MSE:HB3	2.01	0.43
1:A:292:GLN:NE2	1:A:293:LYS:HA	2.33	0.43
1:C:253:ARG:O	1:C:254:GLU:C	2.57	0.43
1:B:16:ARG:HG2	1:B:45:VAL:HG11	1.99	0.43
1:A:370:ASP:OD1	1:A:373:ARG:NH1	2.52	0.43
1:C:345:GLU:OE1	1:C:348:ARG:NH1	2.51	0.43
1:D:94:VAL:O	1:D:94:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:107:PHE:HB3	1:D:112:ILE:HB	2.00	0.43
1:B:245:ASN:OD1	1:B:267:SER:CB	2.64	0.43
1:A:117:ASP:OD1	1:A:118:LYS:HD3	2.19	0.43
1:C:18:GLY:HA2	1:C:46:ALA:O	2.18	0.43
1:D:248:VAL:HG22	1:D:250:MSE:SE	2.69	0.43
1:A:67:PRO:C	1:A:69:ARG:H	2.21	0.43
1:A:326:ARG:NH2	1:A:341:ASN:OD1	2.46	0.43
1:C:110:ARG:HG3	1:C:110:ARG:HH11	1.84	0.43
1:C:301:THR:HG21	1:D:272:GLY:CA	2.49	0.43
1:B:16:ARG:HB2	1:B:16:ARG:HE	1.73	0.43
1:A:159:MSE:HG2	1:A:164:ASP:OD2	2.19	0.43
1:A:19:MSE:CE	1:A:22:GLY:HA3	2.48	0.42
1:A:132:LYS:HE2	1:A:136:GLU:OE2	2.19	0.42
1:D:59:SER:O	1:D:63:LEU:HG	2.19	0.42
1:C:212:THR:HG23	1:C:378:VAL:CG2	2.49	0.42
1:B:229:LEU:HD12	1:B:229:LEU:C	2.40	0.42
1:C:291:THR:HG22	1:C:293:LYS:H	1.85	0.42
1:B:100:HIS:O	1:B:101:TYR:C	2.54	0.42
1:C:264:LEU:HD13	1:C:377:PHE:CZ	2.55	0.42
1:C:212:THR:HG23	1:C:378:VAL:HG23	2.02	0.42
1:A:91:VAL:HG13	1:A:91:VAL:O	2.17	0.42
1:C:259:ARG:C	1:C:259:ARG:HD3	2.40	0.42
1:A:331:HIS:HD2	1:D:335:TYR:CE1	2.37	0.42
1:B:84:LEU:O	1:B:86:ASN:N	2.42	0.42
1:C:165:ILE:O	1:C:165:ILE:HG13	2.18	0.42
1:A:154:ARG:CZ	1:A:364:ILE:HG13	2.50	0.42
1:A:360:ASP:HA	1:A:361:PRO:HD3	1.90	0.42
1:A:142:VAL:HG22	1:A:365:TYR:CD1	2.54	0.42
1:D:278:MSE:HE2	1:D:291:THR:OG1	2.20	0.42
1:A:28:ILE:CD1	1:A:94:VAL:HG13	2.50	0.42
1:D:124:LEU:HD12	1:D:124:LEU:HA	1.88	0.42
1:D:146:ASN:OD1	1:D:146:ASN:N	2.52	0.42
1:D:169:ARG:CZ	1:D:284:THR:HG22	2.50	0.42
1:A:322:ALA:O	1:A:324:VAL:N	2.52	0.42
1:A:280:ARG:CG	1:A:289:GLU:HG2	2.50	0.42
1:A:157:ARG:HH11	1:A:157:ARG:HG3	1.85	0.42
1:C:235:SER:O	1:C:235:SER:OG	2.30	0.42
1:C:327:ILE:HB	1:C:328:PRO:CD	2.50	0.42
1:B:66:ASP:OD2	1:B:68:SER:HB3	2.19	0.41
1:A:280:ARG:HG2	1:A:289:GLU:HG2	2.01	0.41
1:D:160:ILE:O	1:D:161:GLU:C	2.57	0.41
1:A:71:TYR:CE1	1:A:77:MSE:HA	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:172:GLN:NE2	1:C:263:MSE:HG3	2.36	0.41
1:A:301:THR:HA	1:A:302:PRO:HD3	1.82	0.41
1:C:165:ILE:O	1:C:283:GLY:HA3	2.21	0.41
1:A:347:ALA:O	1:A:350:ILE:N	2.53	0.41
1:A:327:ILE:CD1	1:A:331:HIS:O	2.68	0.41
1:A:290:TRP:CH2	1:A:292:GLN:HA	2.54	0.41
1:D:28:ILE:O	1:D:32:HIS:HD2	2.03	0.41
1:D:170:LEU:HB2	1:D:282:TYR:HB2	2.02	0.41
1:C:255:LYS:C	1:C:257:GLY:N	2.73	0.41
1:C:264:LEU:CD2	1:C:264:LEU:C	2.89	0.41
1:B:106:GLU:OE1	1:B:106:GLU:HA	2.20	0.41
1:B:237:VAL:HG21	1:B:240:ARG:CZ	2.51	0.41
1:B:301:THR:CG2	2:B:405:HOH:O	2.58	0.41
1:A:263:MSE:HE1	1:B:263:MSE:HG2	2.03	0.41
1:C:152:MSE:CA	1:C:152:MSE:HE2	2.51	0.41
1:D:88:ILE:HG21	1:D:88:ILE:HD13	1.85	0.41
1:A:204:GLY:C	1:A:242:LEU:HD13	2.41	0.41
1:A:49:LEU:N	1:A:49:LEU:HD12	2.34	0.40
1:A:108:LEU:HG	1:A:114:VAL:HG11	2.03	0.40
1:B:291:THR:HG22	1:B:293:LYS:HG2	2.02	0.40
1:D:42:TYR:N	1:D:42:TYR:CD2	2.89	0.40
1:B:146:ASN:OD1	1:B:146:ASN:N	2.54	0.40
1:C:91:VAL:HG11	1:C:107:PHE:CG	2.57	0.40
1:D:120:LEU:O	1:D:121:THR:HG23	2.22	0.40
1:B:48:ALA:H	1:B:77:MSE:SE	2.55	0.40
1:D:351:TYR:O	1:D:354:ARG:HB2	2.21	0.40
1:C:167:ALA:HB1	1:C:258:THR:OG1	2.21	0.40
1:D:114:VAL:HG22	1:D:114:VAL:O	2.20	0.40
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.88	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	348/417 (84%)	328 (94%)	18 (5%)	2 (1%)	33	72
1	B	347/417 (83%)	325 (94%)	20 (6%)	2 (1%)	33	72
1	C	344/417 (82%)	316 (92%)	26 (8%)	2 (1%)	33	72
1	D	342/417 (82%)	301 (88%)	37 (11%)	4 (1%)	19	54
All	All	1381/1668 (83%)	1270 (92%)	101 (7%)	10 (1%)	30	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	206	SER
1	A	275	ASN
1	B	85	LYS
1	C	254	GLU
1	D	353	LYS
1	C	256	ASP
1	D	254	GLU
1	A	68	SER
1	D	14	ARG
1	B	176	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	277/312 (89%)	249 (90%)	28 (10%)	11	30
1	B	276/312 (88%)	258 (94%)	18 (6%)	24	57
1	C	274/312 (88%)	245 (89%)	29 (11%)	10	27
1	D	274/312 (88%)	257 (94%)	17 (6%)	26	60
All	All	1101/1248 (88%)	1009 (92%)	92 (8%)	16	41

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	28	ILE

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Mol	Chain	Res	Type
1	A	49	LEU
1	A	71	TYR
1	A	80	ARG
1	A	84	LEU
1	A	85	LYS
1	A	97	ASN
1	A	114	VAL
1	A	118	LYS
1	A	122	SER
1	A	161	GLU
1	A	172	GLN
1	A	175	TYR
1	A	183	ASN
1	A	259	ARG
1	A	263	MSE
1	A	280	ARG
1	A	292	GLN
1	A	293	LYS
1	A	301	THR
1	A	305	GLU
1	A	307	LYS
1	A	311	THR
1	A	339	PHE
1	A	364	ILE
1	A	385	SER
1	A	393	LYS
1	B	12	GLN
1	B	51	SER
1	B	52	THR
1	B	69	ARG
1	B	80	ARG
1	B	97	ASN
1	B	112	ILE
1	B	118	LYS
1	B	172	GLN
1	B	175	TYR
1	B	259	ARG
1	B	292	GLN
1	B	301	THR
1	B	307	LYS
1	B	309	LEU
1	B	324	VAL

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Mol	Chain	Res	Type
1	B	339	PHE
1	B	354	ARG
1	C	12	GLN
1	C	38	LEU
1	C	42	TYR
1	C	68	SER
1	C	69	ARG
1	C	71	TYR
1	C	80	ARG
1	C	84	LEU
1	C	85	LYS
1	C	94	VAL
1	C	95	THR
1	C	97	ASN
1	C	112	ILE
1	C	114	VAL
1	C	118	LYS
1	C	157	ARG
1	C	161	GLU
1	C	172	GLN
1	C	175	TYR
1	C	212	THR
1	C	235	SER
1	C	254	GLU
1	C	258	THR
1	C	259	ARG
1	C	301	THR
1	C	339	PHE
1	C	360	ASP
1	C	362	SER
1	C	385	SER
1	D	28	ILE
1	D	38	LEU
1	D	69	ARG
1	D	114	VAL
1	D	118	LYS
1	D	157	ARG
1	D	173	MSE
1	D	175	TYR
1	D	206	SER
1	D	234	ASP
1	D	235	SER

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Mol	Chain	Res	Type
1	D	248	VAL
1	D	254	GLU
1	D	269	VAL
1	D	292	GLN
1	D	324	VAL
1	D	339	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	98	HIS
1	A	100	HIS
1	A	172	GLN
1	A	292	GLN
1	A	331	HIS
1	B	12	GLN
1	C	12	GLN
1	C	213	HIS
1	D	98	HIS
1	D	172	GLN
1	D	268	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	356/417 (85%)	-0.20	1 (0%) 91 93	28, 40, 59, 81	0
1	B	355/417 (85%)	-0.09	5 (1%) 72 72	26, 42, 65, 86	0
1	C	352/417 (84%)	0.21	13 (3%) 39 39	36, 53, 77, 106	0
1	D	350/417 (83%)	0.07	7 (2%) 62 63	30, 52, 77, 98	0
All	All	1413/1668 (84%)	-0.00	26 (1%) 65 66	26, 46, 73, 106	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	GLY	4.2
1	D	53	PRO	3.9
1	D	238	GLY	3.7
1	C	26	ALA	3.4
1	C	48	ALA	3.4
1	B	359	ALA	3.0
1	C	74	PHE	3.0
1	B	86	ASN	2.7
1	C	52	THR	2.6
1	D	55	LYS	2.5
1	D	52	THR	2.5
1	C	240	ARG	2.4
1	C	54	GLU	2.4
1	C	53	PRO	2.4
1	D	83	LYS	2.3
1	C	51	SER	2.3
1	C	239	GLY	2.3
1	C	58	ALA	2.2
1	C	241	GLN	2.2
1	B	54	GLU	2.2
1	A	238	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	45	VAL	2.1
1	D	106	GLU	2.1
1	B	242	LEU	2.0
1	B	241	GLN	2.0
1	D	241	GLN	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.