



# Full wwPDB X-ray Structure Validation Report

Oct 14, 2014 – 08:06 PM EDT

PDB ID : 4OFW  
Title : Crystal Structure of Arabidopsis thaliana DJ-1d  
Authors : Choi, D.; Kim, J.; Ryu, K.-S.; Park, C.  
Deposited on : 2014-01-15  
Resolution : 2.30 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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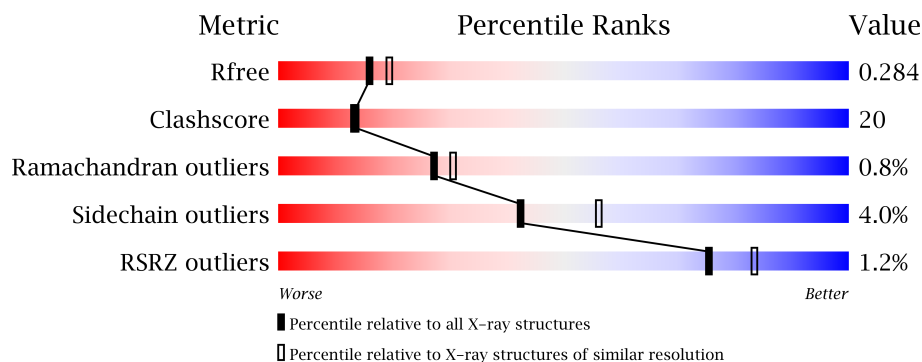
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
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) : stable23828

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	387	
1	B	387	
1	C	387	
1	D	387	
1	E	387	
1	F	387	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18086 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 Protein DJ-1 homolog D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	B	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	C	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	D	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	E	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	F	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			

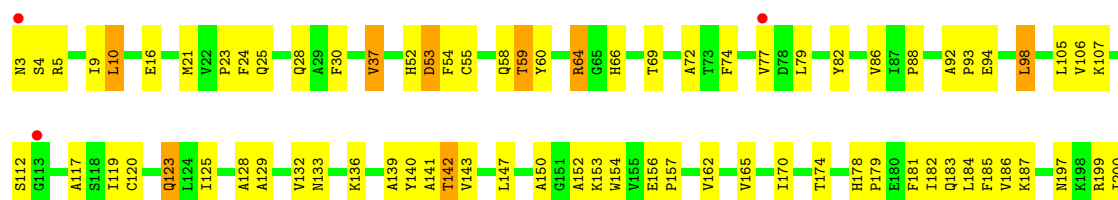
There are 12 discrepancies between the modelled and reference sequences:

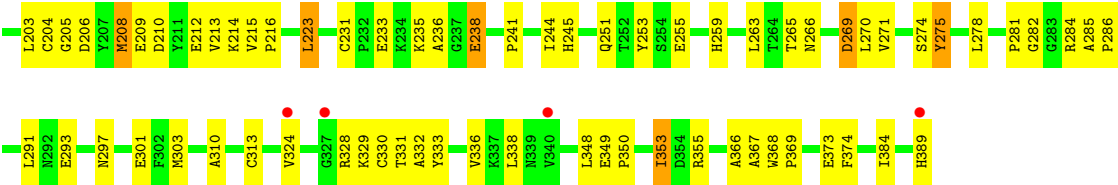
Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLU	ASP	CONFLICT	UNP Q9M8R4
A	389	HIS	-	EXPRESSION TAG	UNP Q9M8R4
B	238	GLU	ASP	CONFLICT	UNP Q9M8R4
B	389	HIS	-	EXPRESSION TAG	UNP Q9M8R4
C	238	GLU	ASP	CONFLICT	UNP Q9M8R4
C	389	HIS	-	EXPRESSION TAG	UNP Q9M8R4
D	238	GLU	ASP	CONFLICT	UNP Q9M8R4
D	389	HIS	-	EXPRESSION TAG	UNP Q9M8R4
E	238	GLU	ASP	CONFLICT	UNP Q9M8R4
E	389	HIS	-	EXPRESSION TAG	UNP Q9M8R4
F	238	GLU	ASP	CONFLICT	UNP Q9M8R4
F	389	HIS	-	EXPRESSION TAG	UNP Q9M8R4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	97	Total 97	O 97	0	0
2	B	81	Total 81	O 81	0	0
2	C	96	Total 96	O 96	0	0
2	D	100	Total 100	O 100	0	0
2	E	82	Total 82	O 82	0	0
2	F	86	Total 86	O 86	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.56Å 115.05Å 115.53Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 47.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-2.30) 95.9 (47.96-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.243 , 0.284 0.243 , 0.284	Depositor DCC
$R_{free}$ test set	11742 reflections (10.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 20.6	EDS
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.029 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	4 of 117426 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.23 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1795e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.39	0/2994	0.62	0/4075
1	B	0.37	0/2994	0.62	0/4075
1	C	0.39	0/2994	0.64	0/4075
1	D	0.39	0/2994	0.62	0/4075
1	E	0.38	0/2994	0.63	0/4075
1	F	0.39	0/2994	0.64	0/4075
All	All	0.38	0/17964	0.63	0/24450

There are no bond length outliers.

There are no bond angle outliers.

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	2924	0	2872	131	0
1	B	2924	0	2872	119	0
1	C	2924	0	2872	110	0
1	D	2924	0	2872	122	0
1	E	2924	0	2872	116	0
1	F	2924	0	2872	134	0
2	A	97	0	0	22	0
2	B	81	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	96	0	0	14	0
2	D	100	0	0	20	0
2	E	82	0	0	13	0
2	F	86	0	0	15	0
All	All	18086	0	17232	701	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 20.

All (701) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:197:ASN:HA	2:B:468:HOH:O	1.59	1.00
1:F:133:ASN:HA	2:F:460:HOH:O	1.66	0.95
1:B:20:VAL:HB	2:B:455:HOH:O	1.66	0.94
1:F:353:ILE:H	1:F:353:ILE:HD12	1.28	0.94
1:D:7:VAL:HG23	2:D:486:HOH:O	1.70	0.91
1:B:59:THR:HG22	2:B:450:HOH:O	1.73	0.89
1:E:79:LEU:HD21	1:E:105:LEU:HG	1.56	0.87
1:E:287:GLU:OE1	1:F:142:THR:HG21	1.74	0.87
1:F:72:ALA:HB3	2:F:463:HOH:O	1.73	0.87
1:C:389:HIS:HB3	2:C:457:HOH:O	1.75	0.87
1:F:21:MET:HE2	1:F:25:GLN:HG3	1.56	0.86
1:E:335:ALA:HA	1:F:98:LEU:HD13	1.58	0.85
1:A:30:PHE:HB2	2:A:434:HOH:O	1.76	0.84
1:D:239:ARG:HH21	1:D:260:THR:HG23	1.39	0.84
1:C:353:ILE:HD12	1:C:353:ILE:H	1.41	0.84
2:E:418:HOH:O	1:F:59:THR:HG21	1.77	0.83
1:B:15:MET:SD	1:B:20:VAL:HG21	2.20	0.82
1:B:37:VAL:HG21	1:B:74:PHE:HA	1.61	0.81
1:D:78:ASP:OD2	1:D:81:LYS:HD3	1.81	0.80
1:A:108:GLU:HA	1:A:111:ARG:NH1	1.97	0.80
1:A:16:GLU:OE2	1:A:259:HIS:HE1	1.64	0.80
1:B:210:ASP:OD2	1:B:259:HIS:HD2	1.66	0.79
1:B:55:CYS:HB3	2:B:445:HOH:O	1.82	0.79
1:E:215:VAL:HB	1:E:216:PRO:HD3	1.64	0.79
1:B:335:ALA:HA	1:C:98:LEU:HD13	1.65	0.78
1:D:21:MET:HG3	1:D:211:TYR:CZ	2.18	0.78
1:D:330:CYS:HB2	1:D:364:THR:HG21	1.64	0.77
1:E:37:VAL:HG21	1:E:74:PHE:HA	1.67	0.76
1:D:53:ASP:OD1	1:D:260:THR:HG22	1.86	0.76
1:B:215:VAL:HB	1:B:216:PRO:HD3	1.68	0.76
1:F:69:THR:HB	2:F:407:HOH:O	1.84	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:59:THR:HG21	2:C:413:HOH:O	1.84	0.75
1:F:150:ALA:O	2:F:460:HOH:O	2.03	0.75
1:A:142:THR:HG21	1:C:287:GLU:OE2	1.87	0.74
1:A:239:ARG:HH21	1:A:260:THR:HG23	1.51	0.74
1:A:61:PHE:HB3	2:A:454:HOH:O	1.88	0.74
1:D:235:LYS:H	1:D:238:GLU:HG3	1.52	0.74
1:E:210:ASP:OD2	1:E:259:HIS:HD2	1.71	0.73
1:C:179:PRO:HG2	2:C:414:HOH:O	1.86	0.73
1:F:16:GLU:OE2	1:F:259:HIS:HE1	1.71	0.73
1:D:79:LEU:H	1:D:79:LEU:HD12	1.53	0.73
1:A:32:ILE:HG13	2:A:434:HOH:O	1.88	0.73
1:A:22:VAL:HB	1:A:23:PRO:HD3	1.68	0.73
1:C:133:ASN:HA	1:C:151:GLY:O	1.88	0.72
1:D:203:LEU:HG	1:D:278:LEU:HD11	1.70	0.72
1:F:23:PRO:HD3	2:F:419:HOH:O	1.88	0.72
1:C:133:ASN:HB2	2:C:472:HOH:O	1.89	0.72
1:F:182:ILE:O	1:F:186:VAL:HG23	1.89	0.72
1:B:209:GLU:HB3	1:B:212:GLU:HB2	1.72	0.72
1:B:239:ARG:HH21	1:B:260:THR:HG23	1.52	0.72
1:B:237:GLY:HA3	1:D:235:LYS:NZ	2.03	0.72
1:B:235:LYS:O	1:B:238:GLU:HG2	1.89	0.72
1:E:248:GLU:HB3	2:E:464:HOH:O	1.90	0.71
1:E:208:MET:HG3	1:E:213:VAL:HG21	1.71	0.71
1:A:136:LYS:HA	1:A:153:LYS:HB2	1.72	0.71
1:D:208:MET:HG3	1:D:213:VAL:HG21	1.72	0.71
1:F:204:CYS:HA	1:F:208:MET:HE1	1.71	0.71
1:A:19:GLU:HB2	2:A:483:HOH:O	1.90	0.71
1:D:235:LYS:H	1:D:238:GLU:CG	2.03	0.71
1:C:203:LEU:HG	1:C:278:LEU:HD11	1.73	0.70
1:A:88:PRO:HB3	2:A:483:HOH:O	1.92	0.70
1:E:37:VAL:CG2	1:E:74:PHE:HA	2.21	0.70
1:F:37:VAL:HG21	1:F:74:PHE:HA	1.72	0.70
1:E:165:VAL:HG22	1:E:184:LEU:HD13	1.74	0.70
1:F:265:THR:HG22	2:F:434:HOH:O	1.91	0.69
1:D:16:GLU:OE2	1:D:259:HIS:HE1	1.74	0.69
1:A:15:MET:SD	1:A:20:VAL:HG21	2.32	0.69
1:F:154:TRP:HE1	1:F:156:GLU:HG2	1.57	0.69
1:E:120:CYS:SG	2:E:478:HOH:O	2.49	0.69
1:C:339:ASN:H	1:C:339:ASN:HD22	1.40	0.69
1:A:183:GLN:HE21	1:A:187:LYS:HE3	1.58	0.69
1:D:119:ILE:HD11	1:D:174:THR:O	1.93	0.68
1:F:389:HIS:HB3	2:F:466:HOH:O	1.91	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:182:ILE:O	1:A:186:VAL:HG23	1.94	0.68
1:B:235:LYS:H	1:B:238:GLU:HG3	1.58	0.68
1:A:200:ILE:HD12	1:A:200:ILE:N	2.09	0.68
1:D:182:ILE:O	1:D:186:VAL:HG23	1.93	0.68
1:A:282:GLY:HA3	1:A:313:CYS:HB3	1.76	0.67
1:B:158:ILE:HD12	1:B:159:THR:N	2.09	0.67
1:F:165:VAL:HG23	1:F:184:LEU:HD13	1.77	0.67
1:F:203:LEU:HG	1:F:278:LEU:HD11	1.77	0.67
1:D:313:CYS:SG	2:D:498:HOH:O	2.50	0.67
1:E:103:VAL:O	1:E:107:LYS:HG3	1.94	0.67
1:B:235:LYS:H	1:B:238:GLU:CG	2.07	0.67
1:A:256:LYS:HG2	2:A:402:HOH:O	1.95	0.67
1:E:30:PHE:CZ	1:E:223:LEU:HD13	2.30	0.66
1:D:253:TYR:O	1:E:91:ARG:NH2	2.28	0.66
1:F:21:MET:CE	1:F:25:GLN:HG3	2.25	0.66
1:F:235:LYS:H	1:F:238:GLU:HG3	1.61	0.66
1:B:165:VAL:CG2	1:B:184:LEU:HD13	2.25	0.66
1:B:282:GLY:HA3	1:B:313:CYS:HB3	1.78	0.66
1:C:182:ILE:O	1:C:186:VAL:HG23	1.96	0.66
1:A:53:ASP:OD1	1:A:260:THR:HG22	1.96	0.66
1:B:22:VAL:HB	1:B:23:PRO:HD3	1.78	0.66
1:F:208:MET:HE2	1:F:281:PRO:HB2	1.77	0.65
1:D:218:GLN:HG2	2:D:463:HOH:O	1.95	0.65
1:E:182:ILE:O	1:E:186:VAL:HG23	1.97	0.65
1:A:119:ILE:HD11	1:A:174:THR:O	1.97	0.65
1:E:350:PRO:HB2	2:E:461:HOH:O	1.96	0.65
1:F:120:CYS:SG	2:F:479:HOH:O	2.53	0.65
1:F:213:VAL:HG13	1:F:214:LYS:N	2.11	0.65
1:C:23:PRO:HD3	2:C:437:HOH:O	1.96	0.64
1:C:355:ARG:HB3	2:C:453:HOH:O	1.96	0.64
1:B:235:LYS:N	1:B:238:GLU:HG3	2.13	0.64
1:B:237:GLY:HA3	1:D:235:LYS:HZ2	1.59	0.64
1:A:62:GLU:OE1	1:A:91:ARG:HD3	1.98	0.64
1:D:3:ASN:O	1:D:4:SER:HB2	1.96	0.64
1:E:5:ARG:NH2	1:E:189:LEU:O	2.31	0.64
1:B:330:CYS:HB2	1:B:364:THR:HG21	1.79	0.64
1:C:37:VAL:HG22	1:C:74:PHE:N	2.13	0.64
1:D:320:ALA:HB2	1:D:325:LEU:HD12	1.77	0.64
1:D:355:ARG:HA	1:D:373:GLU:OE1	1.98	0.64
1:F:333:TYR:O	1:F:336:VAL:HG22	1.97	0.64
1:C:209:GLU:HB3	1:C:212:GLU:HB2	1.80	0.64
1:C:37:VAL:HG13	1:C:74:PHE:HD1	1.63	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:169:LEU:HG	2:D:457:HOH:O	1.98	0.64
1:F:21:MET:CE	1:F:24:PHE:HD2	2.11	0.64
1:A:120:CYS:SG	2:A:488:HOH:O	2.52	0.63
1:F:154:TRP:NE1	1:F:156:GLU:HG2	2.12	0.63
1:A:20:VAL:HG22	1:A:88:PRO:HB3	1.80	0.63
1:C:21:MET:HG3	1:C:211:TYR:CZ	2.33	0.63
1:C:330:CYS:HA	1:C:348:LEU:HD12	1.80	0.63
1:E:355:ARG:HD2	2:E:429:HOH:O	1.97	0.63
1:C:16:GLU:OE2	1:C:259:HIS:HE1	1.80	0.63
1:D:117:ALA:HB1	1:D:181:PHE:CZ	2.33	0.63
1:A:19:GLU:CB	2:A:483:HOH:O	2.43	0.63
1:A:284:ARG:NH1	1:B:60:TYR:O	2.24	0.63
1:F:204:CYS:HA	1:F:208:MET:CE	2.29	0.63
1:A:78:ASP:OD2	1:A:81:LYS:HD3	1.99	0.62
1:C:120:CYS:SG	2:C:490:HOH:O	2.46	0.62
1:C:15:MET:SD	1:C:20:VAL:HG21	2.39	0.62
1:C:305:SER:O	1:C:306:GLU:HB2	1.99	0.62
1:F:313:CYS:HA	1:F:366:ALA:O	1.99	0.62
1:F:140:TYR:HD2	1:F:142:THR:HB	1.65	0.62
1:E:5:ARG:HH11	1:E:389:HIS:H	1.48	0.62
1:D:77:VAL:HG13	1:D:82:TYR:HE1	1.64	0.62
1:F:330:CYS:HA	1:F:348:LEU:HD12	1.80	0.62
1:A:333:TYR:CD1	1:A:334:PRO:HD2	2.35	0.61
1:F:353:ILE:H	1:F:353:ILE:CD1	2.04	0.61
1:A:74:PHE:O	1:A:76:GLU:N	2.34	0.61
1:B:209:GLU:O	1:B:213:VAL:HG23	2.00	0.61
1:E:15:MET:SD	1:E:20:VAL:HG21	2.41	0.61
1:F:37:VAL:HB	2:F:463:HOH:O	1.99	0.61
1:B:312:ILE:HD11	1:B:367:ALA:O	1.99	0.61
1:C:282:GLY:HA3	1:C:313:CYS:HB3	1.82	0.61
1:D:3:ASN:HB2	1:D:31:GLY:O	2.01	0.61
1:A:77:VAL:HB	2:A:440:HOH:O	2.01	0.61
1:A:208:MET:SD	1:A:213:VAL:HG21	2.41	0.61
1:A:60:TYR:O	1:C:284:ARG:NH1	2.34	0.61
1:C:170:ILE:HD13	1:C:185:PHE:HA	1.82	0.61
1:E:5:ARG:NH1	1:E:389:HIS:H	1.99	0.60
1:E:338:LEU:CD2	1:E:342:LEU:HD12	2.31	0.60
1:F:200:ILE:HD12	1:F:200:ILE:N	2.16	0.60
1:C:165:VAL:CG2	1:C:184:LEU:HD13	2.32	0.60
1:D:255:GLU:OE2	1:D:284:ARG:HD3	2.01	0.60
1:E:301:GLU:HA	1:E:304:ASN:ND2	2.16	0.60
1:A:124:LEU:CD2	1:A:143:VAL:HG13	2.32	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:331:THR:OG1	1:B:350:PRO:HG3	2.02	0.60
1:B:53:ASP:OD1	1:B:260:THR:HG22	2.02	0.60
1:A:77:VAL:HG13	1:A:82:TYR:HE1	1.66	0.59
1:C:9:ILE:HG12	1:C:86:VAL:HB	1.83	0.59
1:B:337:LYS:HE2	1:B:347:TRP:CD1	2.38	0.59
1:D:124:LEU:HD23	1:D:143:VAL:HG13	1.83	0.59
1:B:200:ILE:CD1	1:B:220:LEU:HD13	2.33	0.59
1:C:213:VAL:HG13	1:C:214:LYS:N	2.18	0.59
1:D:358:THR:OG1	1:D:377:GLN:NE2	2.36	0.59
1:D:73:THR:HG22	1:D:74:PHE:O	2.02	0.59
1:B:64:ARG:HD2	2:B:425:HOH:O	2.03	0.59
1:B:313:CYS:HA	1:B:366:ALA:O	2.02	0.59
1:B:350:PRO:HB3	1:B:366:ALA:HB2	1.83	0.59
1:C:187:LYS:HG3	2:C:443:HOH:O	2.03	0.59
1:F:274:SER:O	1:F:275:TYR:HB2	2.03	0.59
1:B:30:PHE:CZ	1:B:223:LEU:HD13	2.37	0.59
1:B:226:GLN:HE21	1:B:226:GLN:HA	1.68	0.59
1:F:106:VAL:HG21	1:F:125:ILE:CG2	2.33	0.59
1:C:62:GLU:OE1	1:C:91:ARG:HD3	2.03	0.58
1:C:157:PRO:HA	1:C:162:VAL:HG21	1.85	0.58
1:F:3:ASN:O	1:F:4:SER:HB2	2.03	0.58
1:C:235:LYS:H	1:C:238:GLU:HG3	1.69	0.58
1:A:265:THR:HG23	2:A:460:HOH:O	2.04	0.58
1:A:77:VAL:HG13	1:A:82:TYR:CE1	2.38	0.58
1:D:22:VAL:HB	1:D:23:PRO:HD3	1.85	0.58
1:B:165:VAL:HG21	1:B:184:LEU:HD13	1.86	0.57
1:F:165:VAL:CG2	1:F:184:LEU:HD13	2.35	0.57
1:B:209:GLU:HG3	1:B:212:GLU:H	1.70	0.57
1:C:106:VAL:HG21	1:C:125:ILE:CG2	2.34	0.57
1:D:91:ARG:NH2	1:F:253:TYR:O	2.37	0.57
1:B:285:ALA:HB3	1:B:286:PRO:HD3	1.85	0.57
1:A:209:GLU:HG3	1:A:212:GLU:H	1.69	0.57
1:D:209:GLU:O	1:D:213:VAL:HG23	2.05	0.57
1:B:204:CYS:HA	1:B:208:MET:CE	2.34	0.57
1:C:255:GLU:OE2	1:C:284:ARG:NH2	2.38	0.57
1:A:353:ILE:HG12	2:A:425:HOH:O	2.03	0.57
1:B:16:GLU:OE2	1:B:259:HIS:HE1	1.88	0.57
1:F:209:GLU:HG3	1:F:212:GLU:H	1.70	0.57
1:A:235:LYS:O	1:A:238:GLU:HG2	2.05	0.56
1:A:66:HIS:CD2	1:A:244:ILE:HG23	2.40	0.56
1:C:3:ASN:O	1:C:4:SER:HB2	2.05	0.56
1:B:208:MET:SD	1:B:213:VAL:HG21	2.45	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:123:GLN:N	1:F:123:GLN:OE1	2.39	0.56
1:B:193:ILE:HG12	1:B:386:VAL:HG22	1.87	0.56
1:A:117:ALA:HB1	1:A:181:PHE:CZ	2.41	0.56
1:E:10:LEU:HD11	1:E:102:VAL:HG13	1.87	0.56
1:E:4:SER:O	1:E:5:ARG:HD3	2.06	0.56
1:D:335:ALA:HA	1:E:98:LEU:HD22	1.87	0.56
1:D:210:ASP:OD2	1:D:259:HIS:HD2	1.88	0.56
1:E:326:LYS:HD3	1:E:344:GLY:HA3	1.88	0.56
1:B:235:LYS:N	1:B:238:GLU:CG	2.69	0.56
1:C:333:TYR:O	1:C:336:VAL:HG22	2.06	0.55
1:D:200:ILE:HD12	1:D:220:LEU:HD13	1.88	0.55
1:D:193:ILE:HG12	1:D:386:VAL:HG22	1.88	0.55
1:A:123:GLN:HG2	1:A:139:ALA:HB2	1.88	0.55
1:B:230:VAL:HG21	1:B:270:LEU:HD11	1.88	0.55
1:C:223:LEU:HG	1:C:384:ILE:HG21	1.89	0.55
1:D:239:ARG:NH2	1:D:260:THR:HG23	2.17	0.55
1:E:338:LEU:HD21	1:E:342:LEU:HD12	1.87	0.55
1:B:140:TYR:HD2	1:B:142:THR:HG22	1.71	0.55
1:B:367:ALA:HB3	1:B:369:PRO:HD2	1.89	0.55
1:D:165:VAL:HG22	1:D:184:LEU:HD13	1.88	0.55
1:D:208:MET:CG	1:D:213:VAL:HG21	2.37	0.55
1:D:217:PHE:O	1:D:221:GLN:HG3	2.06	0.55
1:F:37:VAL:CG2	1:F:74:PHE:HA	2.36	0.55
1:F:37:VAL:HG13	1:F:74:PHE:HD1	1.72	0.55
1:A:59:THR:HG22	1:A:60:TYR:H	1.72	0.55
1:E:147:LEU:HD23	1:E:154:TRP:CZ3	2.42	0.55
1:A:204:CYS:HA	1:A:208:MET:HE3	1.89	0.54
1:E:209:GLU:O	1:E:213:VAL:HG23	2.07	0.54
1:B:184:LEU:HD23	2:B:442:HOH:O	2.07	0.54
1:B:294:HIS:O	1:B:298:ILE:HG13	2.07	0.54
1:B:37:VAL:CG2	1:B:74:PHE:HA	2.35	0.54
1:B:280:ILE:HB	1:B:311:SER:HB2	1.89	0.54
1:E:235:LYS:H	1:E:238:GLU:CG	2.20	0.54
1:F:349:GLU:CD	1:F:350:PRO:HD2	2.28	0.54
1:F:55:CYS:HB3	2:F:415:HOH:O	2.07	0.54
1:E:206:ASP:OD2	1:F:58:GLN:HG3	2.07	0.54
1:B:212:GLU:HG3	1:B:368:TRP:HB3	1.89	0.54
1:F:355:ARG:HH21	1:F:355:ARG:HG2	1.71	0.54
1:C:119:ILE:HD11	1:C:174:THR:O	2.07	0.54
1:E:338:LEU:HD12	1:F:128:ALA:HB2	1.88	0.54
1:A:10:LEU:O	1:A:88:PRO:HD2	2.08	0.54
1:F:64:ARG:HD3	2:F:437:HOH:O	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:119:ILE:HG13	1:A:172:ALA:HB3	1.89	0.54
1:F:213:VAL:HG13	1:F:214:LYS:H	1.73	0.54
1:F:21:MET:HE3	1:F:24:PHE:HD2	1.72	0.54
1:D:16:GLU:O	1:D:20:VAL:HG23	2.08	0.54
1:F:233:GLU:O	1:F:233:GLU:HG3	2.07	0.54
1:C:210:ASP:OD2	1:C:259:HIS:HD2	1.90	0.53
1:D:212:GLU:HA	1:D:371:HIS:HE2	1.73	0.53
1:D:353:ILE:HD12	1:D:354:ASP:H	1.72	0.53
1:A:15:MET:CG	1:A:20:VAL:HG21	2.39	0.53
1:A:165:VAL:CG2	1:A:184:LEU:HD13	2.38	0.53
1:F:263:LEU:H	1:F:263:LEU:HD22	1.72	0.53
1:B:200:ILE:HD12	1:B:220:LEU:HD13	1.89	0.53
1:B:204:CYS:HA	1:B:208:MET:HE1	1.90	0.53
1:D:15:MET:HG3	1:D:20:VAL:HG21	1.89	0.53
1:F:235:LYS:N	1:F:238:GLU:HG3	2.22	0.53
1:E:19:GLU:O	1:E:88:PRO:HB3	2.09	0.53
1:D:201:LEU:HD22	1:D:270:LEU:HD21	1.90	0.53
1:E:52:HIS:HE1	1:E:62:GLU:OE1	1.91	0.53
1:B:62:GLU:OE2	1:B:91:ARG:NH1	2.42	0.53
1:D:200:ILE:CD1	1:D:220:LEU:HD13	2.39	0.53
1:D:62:GLU:OE2	1:D:91:ARG:NH1	2.42	0.53
1:D:287:GLU:OE1	1:E:142:THR:HG21	2.08	0.53
1:A:10:LEU:HD11	1:A:102:VAL:HG13	1.90	0.53
1:C:235:LYS:N	1:C:238:GLU:HG3	2.24	0.53
1:C:271:VAL:HG13	1:C:274:SER:OG	2.09	0.53
1:A:25:GLN:NE2	1:A:371:HIS:ND1	2.55	0.53
1:E:293:GLU:OE1	1:E:293:GLU:HA	2.09	0.52
1:A:118:SER:HB3	1:A:123:GLN:OE1	2.09	0.52
1:D:8:LEU:O	1:D:85:LEU:HD12	2.09	0.52
1:C:69:THR:HG23	2:C:486:HOH:O	2.09	0.52
1:C:24:PHE:O	1:C:28:GLN:HG3	2.09	0.52
1:D:215:VAL:HB	1:D:216:PRO:HD3	1.91	0.52
1:F:255:GLU:OE2	1:F:284:ARG:HD3	2.09	0.52
1:B:240:CYS:SG	1:B:263:LEU:HD21	2.50	0.52
1:C:143:VAL:HG12	1:C:147:LEU:CD2	2.40	0.52
1:E:97:ALA:C	1:E:98:LEU:HD12	2.30	0.52
1:F:282:GLY:HA3	1:F:313:CYS:HB3	1.92	0.52
1:C:209:GLU:HG3	1:C:212:GLU:H	1.74	0.52
1:D:32:ILE:HG23	2:D:486:HOH:O	2.09	0.52
1:E:312:ILE:HD11	1:E:367:ALA:O	2.10	0.52
1:E:27:LEU:HD22	1:E:32:ILE:HD12	1.92	0.52
1:F:157:PRO:HA	1:F:162:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:143:VAL:HG12	1:F:143:VAL:O	2.10	0.52
1:E:140:TYR:HD2	1:E:142:THR:HB	1.75	0.52
1:E:301:GLU:HA	1:E:304:ASN:HD22	1.75	0.52
1:E:329:LYS:HG3	2:E:445:HOH:O	2.09	0.52
1:C:312:ILE:HD11	1:C:367:ALA:O	2.10	0.52
1:E:285:ALA:HB3	1:E:286:PRO:HD3	1.92	0.51
1:F:329:LYS:O	1:F:330:CYS:HB3	2.09	0.51
1:A:235:LYS:H	1:A:238:GLU:CG	2.23	0.51
1:B:348:LEU:HD13	1:B:357:PHE:CD2	2.45	0.51
1:F:293:GLU:HA	1:F:293:GLU:OE1	2.08	0.51
1:A:25:GLN:HE21	1:A:215:VAL:HG21	1.75	0.51
1:A:73:THR:HG22	1:A:74:PHE:O	2.10	0.51
1:B:20:VAL:HG22	1:B:88:PRO:HG3	1.93	0.51
1:B:51:VAL:HG13	1:B:259:HIS:CD2	2.44	0.51
1:E:204:CYS:HA	1:E:208:MET:CE	2.41	0.51
1:E:249:GLY:N	2:E:464:HOH:O	2.43	0.51
1:E:336:VAL:O	1:E:336:VAL:HG12	2.09	0.51
1:C:265:THR:HG23	2:C:419:HOH:O	2.11	0.51
1:E:37:VAL:CG2	1:E:74:PHE:CA	2.88	0.51
1:D:208:MET:SD	1:D:213:VAL:HG21	2.51	0.51
1:D:77:VAL:HB	2:D:470:HOH:O	2.11	0.51
1:A:98:LEU:HD21	1:C:337:LYS:HB3	1.93	0.51
1:D:353:ILE:HD12	1:D:354:ASP:N	2.25	0.51
1:E:123:GLN:N	1:E:123:GLN:OE1	2.43	0.51
1:B:37:VAL:CG2	1:B:74:PHE:CA	2.89	0.51
1:C:54:PHE:HB3	2:C:458:HOH:O	2.09	0.51
1:F:77:VAL:HG13	1:F:82:TYR:HE1	1.75	0.51
1:E:294:HIS:O	1:E:298:ILE:HG13	2.10	0.50
1:E:38:CYS:HB3	1:E:70:LEU:HD11	1.93	0.50
1:B:336:VAL:HG12	1:B:336:VAL:O	2.11	0.50
1:E:200:ILE:CD1	1:E:220:LEU:HD13	2.41	0.50
1:A:8:LEU:HB2	1:A:82:TYR:CD2	2.46	0.50
1:B:271:VAL:HG13	1:B:271:VAL:O	2.11	0.50
1:B:271:VAL:HG22	1:B:273:SER:HB2	1.93	0.50
1:C:368:TRP:N	1:C:369:PRO:CD	2.75	0.50
1:D:285:ALA:N	1:D:286:PRO:CD	2.74	0.50
1:A:235:LYS:H	1:A:238:GLU:HG3	1.77	0.50
1:A:332:ALA:CB	1:A:336:VAL:HG23	2.41	0.50
1:D:372:PRO:HD2	2:D:425:HOH:O	2.12	0.50
1:F:235:LYS:H	1:F:238:GLU:CG	2.22	0.50
1:B:91:ARG:NH2	2:B:453:HOH:O	2.44	0.50
1:C:215:VAL:HB	1:C:216:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:135:ARG:HD2	1:E:166:ASP:OD2	2.12	0.50
1:C:235:LYS:H	1:C:238:GLU:CG	2.23	0.50
1:F:197:ASN:HB2	2:F:404:HOH:O	2.12	0.50
1:A:313:CYS:HA	1:A:366:ALA:O	2.11	0.50
1:B:123:GLN:OE1	1:B:123:GLN:N	2.45	0.50
1:C:353:ILE:CD1	1:C:353:ILE:H	2.08	0.50
1:F:5:ARG:HH22	1:F:389:HIS:CD2	2.30	0.50
1:B:91:ARG:HH11	1:B:91:ARG:HG3	1.77	0.50
1:D:120:CYS:SG	2:D:493:HOH:O	2.55	0.50
1:A:135:ARG:HD2	1:A:166:ASP:OD2	2.12	0.49
1:B:389:HIS:HB2	2:B:461:HOH:O	2.10	0.49
1:C:332:ALA:HB1	1:C:336:VAL:CG2	2.42	0.49
1:E:16:GLU:HB3	1:E:19:GLU:HB2	1.94	0.49
1:F:106:VAL:HG21	1:F:125:ILE:HG22	1.92	0.49
1:A:88:PRO:CA	2:A:483:HOH:O	2.60	0.49
1:C:293:GLU:HA	1:C:293:GLU:OE1	2.12	0.49
1:A:16:GLU:OE2	1:A:259:HIS:CE1	2.56	0.49
1:E:77:VAL:HG13	1:E:82:TYR:HE1	1.76	0.49
1:C:270:LEU:HD13	1:C:271:VAL:N	2.27	0.49
1:E:61:PHE:HB3	2:E:459:HOH:O	2.11	0.49
1:A:367:ALA:HB3	1:A:369:PRO:HD2	1.95	0.49
1:D:256:LYS:HG2	2:D:407:HOH:O	2.13	0.49
1:F:105:LEU:C	1:F:105:LEU:HD23	2.33	0.49
1:C:199:ARG:HB2	1:C:275:TYR:HA	1.94	0.49
1:D:148:VAL:C	1:D:150:ALA:H	2.15	0.49
1:F:205:GLY:HA2	1:F:231:CYS:SG	2.53	0.49
1:C:83:ASP:O	1:C:115:PRO:HD2	2.12	0.49
1:E:355:ARG:HG3	1:E:356:CYS:N	2.28	0.49
1:F:269:ASP:N	1:F:269:ASP:OD2	2.45	0.49
1:C:274:SER:O	1:C:275:TYR:HB2	2.12	0.49
1:A:92:ALA:N	1:A:93:PRO:CD	2.76	0.49
1:B:314:HIS:HA	1:B:336:VAL:HG21	1.93	0.49
1:A:98:LEU:HD22	1:C:334:PRO:O	2.13	0.48
1:D:171:THR:HG23	2:D:457:HOH:O	2.13	0.48
1:D:256:LYS:HG3	1:D:257:PRO:HD2	1.94	0.48
1:E:351:ASP:N	2:E:461:HOH:O	2.46	0.48
1:F:154:TRP:HE1	1:F:156:GLU:CG	2.22	0.48
1:B:336:VAL:HA	1:B:339:ASN:HD22	1.78	0.48
1:C:178:HIS:N	1:C:179:PRO:HD2	2.28	0.48
1:D:32:ILE:CG2	2:D:486:HOH:O	2.60	0.48
1:E:337:LYS:HE2	1:E:347:TRP:CD1	2.48	0.48
1:A:15:MET:HG3	1:A:20:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:LEU:O	1:A:85:LEU:HD12	2.13	0.48
1:D:331:THR:OG1	1:D:350:PRO:HB3	2.13	0.48
1:F:212:GLU:OE1	1:F:313:CYS:HB2	2.13	0.48
1:A:58:GLN:HG3	1:C:206:ASP:OD2	2.13	0.48
1:B:16:GLU:HB3	1:B:19:GLU:HB2	1.94	0.48
1:D:66:HIS:CD2	1:D:244:ILE:HG23	2.48	0.48
1:C:353:ILE:HD12	1:C:353:ILE:N	2.20	0.48
1:D:55:CYS:HB3	2:D:442:HOH:O	2.13	0.48
1:D:64:ARG:NH1	2:D:429:HOH:O	2.45	0.48
1:E:157:PRO:HA	1:E:162:VAL:HG21	1.95	0.48
1:E:298:ILE:HG12	2:E:474:HOH:O	2.13	0.48
1:A:332:ALA:HB1	1:A:336:VAL:CG2	2.44	0.48
1:B:180:GLU:O	1:B:184:LEU:HG	2.14	0.48
1:D:271:VAL:HG13	1:D:274:SER:OG	2.14	0.48
1:F:206:ASP:OD1	1:F:241:PRO:HD2	2.13	0.48
1:E:274:SER:O	1:E:275:TYR:HB2	2.13	0.48
1:A:255:GLU:OE1	1:A:284:ARG:NH2	2.46	0.48
1:A:320:ALA:HB2	1:A:325:LEU:HD12	1.95	0.48
1:A:316:GLN:OE1	1:A:316:GLN:N	2.44	0.47
1:F:353:ILE:HD12	1:F:353:ILE:N	2.12	0.47
1:A:358:THR:OG1	1:A:377:GLN:NE2	2.48	0.47
1:D:316:GLN:N	1:D:316:GLN:OE1	2.47	0.47
1:D:92:ALA:N	1:D:93:PRO:CD	2.77	0.47
1:E:117:ALA:HA	1:E:170:ILE:O	2.14	0.47
1:A:136:LYS:O	1:A:137:CYS:HB3	2.14	0.47
1:C:37:VAL:CG2	1:C:74:PHE:N	2.78	0.47
1:F:77:VAL:HG13	1:F:82:TYR:CE1	2.49	0.47
1:B:368:TRP:N	1:B:369:PRO:CD	2.78	0.47
1:C:339:ASN:HD22	1:C:339:ASN:N	2.09	0.47
1:D:201:LEU:HD21	1:D:270:LEU:HD11	1.96	0.47
1:B:280:ILE:HB	1:B:311:SER:CB	2.45	0.47
1:C:313:CYS:HA	1:C:366:ALA:O	2.15	0.47
1:D:223:LEU:HG	1:D:384:ILE:HG21	1.95	0.47
1:D:64:ARG:NH2	2:D:446:HOH:O	2.48	0.47
1:E:144:GLY:O	1:E:148:VAL:HG23	2.14	0.47
1:A:117:ALA:HB1	1:A:181:PHE:CE1	2.50	0.47
1:D:310:ALA:HB1	1:D:374:PHE:CZ	2.50	0.47
1:E:100:ALA:HB3	2:E:437:HOH:O	2.14	0.47
1:E:158:ILE:HG13	1:E:159:THR:HG23	1.96	0.47
1:A:25:GLN:NE2	1:A:215:VAL:HG21	2.30	0.47
1:B:37:VAL:HG21	1:B:74:PHE:CA	2.38	0.47
1:E:140:TYR:CD2	1:E:142:THR:HB	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:59:THR:HG22	1:E:60:TYR:H	1.80	0.47
1:F:123:GLN:HG2	1:F:139:ALA:HB2	1.95	0.47
1:A:208:MET:HG3	1:A:213:VAL:HG21	1.97	0.47
1:F:263:LEU:N	1:F:263:LEU:HD22	2.30	0.47
1:F:199:ARG:HB2	1:F:275:TYR:HA	1.97	0.46
1:B:83:ASP:O	1:B:115:PRO:HD2	2.15	0.46
1:C:143:VAL:HG12	1:C:147:LEU:HD22	1.97	0.46
1:D:299:VAL:O	1:D:303:MET:HG2	2.15	0.46
1:D:7:VAL:HG12	1:D:8:LEU:N	2.31	0.46
1:E:337:LYS:HB3	1:F:98:LEU:HD21	1.98	0.46
1:D:204:CYS:HA	1:D:208:MET:HE3	1.97	0.46
1:D:6:THR:HG22	1:D:82:TYR:CD2	2.50	0.46
1:E:204:CYS:HA	1:E:208:MET:HE3	1.98	0.46
1:A:208:MET:HE2	1:A:213:VAL:HG22	1.97	0.46
1:A:74:PHE:O	1:A:75:ASP:C	2.54	0.46
1:B:106:VAL:HG21	1:B:125:ILE:CG2	2.45	0.46
1:B:62:GLU:OE1	1:B:91:ARG:NH1	2.48	0.46
1:D:313:CYS:HB3	2:D:498:HOH:O	2.15	0.46
1:A:200:ILE:CD1	1:A:200:ILE:N	2.78	0.46
1:B:226:GLN:HG2	2:B:441:HOH:O	2.15	0.46
1:C:185:PHE:CE2	1:C:189:LEU:HD11	2.49	0.46
1:D:153:LYS:HE2	2:D:482:HOH:O	2.15	0.46
1:E:235:LYS:H	1:E:238:GLU:HG2	1.81	0.46
1:A:183:GLN:HE21	1:A:187:LYS:CE	2.27	0.46
1:B:201:LEU:HB2	1:B:275:TYR:CD2	2.50	0.46
1:C:355:ARG:HG3	1:C:373:GLU:OE1	2.15	0.46
1:D:124:LEU:CD2	1:D:143:VAL:HG13	2.45	0.46
1:A:238:GLU:HB2	1:A:263:LEU:HD23	1.97	0.46
1:E:62:GLU:OE2	1:E:91:ARG:NH1	2.48	0.46
1:B:107:LYS:O	1:B:110:SER:HB3	2.16	0.46
1:B:239:ARG:HE	1:B:260:THR:CG2	2.29	0.46
1:D:9:ILE:HG12	1:D:86:VAL:HB	1.98	0.46
1:D:7:VAL:CG1	1:D:8:LEU:N	2.79	0.46
1:F:245:HIS:CD2	1:F:255:GLU:HG3	2.51	0.46
1:A:271:VAL:HG13	1:A:271:VAL:O	2.15	0.46
1:C:263:LEU:N	1:C:263:LEU:HD22	2.30	0.46
1:E:270:LEU:HD13	1:E:271:VAL:N	2.31	0.46
1:F:37:VAL:CG2	1:F:74:PHE:CA	2.94	0.46
1:F:92:ALA:N	1:F:93:PRO:CD	2.79	0.46
1:C:271:VAL:O	1:C:271:VAL:HG13	2.16	0.45
1:E:200:ILE:HD13	1:E:220:LEU:HD13	1.98	0.45
1:A:123:GLN:N	1:A:123:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:137:CYS:HA	1:B:164:VAL:HG11	1.98	0.45
1:D:206:ASP:OD1	1:D:241:PRO:HD2	2.17	0.45
1:E:209:GLU:HG2	1:E:212:GLU:OE2	2.16	0.45
1:E:16:GLU:OE2	1:E:259:HIS:HE1	1.99	0.45
1:A:88:PRO:CB	2:A:483:HOH:O	2.56	0.45
1:B:259:HIS:CD2	1:B:259:HIS:H	2.35	0.45
1:E:6:THR:HG22	1:E:82:TYR:CD2	2.52	0.45
1:C:332:ALA:HB1	1:C:336:VAL:HG21	1.99	0.45
1:C:65:GLY:HA2	1:C:244:ILE:HD13	1.98	0.45
1:E:98:LEU:HD12	1:E:98:LEU:N	2.31	0.45
1:F:235:LYS:N	1:F:238:GLU:CG	2.80	0.45
1:D:142:THR:HA	1:F:291:LEU:HD11	1.99	0.45
1:B:328:ARG:HD2	2:B:418:HOH:O	2.15	0.45
1:D:136:LYS:HA	1:D:153:LYS:HB2	1.97	0.45
1:D:337:LYS:HG3	1:D:347:TRP:CD2	2.52	0.45
1:D:370:GLY:HA2	2:D:425:HOH:O	2.17	0.45
1:F:213:VAL:CG1	1:F:214:LYS:N	2.77	0.45
1:F:10:LEU:O	1:F:88:PRO:HD2	2.16	0.45
1:F:236:ALA:N	1:F:266:ASN:OD1	2.49	0.45
1:B:285:ALA:N	1:B:286:PRO:CD	2.79	0.45
1:B:284:ARG:NH1	1:C:60:TYR:O	2.43	0.45
1:D:235:LYS:H	1:D:238:GLU:HG2	1.80	0.45
1:A:13:ASP:OD1	1:A:48:PRO:HD2	2.17	0.45
1:C:123:GLN:HG2	1:C:139:ALA:HB2	1.99	0.45
1:D:10:LEU:HD11	1:D:102:VAL:HG13	1.98	0.45
1:D:79:LEU:H	1:D:79:LEU:CD1	2.24	0.45
1:C:165:VAL:HG23	1:C:184:LEU:HD13	1.99	0.45
1:C:296:LEU:HD22	1:C:322:ALA:HB2	1.98	0.45
1:D:8:LEU:HD12	1:D:35:HIS:O	2.16	0.45
1:E:314:HIS:HA	1:E:336:VAL:HG21	1.99	0.45
1:D:303:MET:HG3	1:D:324:VAL:HG11	1.97	0.45
1:F:367:ALA:HB3	1:F:369:PRO:HD2	1.99	0.45
1:A:208:MET:CG	1:A:213:VAL:HG21	2.48	0.44
1:C:10:LEU:O	1:C:88:PRO:HD2	2.16	0.44
1:C:311:SER:O	1:C:364:THR:HA	2.18	0.44
1:F:355:ARG:NH2	1:F:355:ARG:HG2	2.31	0.44
1:B:199:ARG:HD3	1:B:274:SER:O	2.17	0.44
1:C:16:GLU:O	1:C:20:VAL:HG23	2.18	0.44
1:C:367:ALA:HB3	1:C:369:PRO:HD2	1.99	0.44
1:D:143:VAL:HG12	1:D:147:LEU:HD22	1.99	0.44
1:E:367:ALA:HB3	1:E:369:PRO:HD2	1.99	0.44
1:D:13:ASP:OD2	1:F:251:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:223:LEU:HG	1:F:384:ILE:HG21	1.98	0.44
1:B:26:ALA:O	1:B:29:ALA:HB3	2.17	0.44
1:D:310:ALA:HB1	1:D:374:PHE:CE1	2.52	0.44
1:E:106:VAL:HG21	1:E:125:ILE:HG22	1.99	0.44
1:E:271:VAL:HG13	1:E:271:VAL:O	2.18	0.44
1:F:170:ILE:HD13	1:F:185:PHE:HA	1.99	0.44
1:F:21:MET:HE3	1:F:24:PHE:CD2	2.51	0.44
1:A:23:PRO:HG2	2:A:449:HOH:O	2.16	0.44
1:A:386:VAL:HG12	1:A:388:PHE:CE1	2.52	0.44
1:B:30:PHE:N	1:B:30:PHE:CD2	2.85	0.44
1:B:206:ASP:OD2	1:C:58:GLN:HG3	2.18	0.44
1:F:136:LYS:HA	1:F:153:LYS:HB2	1.99	0.44
1:A:332:ALA:HB1	1:A:336:VAL:HG23	1.98	0.44
1:B:276:ASP:O	1:B:308:PRO:HD2	2.18	0.44
1:B:158:ILE:CD1	1:B:159:THR:HG23	2.48	0.44
1:C:223:LEU:HA	1:C:223:LEU:HD12	1.82	0.44
1:E:30:PHE:CE2	1:E:223:LEU:HD13	2.53	0.44
1:E:55:CYS:HB3	2:E:459:HOH:O	2.18	0.44
1:A:347:TRP:CZ2	1:A:350:PRO:HD3	2.52	0.44
1:B:135:ARG:NH2	1:B:166:ASP:O	2.51	0.44
1:C:204:CYS:SG	1:C:208:MET:HE1	2.58	0.44
1:C:235:LYS:N	1:C:238:GLU:CG	2.81	0.44
1:C:337:LYS:HA	1:C:347:TRP:CZ3	2.53	0.44
1:E:15:MET:HG3	1:E:20:VAL:HG21	1.99	0.44
1:A:271:VAL:HG13	1:A:274:SER:OG	2.18	0.44
1:B:136:LYS:O	1:B:137:CYS:HB3	2.17	0.44
1:B:200:ILE:HD13	1:B:220:LEU:HD13	1.98	0.44
1:C:213:VAL:HG13	1:C:214:LYS:H	1.80	0.44
1:D:333:TYR:CD1	1:D:334:PRO:HD2	2.52	0.44
1:E:353:ILE:HA	2:E:461:HOH:O	2.17	0.44
1:E:310:ALA:HA	1:E:363:VAL:O	2.18	0.44
1:F:66:HIS:CE1	1:F:244:ILE:HG23	2.52	0.44
1:A:27:LEU:O	2:A:434:HOH:O	2.21	0.44
1:F:303:MET:HG3	1:F:324:VAL:HB	2.00	0.44
1:A:25:GLN:OE1	1:A:371:HIS:HB2	2.18	0.43
1:A:287:GLU:OE1	1:B:142:THR:HG21	2.18	0.43
1:B:328:ARG:NH1	1:B:359:ASP:O	2.51	0.43
1:E:201:LEU:HB2	1:E:275:TYR:CD2	2.53	0.43
1:A:297:ASN:O	1:A:301:GLU:HG3	2.18	0.43
1:C:330:CYS:CA	1:C:348:LEU:HD12	2.46	0.43
1:E:165:VAL:CG2	1:E:184:LEU:HD13	2.46	0.43
1:B:214:LYS:HD3	2:B:405:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:117:ALA:HB1	1:D:181:PHE:CE1	2.53	0.43
1:D:282:GLY:HA3	1:D:313:CYS:HB3	2.00	0.43
1:D:320:ALA:CB	1:D:325:LEU:HD12	2.46	0.43
1:E:277:ALA:HB2	1:E:382:LEU:HD21	2.00	0.43
1:E:92:ALA:HB3	1:E:93:PRO:HD3	2.00	0.43
1:F:24:PHE:O	1:F:28:GLN:HG3	2.19	0.43
1:F:59:THR:HG22	1:F:60:TYR:CD1	2.52	0.43
1:F:66:HIS:CD2	1:F:244:ILE:HG23	2.53	0.43
1:A:59:THR:HG23	2:A:430:HOH:O	2.18	0.43
1:D:143:VAL:HG12	1:D:143:VAL:O	2.18	0.43
1:D:79:LEU:N	1:D:79:LEU:HD12	2.26	0.43
1:E:223:LEU:HD21	1:E:379:MET:HG2	2.00	0.43
1:F:213:VAL:CG1	1:F:214:LYS:H	2.31	0.43
1:C:208:MET:HE2	1:C:281:PRO:HB2	1.99	0.43
1:C:339:ASN:ND2	1:C:339:ASN:N	2.66	0.43
1:D:25:GLN:NE2	1:D:371:HIS:ND1	2.65	0.43
1:E:285:ALA:N	1:E:286:PRO:CD	2.81	0.43
1:E:66:HIS:CD2	1:E:244:ILE:HG23	2.54	0.43
1:F:117:ALA:HA	1:F:170:ILE:O	2.18	0.43
1:A:253:TYR:O	1:B:91:ARG:NH2	2.50	0.43
1:C:388:PHE:O	1:C:389:HIS:HB2	2.18	0.43
1:E:143:VAL:O	1:E:143:VAL:HG12	2.18	0.43
1:F:373:GLU:HG2	2:F:451:HOH:O	2.19	0.43
1:A:199:ARG:HA	1:A:226:GLN:O	2.19	0.43
1:A:223:LEU:HG	1:A:384:ILE:HG21	2.00	0.43
1:A:81:LYS:HE3	2:A:437:HOH:O	2.18	0.43
1:F:107:LYS:HE2	1:F:129:ALA:O	2.19	0.43
1:F:332:ALA:HB1	1:F:336:VAL:CG2	2.48	0.43
1:A:355:ARG:HG2	1:A:357:PHE:CZ	2.54	0.43
1:E:136:LYS:HA	1:E:153:LYS:HB2	2.00	0.43
1:E:310:ALA:HB1	1:E:374:PHE:CZ	2.53	0.43
1:F:183:GLN:O	1:F:187:LYS:HG2	2.18	0.43
1:A:230:VAL:HG21	1:A:270:LEU:HD11	2.01	0.43
1:E:328:ARG:NH1	1:E:359:ASP:O	2.52	0.43
1:A:235:LYS:N	1:A:238:GLU:HG3	2.34	0.42
1:A:265:THR:HG22	1:A:266:ASN:N	2.33	0.42
1:B:375:VAL:O	1:B:379:MET:HG3	2.19	0.42
1:E:235:LYS:H	1:E:238:GLU:HG3	1.82	0.42
1:D:334:PRO:O	1:E:98:LEU:HD22	2.18	0.42
1:B:195:GLY:O	1:B:384:ILE:HG12	2.18	0.42
1:B:337:LYS:HG3	1:B:347:TRP:CD2	2.54	0.42
1:B:310:ALA:HA	1:B:363:VAL:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:119:ILE:HD11	1:C:174:THR:C	2.40	0.42
1:F:132:VAL:CG2	1:F:152:ALA:HB2	2.49	0.42
1:F:297:ASN:O	1:F:301:GLU:HG3	2.19	0.42
1:F:52:HIS:O	1:F:53:ASP:HB3	2.19	0.42
1:B:335:ALA:HB1	1:C:94:GLU:HG2	2.01	0.42
1:D:128:ALA:HB2	1:F:338:LEU:HD13	2.00	0.42
1:D:314:HIS:HD2	1:D:317:GLN:NE2	2.17	0.42
1:A:170:ILE:HD12	1:A:185:PHE:HA	2.01	0.42
1:A:235:LYS:O	1:A:237:GLY:N	2.53	0.42
1:A:288:TYR:CD2	1:B:59:THR:HG23	2.54	0.42
1:A:333:TYR:O	1:A:336:VAL:HG22	2.19	0.42
1:C:123:GLN:N	1:C:123:GLN:OE1	2.51	0.42
1:A:23:PRO:O	1:A:27:LEU:HG	2.19	0.42
1:C:358:THR:OG1	1:C:377:GLN:NE2	2.52	0.42
1:D:294:HIS:O	1:D:298:ILE:HG13	2.19	0.42
1:D:60:TYR:O	1:F:284:ARG:NH1	2.26	0.42
1:F:210:ASP:OD2	1:F:259:HIS:HD2	2.03	0.42
1:F:212:GLU:OE1	1:F:313:CYS:CB	2.68	0.42
1:F:331:THR:OG1	1:F:350:PRO:HB3	2.20	0.42
1:F:9:ILE:HG12	1:F:86:VAL:HB	2.01	0.42
1:A:203:LEU:O	1:A:281:PRO:HD2	2.20	0.42
1:A:312:ILE:HG12	1:A:313:CYS:N	2.33	0.42
1:B:204:CYS:HA	1:B:208:MET:HE3	2.01	0.42
1:E:119:ILE:HG13	1:E:172:ALA:HB3	2.02	0.42
1:F:54:PHE:N	1:F:54:PHE:CD1	2.86	0.42
1:B:203:LEU:HG	1:B:278:LEU:HD11	2.02	0.42
1:C:124:LEU:CD2	1:C:143:VAL:HG13	2.50	0.42
1:D:336:VAL:HB	1:D:339:ASN:HD22	1.85	0.42
1:F:270:LEU:C	1:F:270:LEU:HD13	2.40	0.42
1:A:169:LEU:HG	2:A:442:HOH:O	2.20	0.42
1:F:328:ARG:HA	1:F:328:ARG:HD2	1.94	0.42
1:A:108:GLU:HA	1:A:111:ARG:HH12	1.80	0.42
1:A:124:LEU:HD21	1:A:143:VAL:HG13	2.01	0.42
1:B:37:VAL:CG2	1:B:74:PHE:N	2.82	0.42
1:D:3:ASN:O	1:D:4:SER:CB	2.65	0.42
1:D:5:ARG:HG2	1:D:5:ARG:HH21	1.84	0.42
1:E:106:VAL:HG21	1:E:125:ILE:CG2	2.50	0.42
1:F:165:VAL:HG22	1:F:170:ILE:HG12	2.02	0.42
1:A:337:LYS:HG3	1:A:347:TRP:CD2	2.55	0.41
1:A:42:LYS:N	1:A:42:LYS:HD3	2.33	0.41
1:B:8:LEU:HD12	1:B:35:HIS:O	2.20	0.41
1:E:13:ASP:O	1:E:14:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:215:VAL:HB	1:A:216:PRO:HD3	2.00	0.41
1:B:310:ALA:HB1	1:B:374:PHE:CE1	2.55	0.41
1:C:27:LEU:HD22	1:C:32:ILE:HD12	2.03	0.41
1:C:64:ARG:NH2	2:C:467:HOH:O	2.52	0.41
1:D:313:CYS:HA	1:D:366:ALA:O	2.21	0.41
1:F:271:VAL:HG13	1:F:271:VAL:O	2.20	0.41
1:C:64:ARG:HB2	2:C:420:HOH:O	2.19	0.41
1:E:159:THR:O	1:E:162:VAL:HG13	2.20	0.41
1:E:71:ASN:OD1	1:E:71:ASN:C	2.58	0.41
1:F:310:ALA:HB1	1:F:374:PHE:CZ	2.56	0.41
1:A:73:THR:C	1:A:74:PHE:O	2.58	0.41
1:B:234:LYS:HB3	1:B:238:GLU:HG3	2.02	0.41
1:C:124:LEU:HD23	1:C:143:VAL:HG13	2.03	0.41
1:C:106:VAL:HG21	1:C:125:ILE:HG21	2.01	0.41
1:C:36:THR:HG21	1:C:68:PHE:CZ	2.55	0.41
1:F:285:ALA:HB3	1:F:286:PRO:HD3	2.01	0.41
1:E:335:ALA:CB	1:F:94:GLU:HG2	2.51	0.41
1:A:119:ILE:HD11	1:A:174:THR:C	2.41	0.41
1:B:239:ARG:NH2	1:B:260:THR:HG23	2.28	0.41
1:B:65:GLY:HA2	1:B:244:ILE:HD13	2.01	0.41
1:D:235:LYS:N	1:D:238:GLU:HG3	2.27	0.41
1:E:107:LYS:HG2	1:E:129:ALA:HB1	2.02	0.41
1:E:119:ILE:HD11	1:E:174:THR:O	2.21	0.41
1:E:30:PHE:N	1:E:30:PHE:CD2	2.88	0.41
1:E:338:LEU:C	1:E:338:LEU:HD23	2.40	0.41
1:F:368:TRP:N	1:F:369:PRO:CD	2.83	0.41
1:A:120:CYS:HB3	1:A:121:HIS:H	1.66	0.41
1:A:267:PHE:O	1:A:270:LEU:HB2	2.21	0.41
1:C:105:LEU:HD23	1:C:105:LEU:C	2.41	0.41
1:C:120:CYS:HA	1:C:173:ALA:O	2.21	0.41
1:C:213:VAL:CG1	1:C:214:LYS:N	2.82	0.41
1:F:271:VAL:HG13	1:F:274:SER:OG	2.21	0.41
1:B:144:GLY:O	1:B:148:VAL:HG23	2.20	0.41
1:B:7:VAL:HG12	1:B:8:LEU:N	2.36	0.41
1:D:10:LEU:O	1:D:88:PRO:HD2	2.21	0.41
1:A:294:HIS:O	1:A:298:ILE:HG13	2.20	0.41
1:A:367:ALA:CB	1:A:369:PRO:HD2	2.51	0.41
1:A:88:PRO:HA	2:A:483:HOH:O	2.20	0.41
1:C:323:GLY:HA2	2:C:403:HOH:O	2.21	0.41
1:C:332:ALA:CB	1:C:336:VAL:CG2	2.99	0.41
1:D:173:ALA:N	2:D:411:HOH:O	2.46	0.41
1:E:235:LYS:N	1:E:238:GLU:HG2	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:239:ARG:HG3	1:E:239:ARG:HH11	1.85	0.41
1:F:178:HIS:N	1:F:179:PRO:CD	2.84	0.41
1:B:108:GLU:HA	1:B:111:ARG:NH1	2.35	0.41
1:C:272:SER:HB3	1:C:301:GLU:OE1	2.21	0.41
1:C:129:ALA:O	1:C:131:THR:HG23	2.21	0.41
1:A:32:ILE:CG1	2:A:434:HOH:O	2.57	0.40
1:A:331:THR:OG1	1:A:350:PRO:HB3	2.21	0.40
1:C:37:VAL:HG22	1:C:74:PHE:CA	2.51	0.40
1:D:91:ARG:HB3	2:D:421:HOH:O	2.21	0.40
1:F:119:ILE:HD11	1:F:174:THR:O	2.21	0.40
1:F:30:PHE:CZ	1:F:223:LEU:HD13	2.57	0.40
1:F:37:VAL:CG2	1:F:74:PHE:N	2.84	0.40
1:A:255:GLU:OE2	1:A:284:ARG:HD3	2.20	0.40
1:B:92:ALA:HB3	1:B:93:PRO:HD3	2.03	0.40
1:D:79:LEU:HD21	1:D:105:LEU:HG	2.02	0.40
1:E:118:SER:O	1:E:171:THR:HA	2.22	0.40
1:E:208:MET:HG3	1:E:213:VAL:CG2	2.45	0.40
1:F:330:CYS:CA	1:F:348:LEU:HD12	2.48	0.40
1:F:37:VAL:CB	2:F:463:HOH:O	2.66	0.40
1:E:335:ALA:HB1	1:F:94:GLU:HG2	2.03	0.40
1:A:20:VAL:HG22	1:A:88:PRO:CB	2.49	0.40
1:A:325:LEU:HB2	2:A:431:HOH:O	2.21	0.40
1:C:388:PHE:HB3	1:C:389:HIS:H	1.76	0.40
1:D:185:PHE:O	1:D:189:LEU:HG	2.22	0.40
1:D:271:VAL:O	1:D:271:VAL:HG13	2.21	0.40
1:D:305:SER:O	1:D:306:GLU:HB2	2.21	0.40
1:F:120:CYS:HB3	2:F:479:HOH:O	2.20	0.40
1:B:367:ALA:CB	1:B:369:PRO:HD2	2.52	0.40
1:D:221:GLN:OE1	2:D:463:HOH:O	2.22	0.40
1:D:83:ASP:O	1:D:115:PRO:HD2	2.22	0.40
1:F:236:ALA:O	1:F:263:LEU:O	2.39	0.40
1:F:66:HIS:CE1	1:F:244:ILE:HG12	2.56	0.40
1:A:62:GLU:HG2	1:A:63:SER:N	2.37	0.40
1:A:77:VAL:HG22	2:A:461:HOH:O	2.22	0.40
1:B:130:ASP:CG	1:B:130:ASP:O	2.60	0.40
1:B:19:GLU:OE1	1:B:89:GLY:HA3	2.21	0.40
1:B:316:GLN:N	1:B:316:GLN:OE1	2.55	0.40
1:E:296:LEU:HA	1:E:296:LEU:HD23	1.87	0.40
1:F:117:ALA:HB1	1:F:181:PHE:CZ	2.56	0.40
1:F:215:VAL:HB	1:F:216:PRO:CD	2.52	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	385/387 (100%)	353 (92%)	27 (7%)	5 (1%)	18	17
1	B	385/387 (100%)	356 (92%)	27 (7%)	2 (0%)	38	45
1	C	385/387 (100%)	356 (92%)	28 (7%)	1 (0%)	50	60
1	D	385/387 (100%)	358 (93%)	24 (6%)	3 (1%)	27	30
1	E	385/387 (100%)	352 (91%)	31 (8%)	2 (0%)	38	45
1	F	385/387 (100%)	356 (92%)	24 (6%)	5 (1%)	18	17
All	All	2310/2322 (100%)	2131 (92%)	161 (7%)	18 (1%)	27	30

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
1	E	238	GLU
1	A	74	PHE
1	A	236	ALA
1	D	275	TYR
1	B	238	GLU
1	C	275	TYR
1	F	112	SER
1	D	149	ALA
1	A	141	ALA
1	D	4	SER
1	E	275	TYR
1	F	53	ASP
1	F	79	LEU
1	F	141	ALA
1	F	275	TYR
1	B	271	VAL
1	A	336	VAL

### 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	313/313 (100%)	298 (95%)	15 (5%)	35	46
1	B	313/313 (100%)	300 (96%)	13 (4%)	40	53
1	C	313/313 (100%)	297 (95%)	16 (5%)	33	43
1	D	313/313 (100%)	304 (97%)	9 (3%)	55	71
1	E	313/313 (100%)	304 (97%)	9 (3%)	55	71
1	F	313/313 (100%)	300 (96%)	13 (4%)	40	53
All	All	1878/1878 (100%)	1803 (96%)	75 (4%)	42	56

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	59	THR
1	A	64	ARG
1	A	81	LYS
1	A	98	LEU
1	A	118	SER
1	A	120	CYS
1	A	123	GLN
1	A	142	THR
1	A	147	LEU
1	A	158	ILE
1	A	223	LEU
1	A	270	LEU
1	A	338	LEU
1	A	389	HIS
1	B	3	ASN
1	B	10	LEU
1	B	21	MET
1	B	59	THR
1	B	104	GLU
1	B	147	LEU
1	B	208	MET
1	B	223	LEU

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Mol	Chain	Res	Type
1	B	226	GLN
1	B	251	GLN
1	B	293	GLU
1	B	355	ARG
1	B	389	HIS
1	C	10	LEU
1	C	21	MET
1	C	37	VAL
1	C	42	LYS
1	C	64	ARG
1	C	69	THR
1	C	98	LEU
1	C	118	SER
1	C	123	GLN
1	C	147	LEU
1	C	223	LEU
1	C	226	GLN
1	C	238	GLU
1	C	288	TYR
1	C	339	ASN
1	C	353	ILE
1	D	10	LEU
1	D	37	VAL
1	D	69	THR
1	D	147	LEU
1	D	197	ASN
1	D	223	LEU
1	D	263	LEU
1	D	293	GLU
1	D	313	CYS
1	E	10	LEU
1	E	59	THR
1	E	120	CYS
1	E	142	THR
1	E	147	LEU
1	E	165	VAL
1	E	197	ASN
1	E	223	LEU
1	E	304	ASN
1	F	10	LEU
1	F	37	VAL
1	F	59	THR

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Mol	Chain	Res	Type
1	F	64	ARG
1	F	98	LEU
1	F	123	GLN
1	F	142	THR
1	F	147	LEU
1	F	208	MET
1	F	223	LEU
1	F	238	GLU
1	F	269	ASP
1	F	353	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	28	GLN
1	A	52	HIS
1	A	183	GLN
1	A	259	HIS
1	A	339	ASN
1	A	377	GLN
1	A	385	GLN
1	B	28	GLN
1	B	57	HIS
1	B	226	GLN
1	B	251	GLN
1	B	259	HIS
1	B	339	ASN
1	B	385	GLN
1	C	28	GLN
1	C	52	HIS
1	C	57	HIS
1	C	183	GLN
1	C	226	GLN
1	C	259	HIS
1	C	317	GLN
1	C	339	ASN
1	C	377	GLN
1	D	3	ASN
1	D	25	GLN
1	D	183	GLN
1	D	197	ASN

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Mol	Chain	Res	Type
1	D	259	HIS
1	D	266	ASN
1	D	317	GLN
1	D	339	ASN
1	D	377	GLN
1	E	3	ASN
1	E	28	GLN
1	E	52	HIS
1	E	57	HIS
1	E	183	GLN
1	E	197	ASN
1	E	259	HIS
1	E	294	HIS
1	E	377	GLN
1	F	35	HIS
1	F	245	HIS
1	F	259	HIS
1	F	317	GLN
1	F	339	ASN
1	F	377	GLN
1	F	389	HIS

### 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	387/387 (100%)	0.06	6 (1%) 68 77	16, 30, 48, 69	0
1	B	387/387 (100%)	0.01	5 (1%) 74 82	14, 33, 49, 68	0
1	C	387/387 (100%)	-0.09	2 (0%) 88 94	15, 28, 46, 68	0
1	D	387/387 (100%)	0.03	5 (1%) 74 82	18, 31, 49, 69	0
1	E	387/387 (100%)	-0.14	3 (0%) 83 90	15, 31, 47, 68	0
1	F	387/387 (100%)	0.02	7 (1%) 65 74	14, 31, 48, 67	0
All	All	2322/2322 (100%)	-0.02	28 (1%) 75 83	14, 31, 48, 69	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	389	HIS	4.3
1	A	389	HIS	3.9
1	C	389	HIS	3.5
1	C	3	ASN	3.4
1	A	3	ASN	3.4
1	D	79	LEU	3.4
1	D	75	ASP	3.3
1	D	389	HIS	3.2
1	F	324	VAL	3.0
1	F	327	GLY	2.8
1	E	389	HIS	2.7
1	A	271	VAL	2.7
1	E	270	LEU	2.6
1	D	3	ASN	2.5
1	B	388	PHE	2.5
1	D	77	VAL	2.4
1	F	340	VAL	2.4
1	F	389	HIS	2.4
1	A	75	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	79	LEU	2.2
1	E	79	LEU	2.2
1	B	304	ASN	2.2
1	A	267	PHE	2.1
1	A	270	LEU	2.1
1	B	194	THR	2.1
1	F	3	ASN	2.1
1	F	113	GLY	2.0
1	F	77	VAL	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.