



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:01 PM UTC

PDB ID : 3VR2 / pdb_00003vr2
Title : Crystal structure of nucleotide-free A3B3 complex from *Enterococcus hirae* V-ATPase [eA3B3]
Authors : Arai, S.; Saijo, S.; Suzuki, K.; Mizutani, K.; Kakinuma, Y.; Ishizuka-Katsura, Y.; Ohsawa, N.; Terada, T.; Shirouzu, M.; Yokoyama, S.; Iwata, S.; Yamato, I.; Murata, T.
Deposited on : 2012-04-03
Resolution : 2.80 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

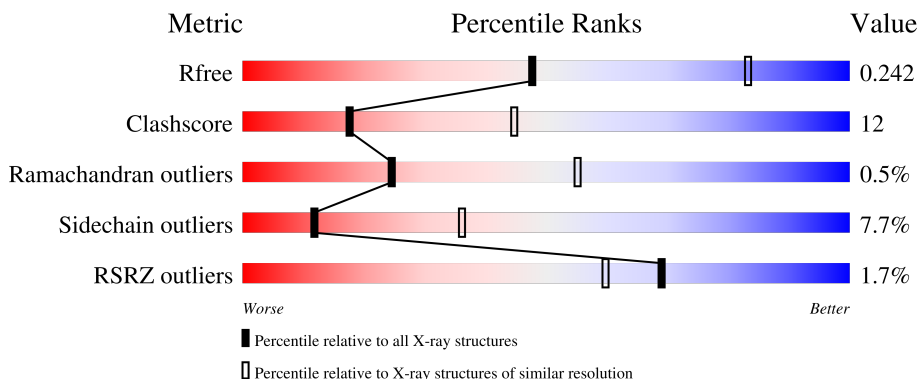
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.80 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.



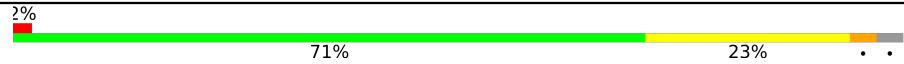

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 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	600	
1	B	600	
1	C	600	
2	D	465	

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Mol	Chain	Length	Quality of chain
2	E	465	
2	F	465	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24053 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	586	4559	2864	766	904	3	22	0	0	0
1	B	586	4555	2862	766	902	3	22	0	0	0
1	C	583	4501	2829	757	890	3	22	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q08636
A	-5	SER	-	expression tag	UNP Q08636
A	-4	SER	-	expression tag	UNP Q08636
A	-3	GLY	-	expression tag	UNP Q08636
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-6	GLY	-	expression tag	UNP Q08636
B	-5	SER	-	expression tag	UNP Q08636
B	-4	SER	-	expression tag	UNP Q08636
B	-3	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-6	GLY	-	expression tag	UNP Q08636
C	-5	SER	-	expression tag	UNP Q08636
C	-4	SER	-	expression tag	UNP Q08636
C	-3	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	447	Total 3447	C 2179	N 596	O 658	Se 14	0	0	0
2	E	449	Total 3448	C 2180	N 596	O 658	Se 14	0	0	0
2	F	451	Total 3454	C 2177	N 598	O 665	Se 14	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q08637
D	-5	SER	-	expression tag	UNP Q08637
D	-4	SER	-	expression tag	UNP Q08637
D	-3	GLY	-	expression tag	UNP Q08637
D	-2	SER	-	expression tag	UNP Q08637
D	-1	SER	-	expression tag	UNP Q08637
D	0	GLY	-	expression tag	UNP Q08637
E	-6	GLY	-	expression tag	UNP Q08637
E	-5	SER	-	expression tag	UNP Q08637
E	-4	SER	-	expression tag	UNP Q08637
E	-3	GLY	-	expression tag	UNP Q08637
E	-2	SER	-	expression tag	UNP Q08637
E	-1	SER	-	expression tag	UNP Q08637
E	0	GLY	-	expression tag	UNP Q08637
F	-6	GLY	-	expression tag	UNP Q08637
F	-5	SER	-	expression tag	UNP Q08637
F	-4	SER	-	expression tag	UNP Q08637
F	-3	GLY	-	expression tag	UNP Q08637
F	-2	SER	-	expression tag	UNP Q08637
F	-1	SER	-	expression tag	UNP Q08637
F	0	GLY	-	expression tag	UNP Q08637

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total 39	O 39	0	0
3	B	8	Total 8	O 8	0	0
3	C	14	Total 14	O 14	0	0
3	D	8	Total 8	O 8	0	0

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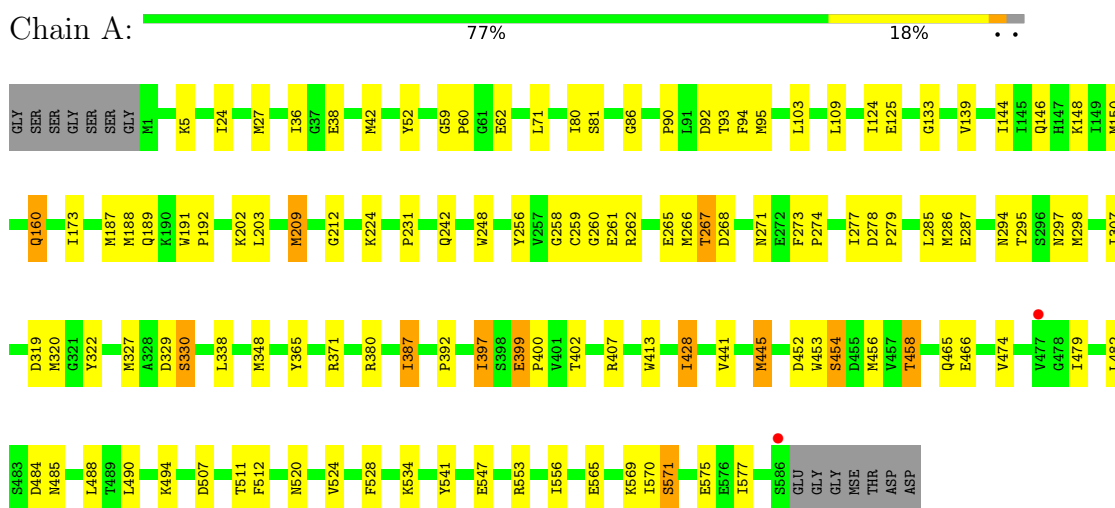
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	12	Total	O	0	0
			12	12		
3	F	8	Total	O	0	0
			8	8		

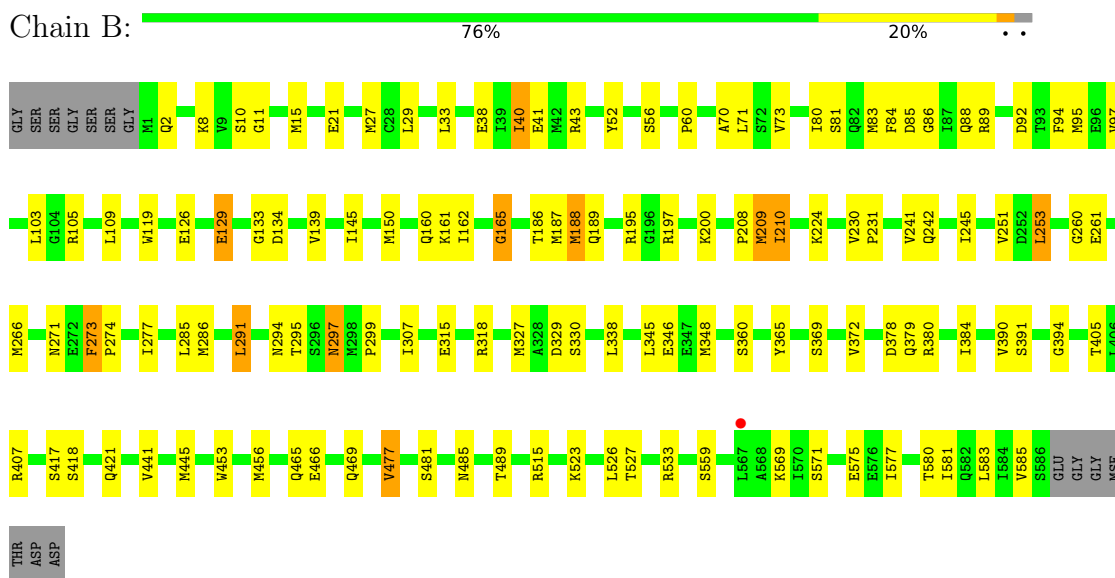
3 Residue-property plots

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.

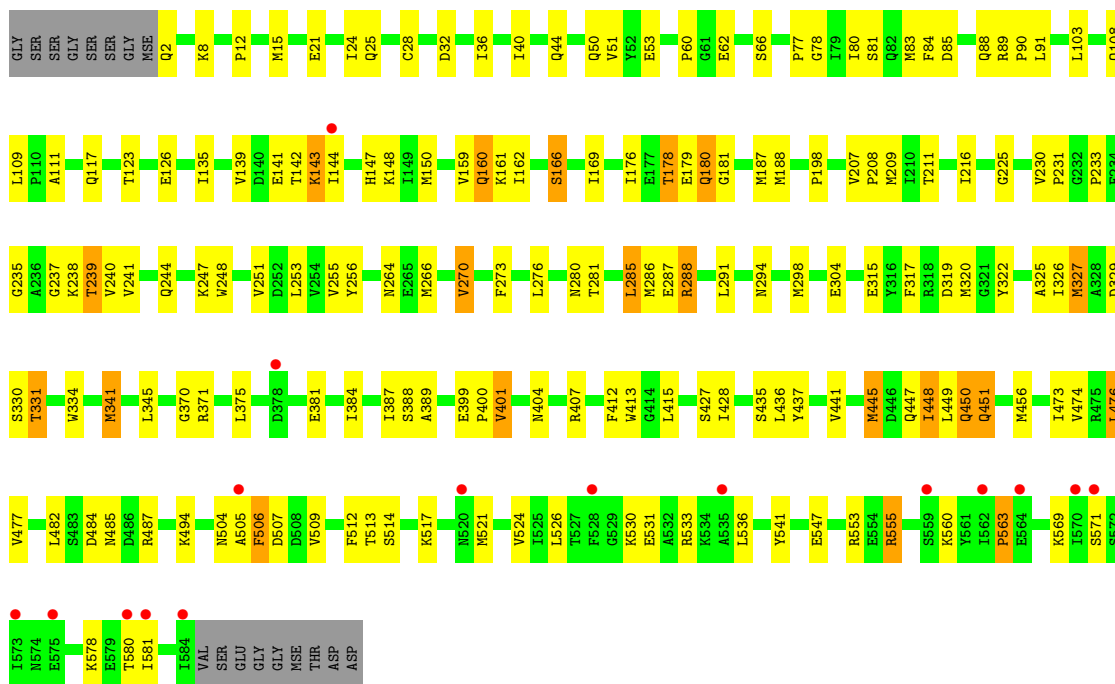
- Molecule 1: V-type sodium ATPase catalytic subunit A



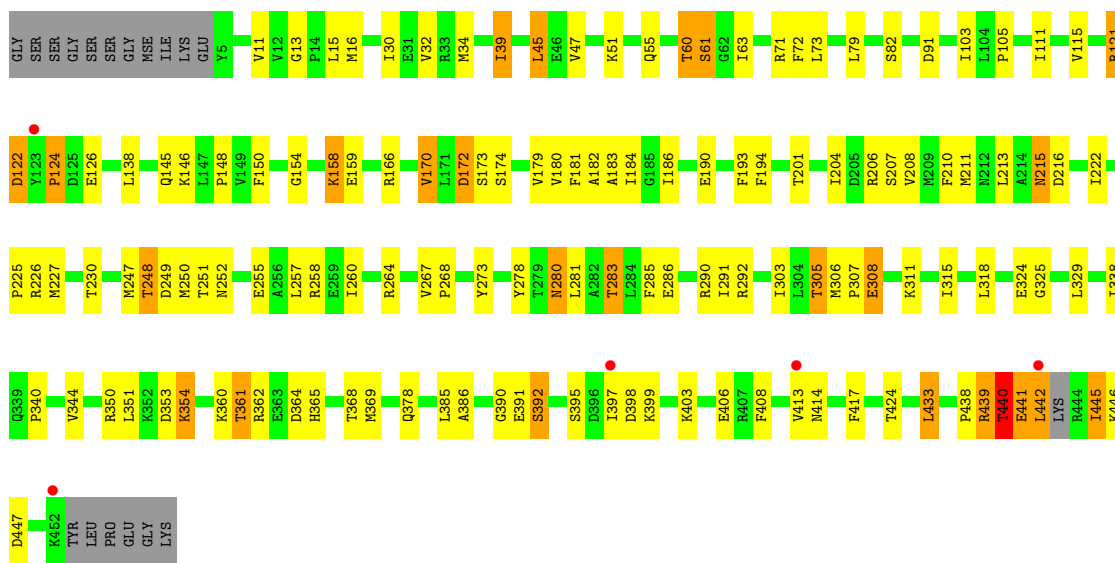
- Molecule 1: V-type sodium ATPase catalytic subunit A



- Molecule 1: V-type sodium ATPase catalytic subunit A

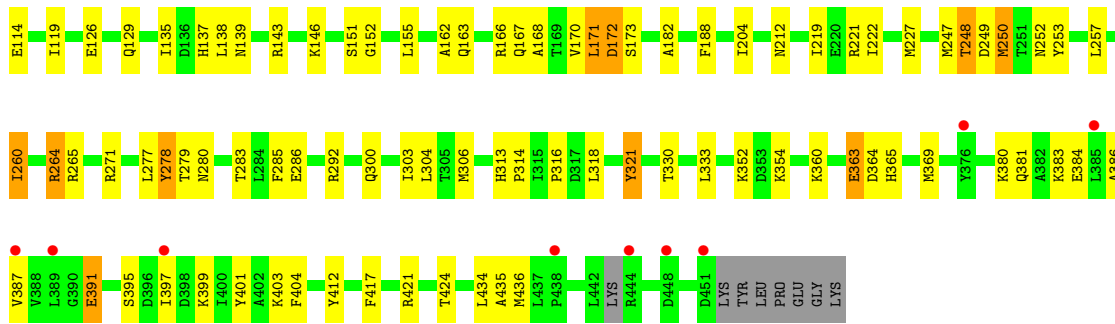


• Molecule 2: V-type sodium ATPase subunit B

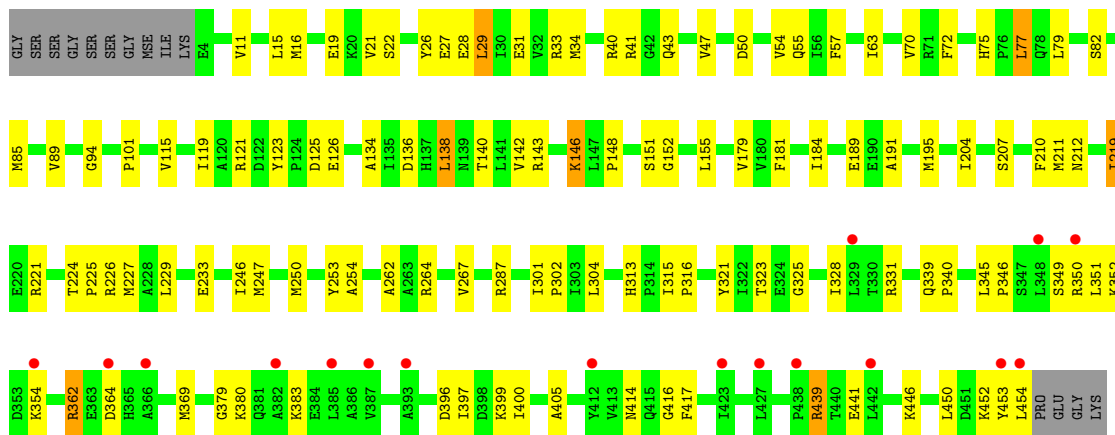


• Molecule 2: V-type sodium ATPase subunit B





- Molecule 2: V-type sodium ATPase subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.80Å 121.50Å 128.26Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	44.18 – 2.80 44.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.18-2.80) 99.3 (44.18-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.243 0.198 , 0.242	Depositor DCC
R_{free} test set	4573 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.009 for k,h,-l 0.011 for -k,-h,-l 0.021 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24053	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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	0.84	0/4613	1.01	4/6206 (0.1%)
1	B	0.62	0/4609	0.90	4/6201 (0.1%)
1	C	0.61	0/4555	0.91	3/6131 (0.0%)
2	D	0.71	0/3493	0.96	0/4698
2	E	0.72	0/3494	0.97	1/4700 (0.0%)
2	F	0.61	0/3501	0.91	1/4706 (0.0%)
All	All	0.69	0/24265	0.94	13/32642 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	GLN	CB-CA-C	-7.75	107.64	116.63
2	F	75	HIS	N-CA-C	7.73	115.18	108.22
2	E	173	SER	N-CA-C	-7.23	98.70	108.24
1	A	399	GLU	CA-C-N	6.26	126.00	119.05
1	A	399	GLU	C-N-CA	6.26	126.00	119.05
1	B	585	VAL	N-CA-C	-6.24	104.21	113.39
1	C	555	ARG	N-CA-C	-6.16	105.25	112.89
1	B	145	ILE	N-CA-C	6.01	116.53	108.11
1	C	78	GLY	N-CA-C	-5.98	106.91	115.64
1	B	297	ASN	N-CA-C	-5.97	105.82	114.12
1	A	209	MSE	CG-SE-CE	-5.77	86.22	98.92
1	B	165	GLY	N-CA-C	5.64	118.19	110.69
1	A	259	CYS	N-CA-C	5.53	118.49	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	124	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4559	0	4521	100	0
1	B	4555	0	4517	77	0
1	C	4501	0	4435	146	0
2	D	3447	0	3416	115	0
2	E	3448	0	3400	92	0
2	F	3454	0	3394	88	0
3	A	39	0	0	4	0
3	B	8	0	0	0	0
3	C	14	0	0	0	0
3	D	8	0	0	4	0
3	E	12	0	0	1	0
3	F	8	0	0	1	0
All	All	24053	0	23683	590	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 12.

All (590) 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)
2:E:102:GLU:CB	2:E:103:ILE:HA	1.63	1.24
1:A:139:VAL:CG2	1:A:187:MSE:HE1	1.72	1.19
1:A:320:MSE:HE2	1:A:322:TYR:CE2	1.84	1.12
2:E:79:LEU:HD13	2:E:227:MSE:CE	1.80	1.12
2:D:361:THR:HG21	2:D:365:HIS:CD2	1.85	1.11
1:C:451:GLN:HE21	1:C:451:GLN:HA	0.95	1.10
2:D:79:LEU:HD13	2:D:227:MSE:HE1	1.30	1.10
2:F:219:ILE:HD12	2:F:219:ILE:H	1.16	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:ILE:HD12	2:D:250:MSE:HE1	1.31	1.09
2:D:361:THR:HG22	2:D:362:ARG:H	0.93	1.07
1:A:407:ARG:HD2	3:A:631:HOH:O	1.53	1.06
1:C:150:MSE:HE1	1:C:319:ASP:HB3	1.35	1.06
1:C:451:GLN:HA	1:C:451:GLN:NE2	1.67	1.05
2:D:361:THR:CG2	2:D:362:ARG:H	1.69	1.02
2:F:29:LEU:HD11	2:F:77:LEU:HD13	1.44	0.99
1:A:139:VAL:HG21	1:A:187:MSE:HE1	1.43	0.98
1:A:27:MSE:HE3	1:A:71:LEU:HB2	1.44	0.98
1:B:139:VAL:HG23	1:B:187:MSE:HE1	1.47	0.97
1:C:77:PRO:HG2	1:C:187:MSE:HE2	1.42	0.97
1:B:266:MSE:HE3	1:B:294:ASN:O	1.65	0.97
2:D:79:LEU:HD13	2:D:227:MSE:CE	1.94	0.97
2:E:250:MSE:HA	2:E:250:MSE:HE2	1.43	0.96
1:C:83:MSE:HE2	1:C:270:VAL:HG11	1.48	0.95
2:D:361:THR:HG22	2:D:362:ARG:N	1.74	0.95
2:E:79:LEU:HD13	2:E:227:MSE:HE3	1.49	0.94
2:E:79:LEU:HD13	2:E:227:MSE:HE1	1.46	0.93
1:C:320:MSE:HE3	1:C:322:TYR:CE2	2.04	0.93
2:E:102:GLU:CB	2:E:103:ILE:CA	2.48	0.92
1:A:320:MSE:CE	1:A:322:TYR:HE2	1.82	0.91
2:F:452:LYS:H	2:F:453:TYR:C	1.79	0.91
1:B:60:PRO:HD3	2:E:47:VAL:HG13	1.53	0.90
2:E:13:GLY:O	2:E:60:THR:HG21	1.72	0.90
1:B:139:VAL:CG2	1:B:187:MSE:HE1	2.00	0.90
1:C:139:VAL:HG21	1:C:187:MSE:CE	2.01	0.90
1:C:451:GLN:HE21	1:C:451:GLN:CA	1.82	0.89
1:A:139:VAL:CG2	1:A:187:MSE:CE	2.51	0.89
2:F:11:VAL:HG22	2:F:16:MSE:HG2	1.55	0.87
2:F:184:ILE:HD13	2:F:250:MSE:HE1	1.57	0.87
1:A:320:MSE:CE	1:A:322:TYR:CE2	2.55	0.86
2:D:391:GLU:O	2:D:392:SER:HB2	1.73	0.85
2:E:383:LYS:HA	2:E:386:ALA:HB3	1.57	0.85
1:C:317:PHE:HD1	1:C:320:MSE:CE	1.89	0.84
2:D:361:THR:HG21	2:D:365:HIS:HD2	1.36	0.84
2:F:250:MSE:HE2	2:F:250:MSE:HA	1.58	0.84
2:F:439:ARG:CG	2:F:439:ARG:HH11	1.89	0.84
2:E:248:THR:HG23	2:E:303:ILE:HB	1.59	0.84
1:C:320:MSE:HE3	1:C:322:TYR:CD2	2.11	0.84
1:B:273:PHE:HD2	1:B:286:MSE:HE1	1.42	0.83
1:C:139:VAL:HG21	1:C:187:MSE:HE3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:VAL:HG22	2:D:16:MSE:HG2	1.59	0.83
2:F:82:SER:O	2:F:85:MSE:HG3	1.78	0.83
1:B:86:GLY:H	1:B:294:ASN:HD21	1.26	0.82
2:F:79:LEU:HD13	2:F:227:MSE:HE1	1.61	0.82
1:C:8:LYS:HB3	1:C:15:MSE:HG3	1.61	0.81
2:F:219:ILE:H	2:F:219:ILE:CD1	1.91	0.80
1:A:60:PRO:HD3	2:D:47:VAL:HG13	1.62	0.80
1:B:261:GLU:HG2	1:B:266:MSE:HE1	1.64	0.80
1:B:189:GLN:NE2	1:B:197:ARG:HH12	1.80	0.80
1:A:266:MSE:HE3	1:A:294:ASN:O	1.81	0.80
1:C:25:GLN:HG3	2:D:61:SER:OG	1.81	0.79
2:D:45:LEU:HB3	2:D:264:ARG:HD3	1.63	0.79
1:A:133:GLY:HA2	1:A:150:MSE:HE2	1.64	0.78
2:E:250:MSE:HA	2:E:250:MSE:CE	2.14	0.78
1:B:40:ILE:HG22	1:B:41:GLU:HG3	1.66	0.77
1:B:273:PHE:HD2	1:B:286:MSE:CE	1.96	0.77
1:A:139:VAL:HG23	1:A:187:MSE:HE1	1.66	0.77
1:B:8:LYS:HB3	1:B:15:MSE:HG2	1.65	0.77
1:B:580:THR:HA	1:B:583:LEU:HD12	1.66	0.76
1:C:28:CYS:HB3	1:C:66:SER:HA	1.66	0.76
2:D:184:ILE:CD1	2:D:250:MSE:HE1	2.15	0.75
1:C:83:MSE:CE	1:C:270:VAL:HG11	2.17	0.75
1:C:141:GLU:OE2	1:C:147:HIS:HD2	1.70	0.75
1:C:506:PHE:HD2	1:C:506:PHE:N	1.84	0.75
2:E:212:ASN:OD1	2:E:221:ARG:HG3	1.87	0.75
2:F:439:ARG:HH11	2:F:439:ARG:HG3	1.51	0.75
2:E:222:ILE:CD1	2:E:260:ILE:HD13	2.16	0.75
1:A:474:VAL:HG22	1:A:482:LEU:HD11	1.68	0.75
1:A:139:VAL:HG21	1:A:187:MSE:CE	2.13	0.75
2:D:248:THR:HG23	2:D:303:ILE:HB	1.67	0.75
2:D:182:ALA:HB3	2:D:247:MSE:HG2	1.68	0.74
2:D:248:THR:CG2	2:D:303:ILE:HB	2.17	0.74
1:C:77:PRO:HG2	1:C:187:MSE:CE	2.15	0.74
1:C:317:PHE:CD1	1:C:320:MSE:CE	2.69	0.74
1:C:273:PHE:HB2	1:C:286:MSE:HE2	1.67	0.74
1:C:506:PHE:N	1:C:506:PHE:CD2	2.52	0.74
1:A:150:MSE:HE3	1:A:380:ARG:HH21	1.51	0.73
1:B:261:GLU:HG2	1:B:266:MSE:CE	2.18	0.73
2:E:222:ILE:HD12	2:E:260:ILE:HD13	1.68	0.73
2:F:79:LEU:HD13	2:F:227:MSE:CE	2.18	0.73
1:C:139:VAL:HG21	1:C:187:MSE:HE1	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:349:SER:O	2:F:352:LYS:HE2	1.88	0.73
1:A:266:MSE:CE	1:A:294:ASN:O	2.37	0.72
1:B:83:MSE:HE2	1:B:291:LEU:HD13	1.71	0.72
1:C:517:LYS:HE2	1:C:521:MSE:HE3	1.71	0.72
1:C:83:MSE:HE2	1:C:270:VAL:CG1	2.20	0.72
1:A:139:VAL:HG23	1:A:187:MSE:CE	2.19	0.72
2:D:222:ILE:HG22	2:D:226:ARG:HH21	1.55	0.72
1:C:317:PHE:HD1	1:C:320:MSE:HE1	1.53	0.72
1:C:50:GLN:HG3	1:C:341:MSE:SE	2.40	0.71
1:C:238:LYS:HG2	1:C:239:THR:N	2.06	0.71
1:B:273:PHE:CD2	1:B:286:MSE:HE1	2.24	0.71
1:A:261:GLU:HG2	1:A:266:MSE:HE2	1.72	0.70
2:E:171:LEU:O	2:E:171:LEU:HD23	1.91	0.70
1:C:317:PHE:HD1	1:C:320:MSE:HE2	1.57	0.70
1:C:317:PHE:CD1	1:C:320:MSE:HE2	2.27	0.69
2:D:441:GLU:O	2:D:442:LEU:HD13	1.92	0.69
2:F:181:PHE:HD2	2:F:211:MSE:HE1	1.56	0.69
2:E:126:GLU:HB3	2:E:143:ARG:HH21	1.58	0.69
1:B:186:THR:HG23	1:B:188:MSE:H	1.59	0.68
2:D:361:THR:CG2	2:D:362:ARG:N	2.36	0.68
1:A:86:GLY:H	1:A:294:ASN:HD21	1.38	0.68
2:F:55:GLN:NE2	2:F:264:ARG:HH21	1.92	0.68
1:A:266:MSE:HE3	1:A:294:ASN:H	1.59	0.68
1:C:178:THR:HG23	1:C:181:GLY:O	1.94	0.68
1:A:320:MSE:HE1	1:A:322:TYR:HE2	1.59	0.67
1:C:320:MSE:HE3	1:C:322:TYR:HE2	1.56	0.67
1:A:261:GLU:HG2	1:A:266:MSE:CE	2.24	0.67
1:C:238:LYS:CG	1:C:239:THR:N	2.57	0.67
2:D:391:GLU:O	2:D:392:SER:CB	2.43	0.66
1:A:565:GLU:N	1:A:565:GLU:OE1	2.28	0.66
1:B:271:ASN:OD1	2:E:292:ARG:NH2	2.29	0.66
2:D:439:ARG:C	2:D:441:GLU:H	2.04	0.66
2:F:79:LEU:HD11	2:F:85:MSE:HE1	1.78	0.66
1:C:51:VAL:HG12	1:C:53:GLU:H	1.60	0.66
1:C:399:GLU:HG2	1:C:400:PRO:HD2	1.78	0.65
2:E:395:SER:O	2:E:399:LYS:CB	2.44	0.65
1:A:133:GLY:O	1:A:380:ARG:NH2	2.29	0.65
1:B:456:MSE:HG2	1:B:526:LEU:HD12	1.79	0.65
2:D:184:ILE:HD13	2:D:225:PRO:HG3	1.79	0.64
1:C:505:ALA:C	1:C:506:PHE:HD2	2.05	0.64
2:E:79:LEU:CD1	2:E:227:MSE:HE1	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:PRO:HG2	2:D:351:LEU:HD13	1.80	0.64
2:E:171:LEU:O	2:E:171:LEU:CG	2.43	0.64
2:D:79:LEU:CD1	2:D:227:MSE:HE1	2.19	0.63
2:F:142:VAL:HG21	2:F:351:LEU:O	1.99	0.63
1:B:297:ASN:HB2	2:E:286:GLU:HG3	1.79	0.63
2:F:452:LYS:N	2:F:453:TYR:C	2.56	0.63
1:C:273:PHE:HB2	1:C:286:MSE:CE	2.29	0.62
2:E:171:LEU:O	2:E:171:LEU:HG	1.98	0.62
2:E:55:GLN:OE1	2:E:264:ARG:NH1	2.32	0.62
2:E:278:TYR:C	2:E:278:TYR:CD2	2.77	0.62
2:D:361:THR:HG21	2:D:365:HIS:CG	2.34	0.62
1:C:288:ARG:HG3	1:C:288:ARG:O	1.99	0.62
1:B:133:GLY:O	1:B:380:ARG:NH2	2.33	0.61
1:A:209:MSE:HE3	1:A:224:LYS:HG2	1.81	0.61
2:D:361:THR:CG2	2:D:365:HIS:HD2	2.09	0.61
1:A:266:MSE:HE3	1:A:294:ASN:N	2.15	0.61
1:C:85:ASP:OD2	1:C:89:ARG:NH1	2.33	0.61
1:A:261:GLU:CG	1:A:266:MSE:HE2	2.29	0.61
2:E:163:GLN:HE21	2:E:167:GLN:HE22	1.48	0.61
2:F:43:GLN:HG2	2:F:57:PHE:HE1	1.66	0.61
2:D:264:ARG:HD2	3:D:501:HOH:O	1.99	0.61
1:C:117:GLN:OE1	1:C:166:SER:OG	2.19	0.60
1:A:452:ASP:O	1:A:456:MSE:HG3	2.00	0.60
2:D:15:LEU:HD22	2:D:45:LEU:HD11	1.84	0.60
1:C:238:LYS:HG2	1:C:239:THR:H	1.65	0.60
1:A:150:MSE:HE1	1:A:319:ASP:HB3	1.83	0.60
1:C:238:LYS:HE3	1:C:329:ASP:OD1	2.02	0.60
2:E:171:LEU:O	2:E:171:LEU:CD2	2.49	0.60
1:C:180:GLN:HG3	1:C:181:GLY:N	2.15	0.60
1:C:327:MSE:HE2	1:C:387:ILE:HB	1.84	0.59
2:D:399:LYS:C	2:D:399:LYS:HD2	2.28	0.59
2:E:94:GLY:HA3	2:E:227:MSE:HE2	1.84	0.59
1:B:27:MSE:HE3	1:B:71:LEU:HB2	1.85	0.59
1:C:448:ILE:HG23	1:C:449:LEU:HD23	1.84	0.59
1:B:60:PRO:HD3	2:E:47:VAL:CG1	2.27	0.59
1:C:264:ASN:ND2	2:F:121:ARG:HD3	2.17	0.59
1:A:399:GLU:HB2	1:A:400:PRO:HD2	1.84	0.59
2:F:123:TYR:HD2	2:F:354:LYS:HE2	1.68	0.59
1:C:331:THR:HG23	1:C:389:ALA:O	2.03	0.58
2:F:89:VAL:HG21	2:F:195:MSE:HE1	1.84	0.58
1:C:294:ASN:ND2	1:C:298:MSE:HE2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:PHE:CD2	2:D:306:MSE:HE3	2.39	0.58
2:F:152:GLY:HA2	3:F:504:HOH:O	2.03	0.58
1:C:25:GLN:CG	2:D:61:SER:OG	2.52	0.58
1:C:126:GLU:HG3	1:C:162:ILE:HG22	1.86	0.58
1:C:235:GLY:CA	2:F:350:ARG:HH21	2.17	0.58
1:C:84:PHE:HB3	1:C:88:GLN:HA	1.86	0.57
1:B:80:ILE:O	1:B:81:SER:HB2	2.04	0.57
1:C:521:MSE:HE2	1:C:560:LYS:HA	1.86	0.57
2:E:391:GLU:OE1	2:E:391:GLU:HA	2.03	0.57
2:D:362:ARG:HD2	2:D:364:ASP:OD1	2.03	0.57
1:A:148:LYS:HB2	1:A:320:MSE:HG2	1.85	0.57
1:B:43:ARG:HG3	1:B:43:ARG:HH11	1.70	0.57
1:C:273:PHE:CB	1:C:286:MSE:HE2	2.34	0.57
1:B:209:MSE:HE3	1:B:224:LYS:HG2	1.86	0.57
2:D:439:ARG:O	2:D:439:ARG:HG3	2.00	0.57
1:C:225:GLY:O	1:C:370:GLY:HA2	2.04	0.57
1:A:348:MSE:HE3	1:A:348:MSE:HA	1.87	0.57
1:C:399:GLU:OE1	1:C:401:VAL:HG12	2.05	0.56
1:C:24:ILE:HG21	2:D:60:THR:HG23	1.88	0.56
1:C:320:MSE:CE	1:C:322:TYR:CD2	2.86	0.56
1:C:135:ILE:HD13	1:C:148:LYS:HD3	1.88	0.56
2:D:306:MSE:HE2	2:D:311:LYS:HA	1.86	0.56
1:A:397:ILE:HD12	1:A:402:THR:HG21	1.88	0.56
1:A:445:MSE:HG2	1:A:453:TRP:CD1	2.41	0.56
1:C:25:GLN:HG3	2:D:61:SER:HG	1.70	0.56
1:C:108:GLN:O	1:C:109:LEU:HD23	2.06	0.56
1:C:415:LEU:HA	1:C:427:SER:O	2.05	0.56
1:C:235:GLY:HA3	2:F:350:ARG:HH21	1.71	0.56
1:C:513:THR:HG23	1:C:517:LYS:HD3	1.88	0.56
2:D:170:VAL:CG1	2:D:172:ASP:HB2	2.36	0.56
2:D:438:PRO:O	2:D:441:GLU:HG2	2.06	0.56
2:D:251:THR:OG1	2:D:305:THR:O	2.22	0.55
1:C:485:ASN:HD22	1:C:533:ARG:HH11	1.54	0.55
2:D:126:GLU:OE2	2:D:290:ARG:NH1	2.40	0.55
1:A:399:GLU:HB2	1:A:400:PRO:CD	2.36	0.55
1:B:274:PRO:HA	1:B:286:MSE:HG2	1.88	0.55
2:F:212:ASN:HD21	2:F:221:ARG:HG2	1.69	0.55
2:F:224:THR:HB	2:F:225:PRO:HD3	1.87	0.55
2:D:181:PHE:HD2	2:D:211:MSE:HE1	1.72	0.55
2:F:55:GLN:HE22	2:F:264:ARG:HE	1.54	0.55
1:C:141:GLU:OE2	1:C:147:HIS:CD2	2.58	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:GLU:HB3	1:C:581:ILE:HD12	1.87	0.55
2:D:158:LYS:HD2	2:D:193:PHE:CD2	2.42	0.55
2:E:306:MSE:HG2	2:E:316:PRO:HG3	1.89	0.55
2:D:184:ILE:CD1	2:D:225:PRO:HG3	2.36	0.55
1:C:526:LEU:O	1:C:530:LYS:HG2	2.05	0.55
2:D:183:ALA:HB1	2:D:186:ILE:HD11	1.88	0.55
2:F:125:ASP:O	2:F:126:GLU:HB2	2.06	0.55
2:F:191:ALA:O	2:F:195:MSE:HG2	2.06	0.55
2:F:250:MSE:HA	2:F:250:MSE:CE	2.34	0.55
2:E:138:LEU:HD23	2:E:369:MSE:HG3	1.88	0.55
1:C:85:ASP:HB3	1:C:91:LEU:HD21	1.89	0.55
1:C:317:PHE:CD1	1:C:320:MSE:HE1	2.34	0.54
2:D:126:GLU:N	2:D:126:GLU:OE1	2.39	0.54
2:D:338:ILE:HG23	2:D:414:ASN:HB2	1.88	0.54
2:F:146:LYS:HD2	2:F:323:THR:HA	1.89	0.54
2:F:94:GLY:HA3	2:F:227:MSE:HE2	1.89	0.54
2:E:103:ILE:HG13	2:E:103:ILE:O	2.06	0.54
2:F:439:ARG:HH11	2:F:439:ARG:HG2	1.71	0.54
1:A:148:LYS:H	1:A:320:MSE:HE3	1.72	0.54
2:F:34:MSE:HE1	2:F:40:ARG:HG3	1.90	0.54
1:A:256:TYR:C	1:A:256:TYR:CD2	2.86	0.54
1:A:24:ILE:HG21	2:E:60:THR:HG23	1.89	0.54
1:C:320:MSE:CE	1:C:322:TYR:CE2	2.85	0.54
2:E:13:GLY:O	2:E:60:THR:CG2	2.51	0.54
1:A:298:MSE:HA	1:A:298:MSE:HE2	1.91	0.53
1:C:247:LYS:HA	1:C:285:LEU:HD11	1.89	0.53
2:E:34:MSE:HB3	2:E:36:ASN:ND2	2.22	0.53
1:B:418:SER:HA	1:B:421:GLN:HG2	1.89	0.53
1:A:267:THR:OG1	2:D:121:ARG:HB3	2.08	0.53
1:C:304:GLU:HG3	1:C:334:TRP:HE1	1.74	0.53
1:C:237:GLY:O	1:C:238:LYS:C	2.52	0.53
1:C:517:LYS:HE2	1:C:521:MSE:CE	2.38	0.53
1:C:77:PRO:CG	1:C:187:MSE:HE2	2.29	0.53
1:C:320:MSE:HE3	1:C:322:TYR:HD2	1.70	0.53
2:D:354:LYS:O	2:D:360:LYS:HE3	2.09	0.53
1:B:200:LYS:HE3	1:B:379:GLN:HG2	1.91	0.53
1:C:178:THR:OG1	1:C:179:GLU:N	2.39	0.53
2:F:439:ARG:HG2	2:F:439:ARG:NH1	2.24	0.53
2:D:440:THR:C	2:D:441:GLU:OE1	2.52	0.53
2:F:313:HIS:ND1	2:F:315:ILE:HG12	2.24	0.53
2:F:439:ARG:CG	2:F:439:ARG:NH1	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:ASN:ND2	1:C:507:ASP:HB2	2.24	0.52
2:D:307:PRO:C	2:D:308:GLU:HG2	2.34	0.52
2:E:36:ASN:C	2:E:36:ASN:HD22	2.16	0.52
2:F:254:ALA:CB	2:F:315:ILE:HD12	2.39	0.52
1:C:40:ILE:HD12	1:C:345:LEU:HD11	1.90	0.52
2:D:445:ILE:O	2:D:446:LYS:C	2.49	0.52
2:D:138:LEU:HA	2:D:369:MSE:HG3	1.91	0.52
2:E:36:ASN:HD21	2:E:38:GLU:HB2	1.74	0.52
2:E:412:TYR:O	2:E:421:ARG:NH1	2.41	0.52
2:F:138:LEU:HA	2:F:369:MSE:HG3	1.91	0.52
1:C:331:THR:HG21	1:C:388:SER:HB3	1.92	0.52
1:B:209:MSE:HE1	1:B:251:VAL:CG1	2.40	0.52
2:D:138:LEU:HD12	2:D:344:VAL:HG11	1.92	0.52
2:D:278:TYR:HD1	2:D:318:LEU:HD22	1.74	0.52
2:F:21:VAL:HG22	2:F:50:ASP:O	2.10	0.52
1:A:273:PHE:HB3	1:A:286:MSE:HE2	1.92	0.51
2:D:13:GLY:O	2:D:60:THR:HG21	2.10	0.51
2:D:146:LYS:HD3	2:D:285:PHE:O	2.11	0.51
2:D:204:ILE:C	2:D:206:ARG:H	2.18	0.51
2:D:439:ARG:C	2:D:441:GLU:N	2.68	0.51
2:E:271:ARG:HB2	2:E:314:PRO:HG3	1.91	0.51
1:A:258:GLY:HA2	1:A:329:ASP:O	2.10	0.51
1:B:577:ILE:O	1:B:581:ILE:HG12	2.09	0.51
2:F:313:HIS:CE1	2:F:315:ILE:HG12	2.45	0.51
1:C:2:GLN:HE22	1:C:21:GLU:H	1.58	0.51
1:C:142:THR:HG21	1:C:287:GLU:O	2.11	0.51
1:C:209:MSE:HE1	1:C:251:VAL:HG13	1.91	0.51
2:D:122:ASP:OD2	2:D:292:ARG:HG2	2.11	0.51
2:E:92:GLY:O	2:E:227:MSE:HG3	2.11	0.51
2:F:362:ARG:HD2	2:F:364:ASP:OD1	2.11	0.51
1:A:274:PRO:HA	1:A:286:MSE:HG2	1.92	0.51
1:B:139:VAL:HG21	1:B:187:MSE:HE1	1.90	0.51
2:E:135:ILE:O	2:E:139:ASN:C	2.54	0.51
2:E:151:SER:OG	2:E:152:GLY:N	2.42	0.51
2:F:181:PHE:CD2	2:F:211:MSE:HE1	2.43	0.51
2:D:226:ARG:NH2	3:D:506:HOH:O	2.41	0.51
2:F:339:GLN:HE21	2:F:416:GLY:HA2	1.74	0.51
2:F:155:LEU:HD21	2:F:331:ARG:HG2	1.93	0.51
1:C:12:PRO:CG	1:C:341:MSE:HE1	2.42	0.50
1:C:435:SER:C	1:C:437:TYR:H	2.20	0.50
2:F:125:ASP:O	2:F:143:ARG:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ASP:C	1:B:85:ASP:OD1	2.53	0.50
1:C:371:ARG:NH1	1:C:381:GLU:OE2	2.44	0.50
1:C:484:ASP:HB3	1:C:536:LEU:HD22	1.93	0.50
2:F:148:PRO:HA	2:F:302:PRO:HD2	1.94	0.50
1:B:231:PRO:HA	1:B:390:VAL:O	2.12	0.50
1:C:139:VAL:CG2	1:C:187:MSE:HE3	2.38	0.50
2:D:222:ILE:CD1	2:D:260:ILE:HD13	2.41	0.50
2:D:248:THR:HG22	2:D:303:ILE:HB	1.93	0.50
1:B:134:ASP:O	1:B:150:MSE:HA	2.11	0.50
1:C:248:TRP:CE2	1:C:512:PHE:HB2	2.47	0.50
1:A:188:MSE:HG2	1:A:189:GLN:N	2.26	0.50
2:D:166:ARG:NH2	2:D:417:PHE:O	2.45	0.50
2:D:184:ILE:HD12	2:D:250:MSE:CE	2.23	0.49
1:A:188:MSE:HE3	1:A:189:GLN:C	2.37	0.49
1:C:83:MSE:HE1	1:C:270:VAL:HG21	1.95	0.49
1:A:27:MSE:HE2	3:A:606:HOH:O	2.11	0.49
1:C:578:LYS:HA	1:C:581:ILE:HG22	1.94	0.49
1:A:80:ILE:O	1:A:81:SER:HB2	2.12	0.49
1:A:144:ILE:HD12	1:A:287:GLU:HB2	1.94	0.49
2:D:34:MSE:HG2	2:D:63:ILE:HG12	1.95	0.49
2:E:129:GLN:O	2:E:168:ALA:HA	2.13	0.49
1:C:327:MSE:HE2	1:C:387:ILE:CG1	2.42	0.49
2:E:182:ALA:HB3	2:E:247:MSE:HG2	1.94	0.49
2:F:226:ARG:NH2	2:F:253:TYR:OH	2.44	0.49
1:B:10:SER:HB2	2:E:46:GLU:HG3	1.94	0.49
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.93	0.49
1:C:399:GLU:HG2	1:C:400:PRO:CD	2.41	0.49
2:D:264:ARG:NE	3:D:501:HOH:O	2.45	0.49
1:A:27:MSE:CE	3:A:606:HOH:O	2.61	0.49
1:B:241:VAL:O	1:B:245:ILE:HG12	2.13	0.49
1:C:436:LEU:HD11	2:D:154:GLY:HA2	1.95	0.49
2:E:401:TYR:O	2:E:404:PHE:HB3	2.12	0.49
2:F:315:ILE:HB	2:F:316:PRO:CD	2.43	0.49
2:D:306:MSE:HE1	2:D:311:LYS:HG2	1.95	0.48
2:E:250:MSE:O	2:E:253:TYR:HB3	2.13	0.48
2:F:315:ILE:HB	2:F:316:PRO:HD3	1.95	0.48
1:B:295:THR:C	1:B:297:ASN:H	2.22	0.48
1:C:447:GLN:O	1:C:447:GLN:CD	2.56	0.48
2:F:396:ASP:HA	2:F:399:LYS:HG2	1.96	0.48
1:C:326:ILE:C	1:C:327:MSE:HE3	2.38	0.48
1:C:331:THR:CG2	1:C:389:ALA:O	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:102:GLU:CB	2:E:103:ILE:HG22	2.42	0.48
1:C:447:GLN:CD	1:C:447:GLN:C	2.80	0.48
2:E:94:GLY:HA3	2:E:227:MSE:CE	2.44	0.48
2:E:137:HIS:O	2:E:365:HIS:HE1	1.96	0.48
1:B:27:MSE:HE3	1:B:71:LEU:H	1.79	0.48
1:B:95:MSE:HG3	2:E:119:ILE:HD11	1.96	0.48
1:C:135:ILE:CD1	1:C:148:LYS:HD3	2.43	0.48
1:C:231:PRO:HG2	1:C:412:PHE:HE1	1.79	0.48
2:D:91:ASP:HA	2:D:211:MSE:O	2.13	0.48
1:A:203:LEU:HB2	1:A:371:ARG:HG2	1.94	0.48
1:C:450:GLN:O	1:C:451:GLN:NE2	2.47	0.48
2:D:103:ILE:O	2:D:105:PRO:HD3	2.13	0.48
2:E:171:LEU:HA	2:E:172:ASP:HA	1.52	0.48
1:A:273:PHE:HB3	1:A:286:MSE:CE	2.44	0.48
1:B:60:PRO:CD	2:E:47:VAL:HG13	2.35	0.48
1:B:97:VAL:HG21	1:B:109:LEU:HD21	1.95	0.48
2:D:79:LEU:HD13	2:D:227:MSE:HE3	1.92	0.48
2:F:26:TYR:O	2:F:27:GLU:HB2	2.12	0.48
1:A:133:GLY:CA	1:A:150:MSE:HE2	2.38	0.48
1:A:266:MSE:HE3	1:A:294:ASN:C	2.38	0.48
1:B:466:GLU:HG2	1:B:489:THR:HG21	1.95	0.48
1:C:80:ILE:O	1:C:81:SER:HB2	2.12	0.48
1:B:52:TYR:O	1:B:299:PRO:HB3	2.13	0.48
1:B:485:ASN:HD21	1:B:533:ARG:HH11	1.62	0.48
2:D:170:VAL:HG12	2:D:172:ASP:HB2	1.95	0.48
1:C:8:LYS:HB3	1:C:15:MSE:CG	2.38	0.47
1:C:239:THR:C	1:C:241:VAL:H	2.22	0.47
2:F:184:ILE:HD11	2:F:225:PRO:HG3	1.95	0.47
1:C:474:VAL:C	1:C:476:LEU:H	2.21	0.47
2:E:222:ILE:HD11	2:E:260:ILE:HD13	1.92	0.47
2:E:363:GLU:HG2	2:E:364:ASP:N	2.29	0.47
2:E:365:HIS:HB3	3:E:511:HOH:O	2.14	0.47
2:F:184:ILE:CD1	2:F:225:PRO:HG3	2.45	0.47
1:A:90:PRO:HG2	1:A:93:THR:HB	1.95	0.47
1:B:126:GLU:HG2	1:B:162:ILE:HG22	1.97	0.47
1:B:315:GLU:HA	1:B:384:ILE:HD11	1.96	0.47
1:A:59:GLY:O	1:A:62:GLU:HG3	2.14	0.47
1:B:210:ILE:HD11	1:B:515:ARG:NH2	2.29	0.47
2:E:36:ASN:ND2	2:E:38:GLU:H	2.12	0.47
2:F:94:GLY:CA	2:F:227:MSE:HE2	2.45	0.47
1:A:38:GLU:OE1	1:A:52:TYR:OH	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:325:GLY:H	2:F:350:ARG:NH1	2.13	0.47
2:F:339:GLN:HE21	2:F:417:PHE:H	1.62	0.47
2:E:36:ASN:HD22	2:E:37:GLY:N	2.13	0.47
2:E:265:ARG:HG2	2:E:265:ARG:HH11	1.79	0.47
1:A:160:GLN:HE21	1:A:160:GLN:HB3	1.48	0.47
1:B:417:SER:O	1:B:421:GLN:HG2	2.15	0.47
1:C:169:ILE:HB	1:C:188:MSE:HB2	1.97	0.47
2:F:34:MSE:HG2	2:F:63:ILE:HG12	1.96	0.47
2:D:215:ASN:C	2:D:215:ASN:HD22	2.22	0.47
2:D:250:MSE:HE2	2:D:250:MSE:HA	1.96	0.47
2:F:383:LYS:HA	2:F:383:LYS:HE2	1.96	0.47
1:C:12:PRO:HG3	1:C:341:MSE:HE1	1.96	0.47
1:A:454:SER:O	1:A:458:THR:HG23	2.15	0.46
1:C:244:GLN:HA	1:C:247:LYS:HD3	1.96	0.46
2:D:166:ARG:CD	2:D:201:THR:HG21	2.46	0.46
2:E:171:LEU:HD23	2:E:171:LEU:H	1.80	0.46
1:C:407:ARG:NH2	2:D:252:ASN:ND2	2.63	0.46
2:D:158:LYS:HG3	2:D:194:PHE:CZ	2.50	0.46
2:D:267:VAL:HA	2:D:268:PRO:HD3	1.79	0.46
2:F:16:MSE:HE1	2:F:70:VAL:HG21	1.96	0.46
1:A:295:THR:C	1:A:297:ASN:H	2.23	0.46
1:A:441:VAL:O	1:A:445:MSE:HB2	2.15	0.46
2:D:340:PRO:HD2	2:D:413:VAL:O	2.14	0.46
1:C:159:VAL:HA	1:C:176:ILE:HD13	1.97	0.46
2:D:280:ASN:O	2:D:283:THR:HB	2.15	0.46
2:E:285:PHE:HD1	2:E:300:GLN:HE22	1.63	0.46
1:A:231:PRO:HD2	1:A:413:TRP:O	2.16	0.46
1:C:90:PRO:HD3	1:C:111:ALA:HA	1.98	0.46
1:C:238:LYS:O	1:C:241:VAL:HB	2.15	0.46
1:C:482:LEU:HB3	1:C:487:ARG:HD3	1.98	0.46
2:E:11:VAL:HG22	2:E:16:MSE:HG2	1.96	0.46
2:E:126:GLU:HB3	2:E:143:ARG:NH2	2.29	0.46
2:E:126:GLU:CB	2:E:143:ARG:HH21	2.26	0.46
2:F:11:VAL:HG22	2:F:16:MSE:CG	2.37	0.46
1:B:485:ASN:O	1:B:485:ASN:ND2	2.49	0.46
1:C:415:LEU:HD23	1:C:428:ILE:HD13	1.98	0.46
2:E:94:GLY:CA	2:E:227:MSE:HE2	2.44	0.46
1:A:42:MSE:HE2	1:A:42:MSE:HB2	1.78	0.46
1:C:404:ASN:HA	1:C:407:ARG:HD3	1.97	0.46
2:E:280:ASN:O	2:E:283:THR:HB	2.16	0.46
1:A:202:LYS:HD3	2:E:188:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PRO:HG3	1:B:441:VAL:HG22	1.98	0.46
1:A:507:ASP:O	1:A:511:THR:HB	2.16	0.45
2:D:215:ASN:C	2:D:215:ASN:ND2	2.74	0.45
2:F:212:ASN:ND2	2:F:221:ARG:HG2	2.31	0.45
1:B:27:MSE:SE	1:B:38:GLU:HB2	2.65	0.45
2:D:111:ILE:HA	2:D:230:THR:OG1	2.17	0.45
2:E:36:ASN:ND2	2:E:36:ASN:C	2.74	0.45
2:E:45:LEU:HD11	2:E:264:ARG:HD3	1.98	0.45
1:A:528:PHE:HA	1:A:577:ILE:HG21	1.98	0.45
1:B:129:GLU:CD	1:B:129:GLU:H	2.24	0.45
1:C:83:MSE:SE	1:C:91:LEU:HD12	2.66	0.45
1:C:504:ASN:HD22	1:C:507:ASP:HB2	1.82	0.45
2:E:152:GLY:O	2:E:155:LEU:HB2	2.16	0.45
1:B:394:GLY:N	2:E:321:TYR:OH	2.49	0.45
1:C:247:LYS:HG3	1:C:248:TRP:CD1	2.51	0.45
2:D:210:PHE:O	2:D:211:MSE:HE2	2.16	0.45
2:D:172:ASP:HB3	2:D:173:SER:H	1.46	0.45
1:A:329:ASP:HA	1:A:330:SER:HA	1.62	0.45
1:B:318:ARG:HD2	1:B:372:VAL:CG2	2.47	0.45
1:C:83:MSE:HG3	1:C:291:LEU:HB3	1.97	0.45
1:A:278:ASP:HA	1:A:279:PRO:HD3	1.88	0.45
2:E:383:LYS:CA	2:E:386:ALA:HB3	2.38	0.45
1:A:95:MSE:HE2	1:A:95:MSE:HB3	1.80	0.45
1:A:274:PRO:HG3	1:A:286:MSE:HE3	1.98	0.45
1:B:33:LEU:HD12	1:B:33:LEU:H	1.82	0.45
1:B:261:GLU:CG	1:B:266:MSE:CE	2.91	0.45
1:B:329:ASP:HA	1:B:330:SER:HA	1.65	0.45
1:C:521:MSE:CE	1:C:560:LYS:HA	2.47	0.45
2:D:170:VAL:HG13	2:D:172:ASP:H	1.80	0.45
2:D:213:LEU:O	2:D:216:ASP:HB2	2.17	0.45
2:F:55:GLN:NE2	2:F:264:ARG:HE	2.14	0.45
2:F:210:PHE:O	2:F:211:MSE:HE2	2.17	0.45
2:F:250:MSE:HB2	2:F:304:LEU:HB3	1.98	0.44
1:A:266:MSE:HE2	1:A:294:ASN:O	2.17	0.44
1:A:212:GLY:HA3	1:A:512:PHE:CD1	2.52	0.44
1:C:270:VAL:HA	1:C:286:MSE:CE	2.47	0.44
1:C:325:ALA:HB1	1:C:327:MSE:HE1	2.00	0.44
2:F:151:SER:OG	2:F:152:GLY:N	2.51	0.44
2:F:246:ILE:HD13	2:F:301:ILE:HB	1.99	0.44
1:C:126:GLU:HG2	1:C:160:GLN:O	2.18	0.44
2:D:281:LEU:HD23	2:D:281:LEU:HA	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:PRO:HG3	1:C:441:VAL:HG13	1.99	0.44
1:C:270:VAL:HA	1:C:286:MSE:HE3	2.00	0.44
2:D:181:PHE:CD2	2:D:211:MSE:HE1	2.51	0.44
2:D:258:ARG:HD2	2:D:273:TYR:CE1	2.52	0.44
2:E:19:GLU:OE1	2:E:20:LYS:HE2	2.16	0.44
1:A:52:TYR:N	1:A:52:TYR:CD1	2.84	0.44
2:D:264:ARG:CD	3:D:501:HOH:O	2.61	0.44
2:D:286:GLU:OE1	2:D:286:GLU:HA	2.17	0.44
1:B:119:TRP:CZ3	1:B:165:GLY:HA2	2.53	0.44
2:D:222:ILE:HD12	2:D:260:ILE:HD13	2.00	0.44
2:E:3:LYS:HE2	2:E:22:SER:O	2.17	0.44
1:B:465:GLN:O	1:B:469:GLN:HG2	2.18	0.43
1:C:253:LEU:HD13	1:C:317:PHE:HB3	1.99	0.43
1:C:255:VAL:O	1:C:326:ILE:HA	2.17	0.43
1:A:5:LYS:HE2	1:A:5:LYS:HB3	1.80	0.43
1:A:80:ILE:O	1:A:81:SER:CB	2.64	0.43
1:A:148:LYS:HG3	1:A:320:MSE:HE3	2.00	0.43
2:D:439:ARG:O	2:D:441:GLU:N	2.52	0.43
2:E:434:LEU:C	2:E:436:MSE:H	2.26	0.43
2:F:229:LEU:HG	2:F:247:MSE:HE1	2.00	0.43
1:A:60:PRO:HD3	2:D:47:VAL:CG1	2.41	0.43
1:B:80:ILE:HD13	1:B:253:LEU:HD21	2.00	0.43
1:C:198:PRO:HB2	1:C:375:LEU:HD11	1.99	0.43
2:E:383:LYS:O	2:E:387:VAL:HG23	2.18	0.43
2:D:386:ALA:O	2:D:390:GLY:HA2	2.18	0.43
2:E:249:ASP:OD1	2:E:304:LEU:HA	2.19	0.43
1:A:490:LEU:HD23	1:A:490:LEU:HA	1.91	0.43
1:B:15:MSE:HB3	1:B:15:MSE:HE2	1.69	0.43
2:E:162:ALA:O	2:E:166:ARG:HG3	2.19	0.43
1:A:27:MSE:HE3	1:A:71:LEU:CB	2.32	0.43
1:A:93:THR:HG22	1:A:109:LEU:HD13	2.00	0.43
1:A:242:GLN:HB3	1:A:327:MSE:HE1	1.99	0.43
1:B:405:THR:C	1:B:407:ARG:H	2.26	0.43
1:C:143:LYS:HD3	1:C:287:GLU:OE2	2.18	0.43
2:D:307:PRO:O	2:D:308:GLU:HG2	2.19	0.43
1:A:262:ARG:HB2	1:A:265:GLU:HG3	2.01	0.43
1:A:413:TRP:HB3	1:A:428:ILE:HD13	2.01	0.43
1:A:445:MSE:CG	1:A:453:TRP:CD1	3.01	0.43
1:B:345:LEU:O	1:B:346:GLU:HB2	2.19	0.43
2:D:179:VAL:O	2:D:207:SER:HA	2.18	0.43
1:A:520:ASN:O	1:A:524:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:408:PHE:HA	2:D:433:LEU:HD11	2.01	0.43
2:E:278:TYR:C	2:E:278:TYR:HD2	2.23	0.43
2:F:142:VAL:CG2	2:F:351:LEU:O	2.67	0.43
2:F:345:LEU:HB2	2:F:346:PRO:HD3	2.00	0.43
1:A:484:ASP:OD1	1:A:541:TYR:HD1	2.01	0.43
1:C:317:PHE:HA	1:C:320:MSE:HE2	2.00	0.43
2:D:255:GLU:OE1	2:D:273:TYR:OH	2.34	0.43
2:D:445:ILE:C	2:D:447:ASP:N	2.76	0.43
1:A:261:GLU:CG	1:A:266:MSE:CE	2.93	0.42
1:A:494:LYS:NZ	3:A:633:HOH:O	2.52	0.42
2:E:330:THR:OG1	2:E:333:LEU:HD12	2.18	0.42
1:A:261:GLU:HB2	1:A:266:MSE:HE2	2.01	0.42
1:A:271:ASN:OD1	2:D:292:ARG:NH2	2.52	0.42
2:D:190:GLU:O	2:D:193:PHE:HB3	2.19	0.42
2:E:45:LEU:HD23	2:E:45:LEU:HA	1.85	0.42
1:A:261:GLU:CB	1:A:266:MSE:HE2	2.48	0.42
1:A:191:TRP:CD2	1:A:192:PRO:HD2	2.54	0.42
1:A:553:ARG:HA	1:A:556:ILE:HD12	2.01	0.42
1:C:298:MSE:HG3	2:F:115:VAL:HG11	2.00	0.42
2:D:180:VAL:HG22	2:D:208:VAL:HB	2.01	0.42
2:F:233:GLU:CD	2:F:287:ARG:HE	2.27	0.42
1:A:261:GLU:HG2	1:A:266:MSE:HE1	2.00	0.42
2:D:30:ILE:HG22	2:D:72:PHE:CD1	2.55	0.42
2:E:126:GLU:CB	2:E:143:ARG:NH2	2.83	0.42
2:E:163:GLN:HG3	2:E:417:PHE:O	2.19	0.42
2:F:31:GLU:HG3	2:F:41:ARG:HG2	2.01	0.42
1:B:83:MSE:HG2	1:B:291:LEU:HB3	2.02	0.42
1:B:70:ALA:O	1:B:71:LEU:C	2.61	0.42
1:C:329:ASP:HA	1:C:330:SER:HA	1.63	0.42
2:F:399:LYS:HG3	2:F:400:ILE:HG13	2.02	0.42
1:A:258:GLY:HA3	1:A:266:MSE:HE1	2.01	0.42
1:A:570:ILE:O	1:A:571:SER:C	2.63	0.42
1:B:348:MSE:HB2	2:F:262:ALA:HB1	2.02	0.42
2:F:452:LYS:H	2:F:454:LEU:N	2.17	0.42
1:A:387:ILE:HG23	1:A:413:TRP:HZ3	1.85	0.42
2:F:94:GLY:HA3	2:F:227:MSE:CE	2.50	0.42
2:F:136:ASP:O	2:F:140:THR:HG22	2.19	0.42
1:B:242:GLN:HB3	1:B:327:MSE:CE	2.50	0.42
1:C:216:ILE:HG23	1:C:413:TRP:CZ2	2.54	0.42
1:C:449:LEU:O	1:C:450:GLN:HB2	2.20	0.42
1:B:56:SER:HB3	1:B:105:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:LYS:O	1:B:527:THR:N	2.52	0.41
1:C:60:PRO:HD3	2:F:47:VAL:HG13	2.02	0.41
2:D:148:PRO:HD2	2:D:325:GLY:O	2.19	0.41
2:E:313:HIS:O	2:E:314:PRO:C	2.63	0.41
1:A:248:TRP:CZ3	1:A:279:PRO:HB3	2.55	0.41
1:B:11:GLY:HA2	2:E:26:TYR:CZ	2.55	0.41
1:B:89:ARG:HD2	1:B:94:PHE:HE1	1.85	0.41
1:C:315:GLU:HA	1:C:384:ILE:HD11	2.02	0.41
1:B:266:MSE:CE	1:B:294:ASN:O	2.52	0.41
1:C:32:ASP:OD2	1:C:62:GLU:HG2	2.21	0.41
1:C:294:ASN:HD22	1:C:298:MSE:HE2	1.85	0.41
2:F:28:GLU:OE2	2:F:72:PHE:HB3	2.21	0.41
1:A:295:THR:C	1:A:297:ASN:N	2.78	0.41
1:C:256:TYR:HE2	1:C:266:MSE:HE1	1.85	0.41
2:D:251:THR:HA	2:D:315:ILE:HD13	2.02	0.41
2:F:43:GLN:HG2	2:F:57:PHE:CE1	2.51	0.41
1:B:318:ARG:HD2	1:B:372:VAL:HG22	2.03	0.41
1:C:563:PRO:O	1:C:569:LYS:HG3	2.21	0.41
2:D:440:THR:O	2:D:441:GLU:OE1	2.38	0.41
2:F:225:PRO:HA	2:F:247:MSE:HE2	2.01	0.41
1:A:307:ILE:HB	1:A:365:TYR:CE1	2.56	0.41
1:A:392:PRO:HG2	1:A:397:ILE:HD13	2.01	0.41
1:C:233:PRO:HA	2:F:321:TYR:OH	2.21	0.41
1:C:456:MSE:HG2	1:C:526:LEU:HD22	2.03	0.41
2:D:145:GLN:HG3	2:D:351:LEU:HD12	2.03	0.41
2:D:249:ASP:OD2	2:D:249:ASP:C	2.64	0.41
2:E:45:LEU:HD21	2:E:264:ARG:NH1	2.36	0.41
2:F:379:GLY:HA3	2:F:405:ALA:HB2	2.03	0.41
2:E:277:LEU:HD23	2:E:318:LEU:HD12	2.03	0.41
2:F:339:GLN:HA	2:F:340:PRO:HA	1.86	0.41
1:C:209:MSE:HG2	1:C:211:THR:HG22	2.02	0.40
1:C:256:TYR:CE2	1:C:266:MSE:HE1	2.56	0.40
2:E:271:ARG:HB2	2:E:314:PRO:CG	2.51	0.40
1:B:271:ASN:O	1:B:274:PRO:HD2	2.22	0.40
1:C:207:VAL:HA	1:C:208:PRO:HD3	1.92	0.40
2:F:179:VAL:O	2:F:207:SER:HA	2.20	0.40
1:C:445:MSE:HA	1:C:445:MSE:HE2	2.02	0.40
2:D:183:ALA:HB1	2:D:186:ILE:CD1	2.51	0.40
2:E:252:ASN:HD22	2:E:252:ASN:HA	1.74	0.40
2:E:265:ARG:HG2	2:E:265:ARG:NH1	2.36	0.40
2:F:446:LYS:O	2:F:450:LEU:CA	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:VAL:O	2:D:39:ILE:HA	2.21	0.40
2:E:88:ARG:NH1	2:E:101:PRO:O	2.49	0.40
1:B:307:ILE:HD12	1:B:365:TYR:CD1	2.57	0.40
1:B:369:SER:HB2	1:B:384:ILE:O	2.22	0.40
2:D:45:LEU:HD21	2:D:55:GLN:HB2	2.04	0.40
2:D:159:GLU:HB3	2:D:417:PHE:CD1	2.57	0.40
2:D:324:GLU:HA	2:D:350:ARG:HD2	2.04	0.40
2:E:171:LEU:CD2	2:E:171:LEU:H	2.34	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	584/600 (97%)	556 (95%)	27 (5%)	1 (0%)	43	72
1	B	584/600 (97%)	540 (92%)	41 (7%)	3 (0%)	24	55
1	C	581/600 (97%)	537 (92%)	42 (7%)	2 (0%)	36	66
2	D	443/465 (95%)	407 (92%)	31 (7%)	5 (1%)	11	36
2	E	445/465 (96%)	411 (92%)	33 (7%)	1 (0%)	43	72
2	F	449/465 (97%)	407 (91%)	39 (9%)	3 (1%)	18	47
All	All	3086/3195 (97%)	2858 (93%)	213 (7%)	15 (0%)	24	55

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	174	SER
2	D	392	SER
1	C	280	ASN
2	D	172	ASP

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Mol	Chain	Res	Type
1	B	391	SER
1	B	477	VAL
1	C	563	PRO
2	D	440	THR
2	F	414	ASN
2	F	134	ALA
1	B	260	GLY
2	D	445	ILE
2	E	435	ALA
1	A	260	GLY
2	F	101	PRO

5.3.2 Protein sidechains [i](#)

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	501/487 (103%)	470 (94%)	31 (6%)	16	45
1	B	500/487 (103%)	469 (94%)	31 (6%)	16	45
1	C	489/487 (100%)	449 (92%)	40 (8%)	10	33
2	D	358/372 (96%)	319 (89%)	39 (11%)	6	21
2	E	355/372 (95%)	320 (90%)	35 (10%)	7	24
2	F	356/372 (96%)	336 (94%)	20 (6%)	19	50
All	All	2559/2577 (99%)	2363 (92%)	196 (8%)	12	36

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	92	ASP
1	A	94	PHE
1	A	103	LEU
1	A	124	ILE
1	A	125	GLU
1	A	146	GLN

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Mol	Chain	Res	Type
1	A	160	GLN
1	A	173	ILE
1	A	267	THR
1	A	268	ASP
1	A	277	ILE
1	A	285	LEU
1	A	330	SER
1	A	338	LEU
1	A	387	ILE
1	A	397	ILE
1	A	428	ILE
1	A	445	MSE
1	A	454	SER
1	A	458	THR
1	A	465	GLN
1	A	466	GLU
1	A	479	ILE
1	A	485	ASN
1	A	488	LEU
1	A	534	LYS
1	A	547	GLU
1	A	569	LYS
1	A	571	SER
1	A	575	GLU
1	B	2	GLN
1	B	21	GLU
1	B	29	LEU
1	B	40	ILE
1	B	73	VAL
1	B	92	ASP
1	B	103	LEU
1	B	129	GLU
1	B	160	GLN
1	B	161	LYS
1	B	188	MSE
1	B	195	ARG
1	B	209	MSE
1	B	210	ILE
1	B	230	VAL
1	B	253	LEU
1	B	273	PHE
1	B	277	ILE

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Mol	Chain	Res	Type
1	B	285	LEU
1	B	291	LEU
1	B	338	LEU
1	B	360	SER
1	B	378	ASP
1	B	445	MSE
1	B	453	TRP
1	B	477	VAL
1	B	481	SER
1	B	559	SER
1	B	569	LYS
1	B	571	SER
1	B	575	GLU
1	C	36	ILE
1	C	103	LEU
1	C	123	THR
1	C	143	LYS
1	C	144	ILE
1	C	160	GLN
1	C	161	LYS
1	C	166	SER
1	C	178	THR
1	C	180	GLN
1	C	230	VAL
1	C	239	THR
1	C	240	VAL
1	C	270	VAL
1	C	276	LEU
1	C	281	THR
1	C	285	LEU
1	C	288	ARG
1	C	327	MSE
1	C	331	THR
1	C	341	MSE
1	C	401	VAL
1	C	445	MSE
1	C	448	ILE
1	C	450	GLN
1	C	451	GLN
1	C	473	ILE
1	C	476	LEU
1	C	477	VAL

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Mol	Chain	Res	Type
1	C	494	LYS
1	C	506	PHE
1	C	509	VAL
1	C	514	SER
1	C	524	VAL
1	C	541	TYR
1	C	547	GLU
1	C	553	ARG
1	C	555	ARG
1	C	571	SER
1	C	580	THR
2	D	39	ILE
2	D	45	LEU
2	D	51	LYS
2	D	60	THR
2	D	61	SER
2	D	71	ARG
2	D	73	LEU
2	D	82	SER
2	D	115	VAL
2	D	121	ARG
2	D	122	ASP
2	D	158	LYS
2	D	170	VAL
2	D	215	ASN
2	D	248	THR
2	D	257	LEU
2	D	280	ASN
2	D	283	THR
2	D	291	ILE
2	D	305	THR
2	D	308	GLU
2	D	329	LEU
2	D	353	ASP
2	D	354	LYS
2	D	361	THR
2	D	368	THR
2	D	378	GLN
2	D	385	LEU
2	D	395	SER
2	D	397	ILE
2	D	398	ASP

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Mol	Chain	Res	Type
2	D	403	LYS
2	D	406	GLU
2	D	424	THR
2	D	433	LEU
2	D	439	ARG
2	D	440	THR
2	D	441	GLU
2	D	442	LEU
2	E	6	ARG
2	E	21	VAL
2	E	33	ARG
2	E	34	MSE
2	E	36	ASN
2	E	66	LYS
2	E	73	LEU
2	E	104	LEU
2	E	110	ASP
2	E	114	GLU
2	E	146	LYS
2	E	170	VAL
2	E	171	LEU
2	E	172	ASP
2	E	204	ILE
2	E	219	ILE
2	E	248	THR
2	E	250	MSE
2	E	257	LEU
2	E	260	ILE
2	E	264	ARG
2	E	278	TYR
2	E	279	THR
2	E	321	TYR
2	E	352	LYS
2	E	354	LYS
2	E	360	LYS
2	E	363	GLU
2	E	380	LYS
2	E	381	GLN
2	E	384	GLU
2	E	391	GLU
2	E	397	ILE
2	E	403	LYS

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Mol	Chain	Res	Type
2	E	424	THR
2	F	15	LEU
2	F	19	GLU
2	F	22	SER
2	F	29	LEU
2	F	33	ARG
2	F	54	VAL
2	F	77	LEU
2	F	119	ILE
2	F	138	LEU
2	F	146	LYS
2	F	189	GLU
2	F	204	ILE
2	F	219	ILE
2	F	267	VAL
2	F	328	ILE
2	F	362	ARG
2	F	380	LYS
2	F	397	ILE
2	F	439	ARG
2	F	441	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	146	GLN
1	A	160	GLN
1	A	244	GLN
1	A	294	ASN
1	A	404	ASN
1	A	465	GLN
1	A	502	GLN
1	A	574	ASN
1	B	25	GLN
1	B	153	ASN
1	B	189	GLN
1	B	204	ASN
1	B	294	ASN
1	B	297	ASN
1	B	404	ASN
1	B	432	GLN

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Mol	Chain	Res	Type
1	B	485	ASN
1	B	574	ASN
1	C	2	GLN
1	C	147	HIS
1	C	153	ASN
1	C	160	GLN
1	C	201	GLN
1	C	264	ASN
1	C	294	ASN
1	C	451	GLN
1	C	485	ASN
1	C	502	GLN
1	C	504	ASN
1	C	520	ASN
2	D	55	GLN
2	D	99	ASN
2	D	112	ASN
2	D	137	HIS
2	D	139	ASN
2	D	163	GLN
2	D	252	ASN
2	D	300	GLN
2	D	365	HIS
2	D	370	ASN
2	D	378	GLN
2	E	36	ASN
2	E	112	ASN
2	E	167	GLN
2	E	200	GLN
2	E	252	ASN
2	E	300	GLN
2	E	339	GLN
2	E	365	HIS
2	E	370	ASN
2	E	381	GLN
2	E	410	ASN
2	F	43	GLN
2	F	55	GLN
2	F	137	HIS
2	F	139	ASN
2	F	242	HIS
2	F	339	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	563/600 (93%)	-0.62	2 (0%) 88 84	24, 41, 83, 117	0
1	B	563/600 (93%)	-0.16	1 (0%) 91 88	38, 71, 129, 155	0
1	C	561/600 (93%)	0.09	16 (2%) 53 43	38, 76, 175, 198	0
2	D	433/465 (93%)	-0.10	5 (1%) 76 68	34, 60, 133, 196	0
2	E	435/465 (93%)	-0.01	9 (2%) 63 54	32, 66, 167, 221	0
2	F	437/465 (93%)	0.27	17 (3%) 43 34	42, 91, 191, 212	0
All	All	2992/3195 (93%)	-0.11	50 (1%) 69 60	24, 66, 169, 221	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	444	ARG	4.2
1	C	584	ILE	3.7
2	F	438	PRO	3.6
2	D	452	LYS	3.2
1	B	567	LEU	3.1
2	F	393	ALA	3.1
1	C	571	SER	2.9
2	F	366	ALA	2.9
2	D	397	ILE	2.9
2	F	348	LEU	2.9
2	F	412	TYR	2.8
2	E	387	VAL	2.7
2	F	454	LEU	2.7
1	C	575	GLU	2.7
1	C	528	PHE	2.7
2	D	413	VAL	2.6
2	E	389	LEU	2.6
2	E	397	ILE	2.6
1	C	562	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	382	ALA	2.5
2	F	442	LEU	2.5
1	C	520	ASN	2.5
1	C	505	ALA	2.5
1	C	535	ALA	2.5
1	C	378	ASP	2.4
1	C	581	ILE	2.4
2	F	423	ILE	2.4
1	C	559	SER	2.4
1	A	586	SER	2.4
1	C	564	GLU	2.4
2	D	123	TYR	2.3
2	F	329	LEU	2.3
1	A	477	VAL	2.3
2	E	438	PRO	2.3
2	E	451	ASP	2.3
1	C	580	THR	2.2
2	F	350	ARG	2.2
2	F	364	ASP	2.2
2	F	387	VAL	2.2
2	E	376	TYR	2.2
2	F	453	TYR	2.2
1	C	144	ILE	2.1
1	C	570	ILE	2.1
2	F	354	LYS	2.1
2	D	442	LEU	2.1
2	F	385	LEU	2.1
2	E	385	LEU	2.1
1	C	573	ILE	2.1
2	F	427	LEU	2.1
2	E	448	ASP	2.1

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.