Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:01 PM GMT

PDB ID	:	3VR2
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

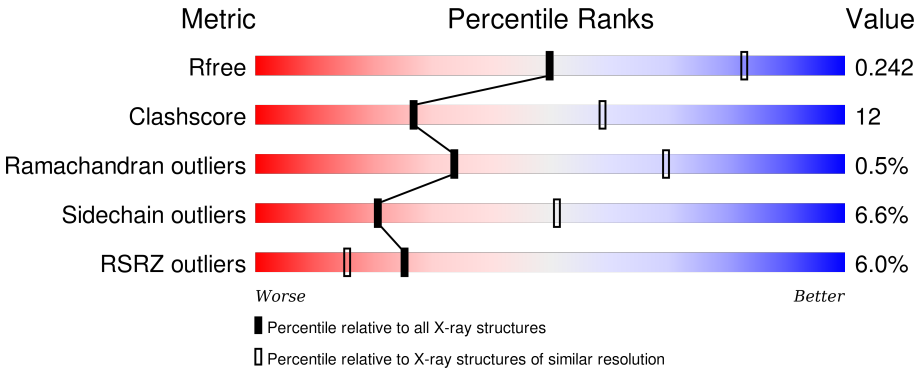
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	78% 18%
1	B	600	4% 78% 19%
1	C	600	8% 69% 25%
2	D	465	3% 67% 24% 5%
2	E	465	6% 74% 21%

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Mol	Chain	Length	Quality of chain
2	F	465	

2 Entry composition (i)

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
1	A	586	Total	C	N	O	S	Se	0	0	0
			4559	2864	766	904	3	22			
1	B	586	Total	C	N	O	S	Se	0	0	0
			4555	2862	766	902	3	22			
1	C	583	Total	C	N	O	S	Se	0	0	0
			4501	2829	757	890	3	22			

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	C	N	O	Se	0	0	0
			3447	2179	596	658	14			
2	E	449	Total	C	N	O	Se	0	0	0
			3448	2180	596	658	14			
2	F	451	Total	C	N	O	Se	0	0	0
			3454	2177	598	665	14			

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	O	0	0
			39	39		
3	B	8	Total	O	0	0
			8	8		
3	C	14	Total	O	0	0
			14	14		
3	D	8	Total	O	0	0
			8	8		

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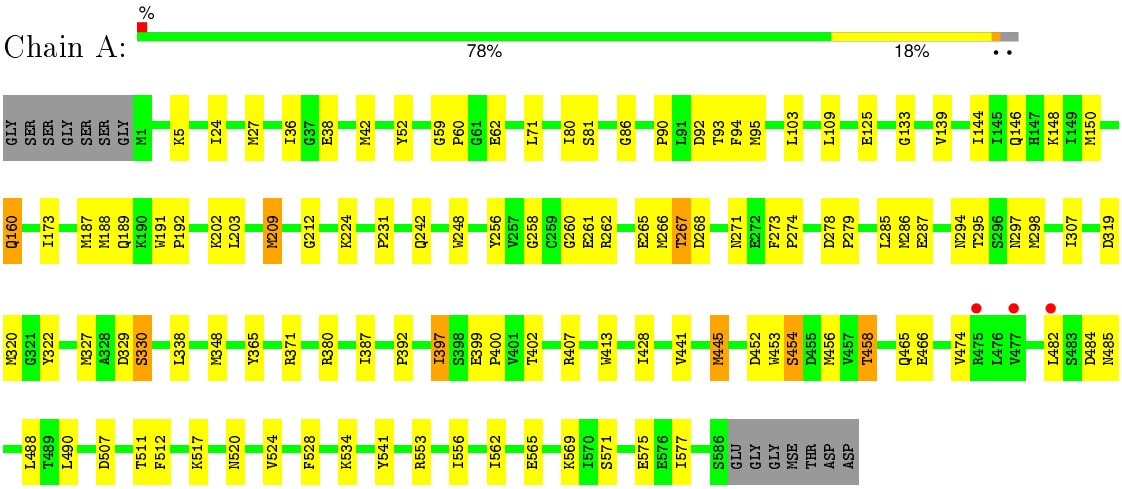
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	12	Total O 12 12	0	0
3	F	8	Total O 8 8	0	0

3 Residue-property plots (i)

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.

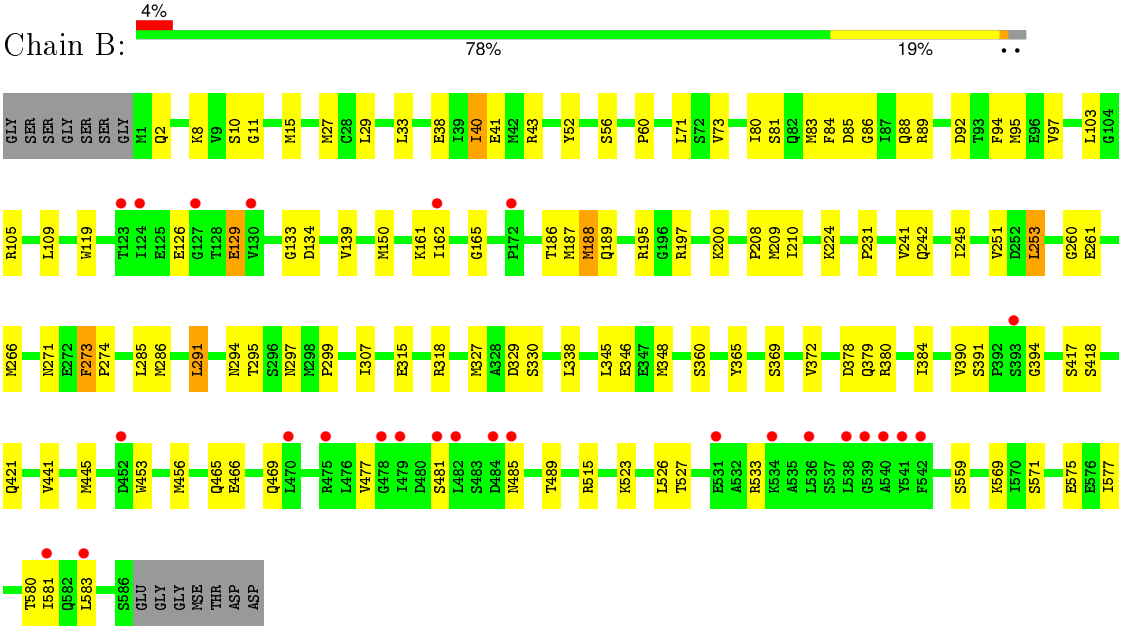
- Molecule 1: V-type sodium ATPase catalytic subunit A

Chain A:



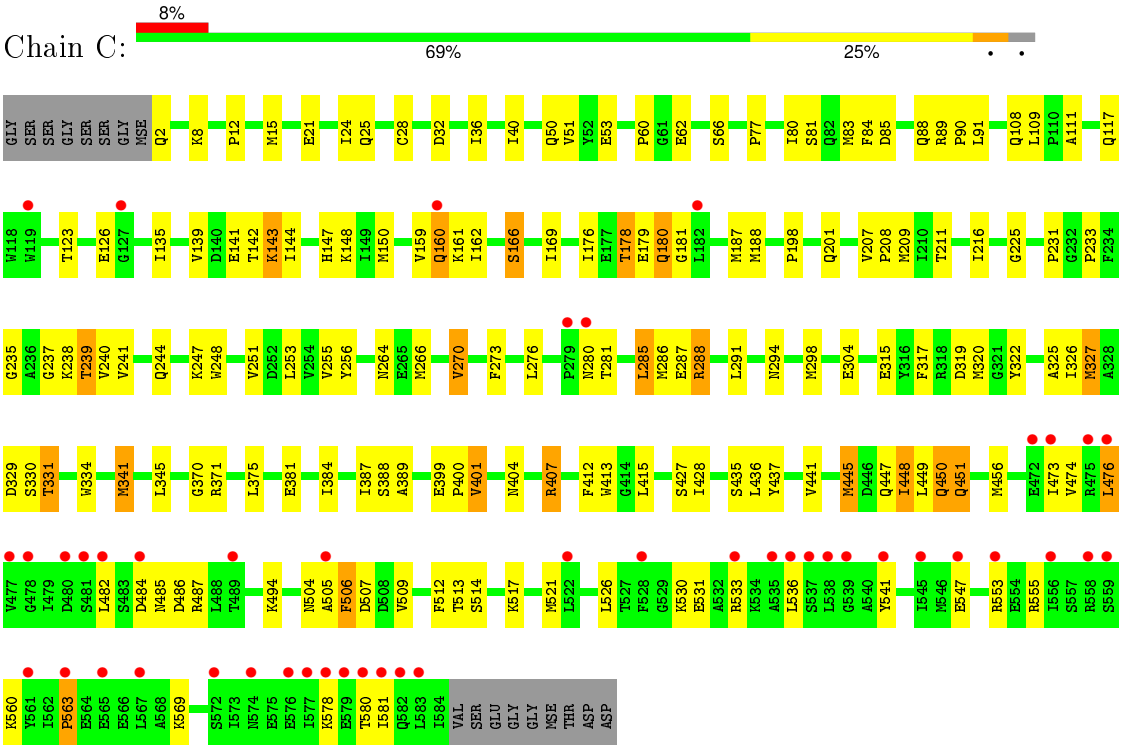
- Molecule 1: V-type sodium ATPase catalytic subunit A

Chain B:



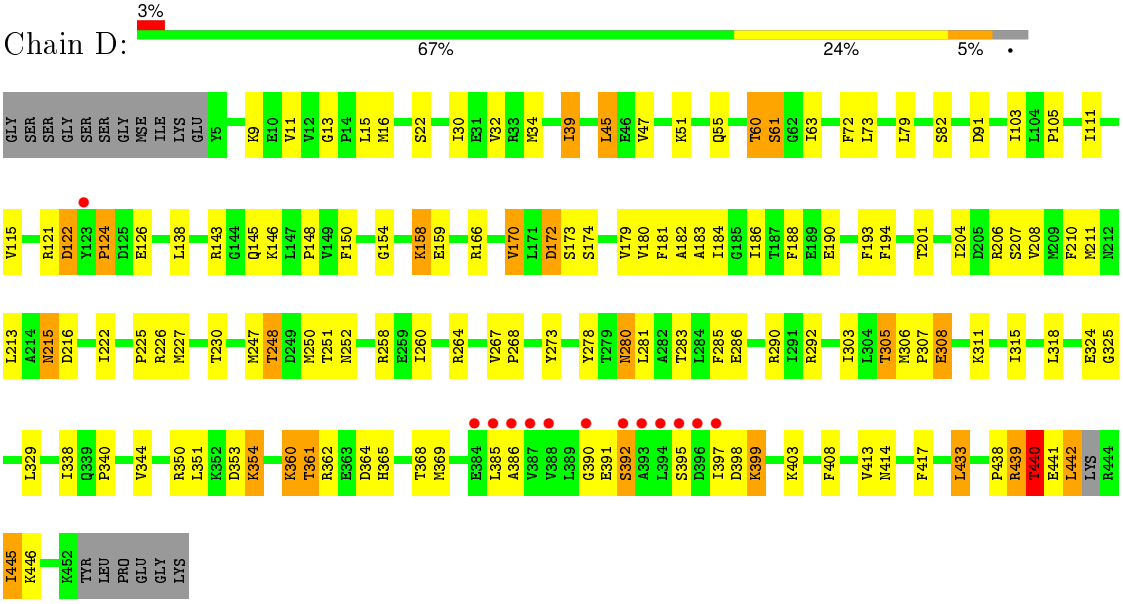
- Molecule 1: V-type sodium ATPase catalytic subunit A

Chain C:



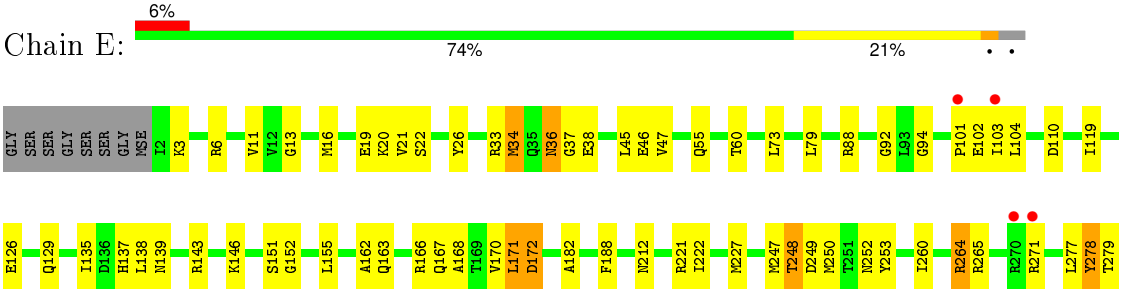
• Molecule 2: V-type sodium ATPase subunit B

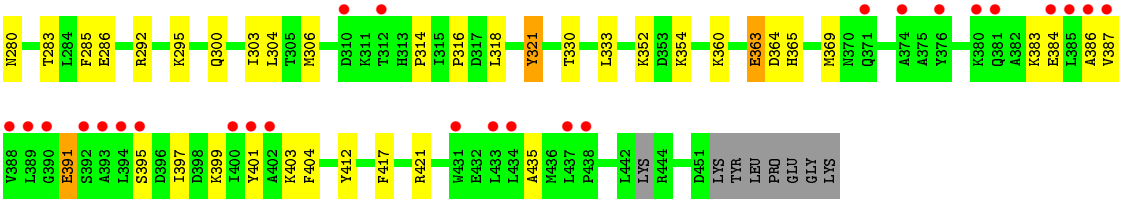
Chain D:



• Molecule 2: V-type sodium ATPase subunit B

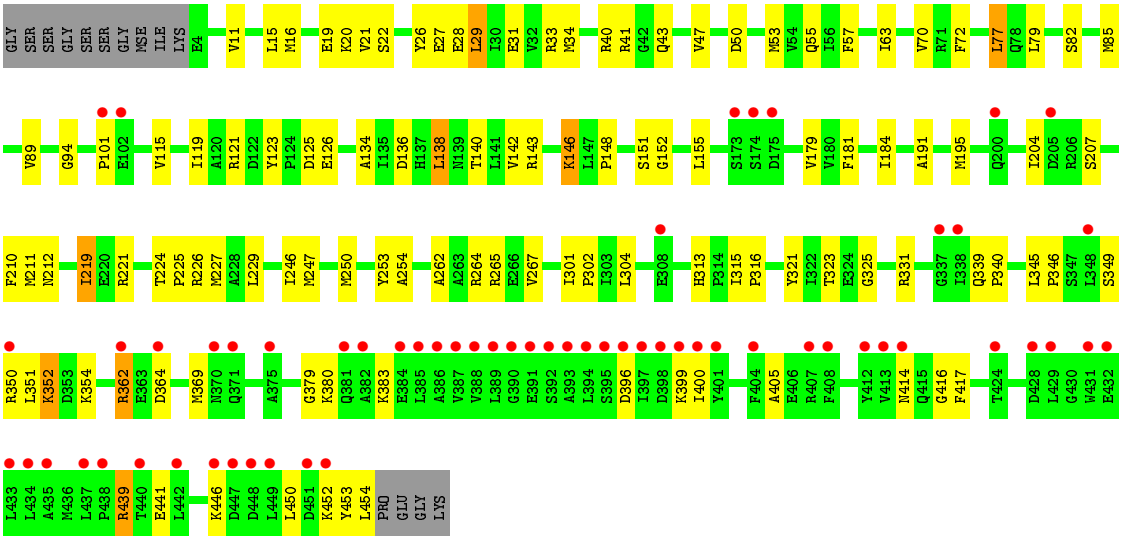
Chain E:





- Molecule 2: V-type sodium ATPase subunit B

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.11 (at 2.81Å)	Xtriage
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 (5.26%)	DCC
Wilson B-factor (Å^2)	64.4	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.5	EDS
Estimated twinning fraction	0.009 for k,h,-l 0.011 for -k,-h,-l 0.021 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 91450 reflections	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.68	0/4613	0.74	1/6206 (0.0%)
1	B	0.49	0/4609	0.61	0/6201
1	C	0.49	0/4555	0.59	0/6131
2	D	0.57	0/3493	0.68	0/4698
2	E	0.58	0/3494	0.68	0/4700
2	F	0.48	0/3501	0.63	0/4706
All	All	0.55	0/24265	0.66	1/32642 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	MSE	CG-SE-CE	-5.76	86.22	98.90

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	98	0
1	B	4555	0	4517	75	0
1	C	4501	0	4435	145	0
2	D	3447	0	3416	112	0
2	E	3448	0	3400	89	0
2	F	3454	0	3394	87	0
3	A	39	0	0	3	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	578	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 (578) 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:HA	1:C:451:GLN:HE21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:79:LEU:HD13	2:D:227:MSE:CE	1.94	0.97
1:B:266:MSE:HE3	1:B:294:ASN:O	1.65	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:E:13:GLY:O	2:E:60:THR:HG21	1.72	0.90
1:B:60:PRO:HD3	2:E:47:VAL:HG13	1.53	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:F:452:LYS:H	2:F:453:TYR:C	1.79	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
2:D:361:THR:HG21	2:D:365:HIS:HD2	1.36	0.84
1:C:317:PHE:HD1	1:C:320:MSE:CE	1.89	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
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:CD1	2:F:219:ILE:H	1.91	0.80
1:B:261:GLU:HG2	1:B:266:MSE:HE1	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PRO:HD3	2:D:47:VAL:HG13	1.62	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
2:F:439:ARG:HG3	2:F:439:ARG:HH11	1.51	0.75
1:C:506:PHE:N	1:C:506:PHE:HD2	1.84	0.75
1:C:141:GLU:OE2	1:C:147:HIS:HD2	1.70	0.75
2:E:212:ASN:OD1	2:E:221:ARG:HG3	1.87	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:248:THR:CG2	2:D:303:ILE:HB	2.17	0.74
2:D:182:ALA:HB3	2:D:247:MSE:HG2	1.68	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
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:C:517:LYS:HE2	1:C:521:MSE:HE3	1.71	0.72
1:B:83:MSE:HE2	1:B:291:LEU:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:A:565:GLU:N	2.28	0.66
1:B:271:ASN:OD1	2:E:292:ARG:NH2	2.29	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
2:E:79:LEU:CD1	2:E:227:MSE:HE1	2.23	0.64
2:E:171:LEU:O	2:E:171:LEU:CG	2.43	0.64
2:D:124:PRO:HG2	2:D:351:LEU:HD13	1.80	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
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:D:361:THR:HG21	2:D:365:HIS:CG	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ARG:O	1:C:288:ARG:HG3	1.99	0.62
1:B:133:GLY:O	1:B:380:ARG:NH2	2.33	0.61
2:D:361:THR:CG2	2:D:365:HIS:HD2	2.09	0.61
1:A:209:MSE:HE3	1:A:224:LYS:HG2	1.81	0.61
1:C:85:ASP:OD2	1:C:89:ARG:NH1	2.33	0.61
1:A:266:MSE:HE3	1:A:294:ASN:N	2.15	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
2:D:439:ARG:C	2:D:441:GLU:H	2.04	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:CD2	2:E:171:LEU:O	2.49	0.60
1:C:180:GLN:HG3	1:C:181:GLY:N	2.15	0.60
1:C:505:ALA:C	1:C:506:PHE:HD2	2.05	0.59
1:C:327:MSE:HE2	1:C:387:ILE:HB	1.84	0.59
2:E:94:GLY:HA3	2:E:227:MSE:HE2	1.84	0.59
1:C:448:ILE:HG23	1:C:449:LEU:HD23	1.84	0.59
1:B:27:MSE:HE3	1:B:71:LEU:HB2	1.85	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
2:D:439:ARG:O	2:D:439:ARG:HG3	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:362:ARG:HD2	2:D:364:ASP:OD1	2.03	0.57
2:E:278:TYR:CD2	2:E:278:TYR:C	2.77	0.57
1:A:148:LYS:HB2	1:A:320:MSE:HG2	1.85	0.57
1:C:273:PHE:CB	1:C:286:MSE:HE2	2.34	0.57
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.70	0.57
1:B:209:MSE:HE3	1:B:224:LYS:HG2	1.86	0.57
1:C:225:GLY:O	1:C:370:GLY:HA2	2.04	0.57
1:A:348:MSE:HA	1:A:348:MSE:HE3	1.87	0.57
1:C:399:GLU:OE1	1:C:401:VAL:HG12	2.05	0.56
1:C:320:MSE:CE	1:C:322:TYR:CD2	2.86	0.56
1:C:24:ILE:HG21	2:D:60:THR:HG23	1.88	0.56
2:D:306:MSE:HE2	2:D:311:LYS:HA	1.86	0.56
1:C:135:ILE:HD13	1:C:148:LYS:HD3	1.88	0.56
1:A:397:ILE:HD12	1:A:402:THR:HG21	1.88	0.56
1:C:25:GLN:HG3	2:D:61:SER:HG	1.70	0.56
1:A:445:MSE:HG2	1:A:453:TRP:CD1	2.41	0.56
1:C:415:LEU:HA	1:C:427:SER:O	2.05	0.56
1:C:108:GLN:O	1:C:109:LEU:HD23	2.06	0.56
1:C:513:THR:HG23	1:C:517:LYS:HD3	1.88	0.56
2:D:438:PRO:O	2:D:441:GLU:HG2	2.06	0.56
1:C:235:GLY:HA3	2:F:350:ARG:HH21	1.71	0.56
2:D:170:VAL:CG1	2:D:172:ASP:HB2	2.36	0.56
2:D:251:THR:OG1	2:D:305:THR:O	2.22	0.55
2:D:126:GLU:OE2	2:D:290:ARG:NH1	2.40	0.55
1:C:485:ASN:HD22	1:C:533:ARG:HH11	1.54	0.55
2:F:224:THR:HB	2:F:225:PRO:HD3	1.87	0.55
1:B:274:PRO:HA	1:B:286:MSE:HG2	1.88	0.55
1:A:399:GLU:HB2	1:A:400:PRO:CD	2.36	0.55
2:F:212:ASN:HD21	2:F:221:ARG:HG2	1.69	0.55
2:F:55:GLN:HE22	2:F:264:ARG:HE	1.54	0.55
2:D:181:PHE:HD2	2:D:211:MSE:HE1	1.72	0.55
1:C:141:GLU:OE2	1:C:147:HIS:CD2	2.58	0.55
2:E:306:MSE:HG2	2:E:316:PRO:HG3	1.89	0.55
1:C:531:GLU:HB3	1:C:581:ILE:HD12	1.87	0.55
2:F:125:ASP:O	2:F:126:GLU:HB2	2.06	0.55
2:D:158:LYS:HD2	2:D:193:PHE:CD2	2.42	0.55
2:D:184:ILE:CD1	2:D:225:PRO:HG3	2.36	0.55
2:F:250:MSE:HA	2:F:250:MSE:CE	2.34	0.55
2:F:191:ALA:O	2:F:195:MSE:HG2	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:399:LYS:C	2:D:399:LYS:HD2	2.28	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: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:24:ILE:HG21	2:E:60:THR:HG23	1.89	0.54
1:C:247:LYS:HA	1:C:285:LEU:HD11	1.89	0.53
1:A:298:MSE:HE2	1:A:298:MSE:HA	1.91	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: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
2:F:439:ARG:HG2	2:F:439:ARG:NH1	2.24	0.53
1:C:178:THR:OG1	1:C:179:GLU:N	2.39	0.53
1:B:200:LYS:HE3	1:B:379:GLN:HG2	1.91	0.53
2:F:439:ARG:CG	2:F:439:ARG:NH1	2.56	0.53
2:F:313:HIS:ND1	2:F:315:ILE:HG12	2.24	0.53
1:C:504:ASN:ND2	1:C:507:ASP:HB2	2.24	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:E:36:ASN:HD21	2:E:38:GLU:HB2	1.74	0.52
2:D:138:LEU:HA	2:D:369:MSE:HG3	1.91	0.52
2:F:138:LEU:HA	2:F:369:MSE:HG3	1.91	0.52
2:E:412:TYR:O	2:E:421:ARG:NH1	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:VAL:HG22	2:F:50:ASP:O	2.10	0.52
2:D:13:GLY:O	2:D:60:THR:HG21	2.10	0.51
1:A:273:PHE:HB3	1:A:286:MSE:HE2	1.92	0.51
2:D:146:LYS:HD3	2:D:285:PHE:O	2.11	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
2:F:313:HIS:CE1	2:F:315:ILE:HG12	2.45	0.51
1:B:577:ILE:O	1:B:581:ILE:HG12	2.09	0.51
1:C:2:GLN:HE22	1:C:21:GLU:H	1.58	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: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
1:B:139:VAL:HG21	1:B:187:MSE:HE1	1.90	0.51
2:F:181:PHE:CD2	2:F:211:MSE:HE1	2.43	0.51
1:A:274:PRO:HA	1:A:286:MSE:HG2	1.92	0.51
2:E:151:SER:OG	2:E:152:GLY:N	2.42	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
2:F:125:ASP:O	2:F:143:ARG:HB2	2.12	0.50
1:C:484:ASP:HB3	1:C:536:LEU:HD22	1.93	0.50
1:C:371:ARG:NH1	1:C:381:GLU:OE2	2.44	0.50
2:F:148:PRO:HA	2:F:302:PRO:HD2	1.94	0.50
1:C:139:VAL:CG2	1:C:187:MSE:HE3	2.38	0.50
1:B:231:PRO:HA	1:B:390:VAL:O	2.12	0.50
2:D:248:THR:HG22	2:D:303:ILE:HB	1.93	0.50
2:D:222:ILE:CD1	2:D:260:ILE:HD13	2.41	0.50
1:C:248:TRP:CE2	1:C:512:PHE:HB2	2.47	0.50
1:C:80:ILE:O	1:C:81:SER:HB2	2.12	0.50
1:B:134:ASP:O	1:B:150:MSE:HA	2.11	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HD12	1:A:287:GLU:HB2	1.94	0.49
1:A:80:ILE:O	1:A:81:SER:HB2	2.12	0.49
2:F:452:LYS:N	2:F:453:TYR:C	2.56	0.49
1:C:327:MSE:HE2	1:C:387:ILE:CG1	2.42	0.49
2:F:226:ARG:NH2	2:F:253:TYR:OH	2.44	0.49
2:E:182:ALA:HB3	2:E:247:MSE:HG2	1.94	0.49
2:D:264:ARG:NE	3:D:501:HOH:O	2.45	0.49
1:C:399:GLU:HG2	1:C:400:PRO:CD	2.41	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:A:256:TYR:CD2	1:A:256:TYR:C	2.86	0.49
1:A:27:MSE:CE	3:A:606:HOH:O	2.61	0.49
1:A:517:LYS:NZ	1:A:562:ILE:O	2.39	0.49
2:F:315:ILE:HB	2:F:316:PRO:CD	2.43	0.49
1:B:241:VAL:O	1:B:245:ILE:HG12	2.13	0.49
2:E:401:TYR:O	2:E:404:PHE:HB3	2.12	0.49
1:C:436:LEU:HD11	2:D:154:GLY:HA2	1.95	0.49
2:E:250:MSE:O	2:E:253:TYR:HB3	2.13	0.48
2:D:306:MSE:HE1	2:D:311:LYS:HG2	1.95	0.48
2:F:315:ILE:HB	2:F:316:PRO:HD3	1.95	0.48
2:F:396:ASP:HA	2:F:399:LYS:HG2	1.96	0.48
1:C:237:GLY:O	1:C:238:LYS:C	2.52	0.48
2:E:102:GLU:CB	2:E:103:ILE:HG22	2.42	0.48
1:C:331:THR:CG2	1:C:389:ALA:O	2.60	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:C:135:ILE:CD1	1:C:148:LYS:HD3	2.43	0.48
2:D:91:ASP:HA	2:D:211:MSE:O	2.13	0.48
1:B:95:MSE:HG3	2:E:119:ILE:HD11	1.96	0.48
1:C:231:PRO:HG2	1:C:412:PHE:HE1	1.79	0.48
1:C:450:GLN:O	1:C:451:GLN:NE2	2.47	0.48
2:E:171:LEU:HA	2:E:172:ASP:HA	1.52	0.48
1:A:203:LEU:HB2	1:A:371:ARG:HG2	1.94	0.48
2:D:103:ILE:O	2:D:105:PRO:HD3	2.13	0.48
2:F:26:TYR:O	2:F:27:GLU:HB2	2.12	0.48
2:D:79:LEU:HD13	2:D:227:MSE:HE3	1.92	0.48
1:B:60:PRO:CD	2:E:47:VAL:HG13	2.35	0.48
1:A:273:PHE:HB3	1:A:286:MSE:CE	2.44	0.48
1:B:97:VAL:HG21	1:B:109:LEU:HD21	1.95	0.48
1:A:133:GLY:CA	1:A:150:MSE:HE2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:440:THR:C	2:D:441:GLU:OE1	2.52	0.48
1:B:466:GLU:HG2	1:B:489:THR:HG21	1.95	0.48
2:D:170:VAL:HG12	2:D:172:ASP:HB2	1.95	0.48
2:E:36:ASN:HD22	2:E:36:ASN:C	2.16	0.48
2:D:307:PRO:C	2:D:308:GLU:HG2	2.34	0.48
1:B:485:ASN:HD21	1:B:533:ARG:HH11	1.62	0.48
1:B:52:TYR:O	1:B:299:PRO:HB3	2.13	0.48
2:F:184:ILE:HD11	2:F:225:PRO:HG3	1.95	0.47
1:C:8:LYS:HB3	1:C:15:MSE:CG	2.38	0.47
2:D:445:ILE:O	2:D:446:LYS:C	2.49	0.47
2:F:184:ILE:CD1	2:F:225:PRO:HG3	2.45	0.47
2:E:222:ILE:HD11	2:E:260:ILE:HD13	1.92	0.47
2:E:365:HIS:HB3	3:E:511:HOH:O	2.14	0.47
2:E:363:GLU:HG2	2:E:364:ASP:N	2.29	0.47
1:B:315:GLU:HA	1:B:384:ILE:HD11	1.96	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
2:F:94:GLY:CA	2:F:227:MSE:HE2	2.45	0.47
2:E:36:ASN:ND2	2:E:38:GLU:H	2.12	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: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
1:A:38:GLU:OE1	1:A:52:TYR:OH	2.31	0.47
2:E:36:ASN:HD22	2:E:37:GLY:N	2.13	0.47
2:E:265:ARG:HH11	2:E:265:ARG:HG2	1.79	0.47
1:B:417:SER:O	1:B:421:GLN:HG2	2.15	0.47
1:A:160:GLN:HB3	1:A:160:GLN:HE21	1.48	0.47
2:F:34:MSE:HG2	2:F:63:ILE:HG12	1.96	0.47
1:C:169:ILE:HB	1:C:188:MSE:HB2	1.97	0.47
2:D:250:MSE:HA	2:D:250:MSE:HE2	1.96	0.47
2:D:204:ILE:C	2:D:206:ARG:H	2.18	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
2:E:171:LEU:HD23	2:E:171:LEU:H	1.80	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
1:A:454:SER:O	1:A:458:THR:HG23	2.15	0.46
2:F:16:MSE:HE1	2:F:70:VAL:HG21	1.96	0.46
2:D:158:LYS:HG3	2:D:194:PHE:CZ	2.50	0.46
1:C:407:ARG:NH2	2:D:252:ASN:ND2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:VAL:HA	2:D:268:PRO:HD3	1.79	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:E:285:PHE:HD1	2:E:300:GLN:HE22	1.63	0.46
2:E:135:ILE:O	2:E:139:ASN:C	2.54	0.46
2:D:280:ASN:O	2:D:283:THR:HB	2.15	0.46
1:B:85:ASP:OD1	1:B:85:ASP:C	2.53	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
2:F:11:VAL:HG22	2:F:16:MSE:CG	2.37	0.46
1:C:238:LYS:O	1:C:241:VAL:HB	2.15	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:E:11:VAL:HG22	2:E:16:MSE:HG2	1.96	0.46
1:C:482:LEU:HB3	1:C:487:ARG:HD3	1.98	0.46
2:E:94:GLY:CA	2:E:227:MSE:HE2	2.44	0.46
1:C:415:LEU:HD23	1:C:428:ILE:HD13	1.98	0.46
1:B:485:ASN:ND2	1:B:485:ASN:O	2.49	0.46
2:D:439:ARG:C	2:D:441:GLU:N	2.68	0.46
1:C:404:ASN:HA	1:C:407:ARG:HD3	1.97	0.46
1:C:435:SER:C	1:C:437:TYR:H	2.20	0.46
1:A:42:MSE:HB2	1:A:42:MSE:HE2	1.78	0.46
2:E:280:ASN:O	2:E:283:THR:HB	2.16	0.46
1:B:208:PRO:HG3	1:B:441:VAL:HG22	1.98	0.46
1:A:202:LYS:HD3	2:E:188:PHE:CD2	2.51	0.46
2:F:212:ASN:ND2	2:F:221:ARG:HG2	2.31	0.45
1:A:507:ASP:O	1:A:511:THR:HB	2.16	0.45
2:E:45:LEU:HD11	2:E:264:ARG:HD3	1.98	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
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:A:528:PHE:HA	1:A:577:ILE:HG21	1.98	0.45
2:D:210:PHE:O	2:D:211:MSE:HE2	2.16	0.45
1:C:247:LYS:HG3	1:C:248:TRP:CD1	2.51	0.45
1:B:394:GLY:N	2:E:321:TYR:OH	2.49	0.45
2:D:172:ASP:HB3	2:D:173:SER:H	1.46	0.45
1:C:83:MSE:HG3	1:C:291:LEU:HB3	1.97	0.45
1:A:329:ASP:HA	1:A:330:SER:HA	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ARG:HD2	1:B:372:VAL:CG2	2.47	0.45
2:E:383:LYS:CA	2:E:386:ALA:HB3	2.38	0.45
1:A:278:ASP:HA	1:A:279:PRO:HD3	1.88	0.45
1:A:188:MSE:HE3	1:A:189:GLN:C	2.37	0.45
1:A:95:MSE:HB3	1:A:95:MSE:HE2	1.80	0.45
1:B:261:GLU:CG	1:B:266:MSE:CE	2.91	0.45
1:A:274:PRO:HG3	1:A:286:MSE:HE3	1.98	0.45
1:B:33:LEU:H	1:B:33:LEU:HD12	1.82	0.45
1:C:521:MSE:CE	1:C:560:LYS:HA	2.47	0.45
2:F:210:PHE:O	2:F:211:MSE:HE2	2.17	0.45
2:F:55:GLN:NE2	2:F:264:ARG:HE	2.14	0.45
2:D:170:VAL:HG13	2:D:172:ASP:H	1.80	0.45
1:B:329:ASP:HA	1:B:330:SER:HA	1.65	0.45
2:D:213:LEU:O	2:D:216:ASP:HB2	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: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
1:A:212:GLY:HA3	1:A:512:PHE:CD1	2.52	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
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
1:C:208:PRO:HG3	1:C:441:VAL:HG13	1.99	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
2:D:264:ARG:CD	3:D:501:HOH:O	2.61	0.44
1:A:52:TYR:CD1	1:A:52:TYR:N	2.84	0.44
2:D:286:GLU:HA	2:D:286:GLU:OE1	2.17	0.44
1:C:447:GLN:O	1:C:447:GLN:CD	2.56	0.44
1:C:326:ILE:C	1:C:327:MSE:HE3	2.38	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:119:TRP:CZ3	1:B:165:GLY:HA2	2.53	0.44
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:B:465:GLN:O	1:B:469:GLN:HG2	2.18	0.43
1:A:148:LYS:HG3	1:A:320:MSE:HE3	2.00	0.43
2:F:229:LEU:HG	2:F:247:MSE:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:439:ARG:O	2:D:441:GLU:N	2.52	0.43
1:A:80:ILE:O	1:A:81:SER:CB	2.64	0.43
1:A:5:LYS:HE2	1:A:5:LYS:HB3	1.80	0.43
2:E:383:LYS:O	2:E:387:VAL:HG23	2.18	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:249:ASP:OD1	2:E:304:LEU:HA	2.19	0.43
2:D:386:ALA:O	2:D:390:GLY:HA2	2.18	0.43
1:B:15:MSE:HE2	1:B:15:MSE:HB3	1.69	0.43
2:E:162:ALA:O	2:E:166:ARG:HG3	2.19	0.43
1:A:490:LEU:HA	1:A:490:LEU:HD23	1.91	0.43
1:A:27:MSE:HE3	1:A:71:LEU:CB	2.32	0.43
1:A:266:MSE:HE3	1:A:294:ASN:C	2.38	0.43
1:C:143:LYS:HD3	1:C:287:GLU:OE2	2.18	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
2:D:307:PRO:O	2:D:308:GLU:HG2	2.19	0.43
1:C:239:THR:C	1:C:241:VAL:H	2.22	0.43
1:A:445:MSE:CG	1:A:453:TRP:CD1	3.01	0.43
1:A:413:TRP:HB3	1:A:428:ILE:HD13	2.01	0.43
2:D:179:VAL:O	2:D:207:SER:HA	2.18	0.43
1:A:262:ARG:HB2	1:A:265:GLU:HG3	2.01	0.43
1:B:345:LEU:O	1:B:346:GLU:HB2	2.19	0.43
2:F:142:VAL:CG2	2:F:351:LEU:O	2.67	0.43
1:A:520:ASN:O	1:A:524:VAL:HG13	2.19	0.43
2:D:408:PHE:HA	2:D:433:LEU:HD11	2.01	0.43
2:F:345:LEU:HB2	2:F:346:PRO:HD3	2.00	0.43
1:C:317:PHE:HA	1:C:320:MSE:HE2	2.00	0.43
1:A:484:ASP:OD1	1:A:541:TYR:HD1	2.01	0.43
1:C:474:VAL:C	1:C:476:LEU:H	2.21	0.43
1:A:261:GLU:CG	1:A:266:MSE:CE	2.93	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
2:E:45:LEU:HD23	2:E:45:LEU:HA	1.85	0.42
2:D:190:GLU:O	2:D:193:PHE:HB3	2.19	0.42
1:A:271:ASN:OD1	2:D:292:ARG:NH2	2.52	0.42
1:A:261:GLU:CB	1:A:266:MSE:HE2	2.48	0.42
1:B:295:THR:C	1:B:297:ASN:H	2.22	0.42
1:C:298:MSE:HG3	2:F:115:VAL:HG11	2.00	0.42
1:A:553:ARG:HA	1:A:556:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:TRP:CD2	1:A:192:PRO:HD2	2.54	0.42
2:D:180:VAL:HG22	2:D:208:VAL:HB	2.01	0.42
1:A:261:GLU:HG2	1:A:266:MSE:HE1	2.00	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
2:D:30:ILE:HG22	2:D:72:PHE:CD1	2.55	0.42
1:B:83:MSE:HG2	1:B:291:LEU:HB3	2.02	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
2:D:215:ASN:HD22	2:D:215:ASN:C	2.22	0.42
2:F:452:LYS:H	2:F:454:LEU:N	2.17	0.42
1:A:258:GLY:HA3	1:A:266:MSE:HE1	2.01	0.42
1:B:348:MSE:HB2	2:F:262:ALA:HB1	2.02	0.42
2:F:94:GLY:HA3	2:F:227:MSE:CE	2.50	0.42
1:A:387:ILE:HG23	1:A:413:TRP:HZ3	1.85	0.42
2:F:136:ASP:O	2:F:140:THR:HG22	2.19	0.42
1:C:449:LEU:O	1:C:450:GLN:HB2	2.20	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:B:129:GLU:CD	1:B:129:GLU:H	2.24	0.42
1:B:523:LYS:O	1:B:527:THR:N	2.52	0.41
2:D:148:PRO:HD2	2:D:325:GLY:O	2.19	0.41
1:A:295:THR:C	1:A:297:ASN:H	2.23	0.41
1:B:56:SER:HB3	1:B:105:ARG:HH21	1.85	0.41
1:C:60:PRO:HD3	2:F:47:VAL:HG13	2.02	0.41
1:A:248:TRP:CZ3	1:A:279:PRO:HB3	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:11:GLY:HA2	2:E:26:TYR:CZ	2.55	0.41
1:B:266:MSE:CE	1:B:294:ASN:O	2.52	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:C:32:ASP:OD2	1:C:62:GLU:HG2	2.21	0.41
2:D:251:THR:HA	2:D:315:ILE:HD13	2.02	0.41
1:C:256:TYR:HE2	1:C:266:MSE:HE1	1.85	0.41
2:F:43:GLN:HG2	2:F:57:PHE:CE1	2.51	0.41
2:F:225:PRO:HA	2:F:247:MSE:HE2	2.01	0.41
2:D:440:THR:O	2:D:441:GLU:OE1	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:GLN:HG3	2:D:351:LEU:HD12	2.03	0.41
2:E:45:LEU:HD21	2:E:264:ARG:NH1	2.36	0.41
1:A:392:PRO:HG2	1:A:397:ILE:HD13	2.01	0.41
1:C:456:MSE:HG2	1:C:526:LEU:HD22	2.03	0.41
2:E:36:ASN:C	2:E:36:ASN:ND2	2.74	0.41
2:D:215:ASN:ND2	2:D:215:ASN:C	2.74	0.41
2:F:379:GLY:HA3	2:F:405:ALA:HB2	2.03	0.41
1:C:233:PRO:HA	2:F:321:TYR:OH	2.21	0.41
1:A:307:ILE:HB	1:A:365:TYR:CE1	2.56	0.41
2:F:339:GLN:HA	2:F:340:PRO:HA	1.86	0.41
2:E:277:LEU:HD23	2:E:318:LEU:HD12	2.03	0.41
2:E:271:ARG:HB2	2:E:314:PRO:CG	2.51	0.40
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
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
2:D:183:ALA:HB1	2:D:186:ILE:CD1	2.51	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
2:E:252:ASN:HD22	2:E:252:ASN:HA	1.74	0.40
1:C:445:MSE:HE2	1:C:445:MSE:HA	2.02	0.40
2:E:88:ARG:NH1	2:E:101:PRO:O	2.49	0.40
2:D:32:VAL:O	2:D:39:ILE:HA	2.21	0.40
2:D:45:LEU:HD21	2:D:55:GLN:HB2	2.04	0.40
2:E:171:LEU:CD2	2:E:171:LEU:H	2.34	0.40
2:D:159:GLU:HB3	2:D:417:PHE:CD1	2.57	0.40
1:B:369:SER:HB2	1:B:384:ILE:O	2.22	0.40
2:D:324:GLU:HA	2:D:350:ARG:HD2	2.04	0.40
1:B:307:ILE:HD12	1:B:365:TYR:CD1	2.57	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%)	52 84
1	B	584/600 (97%)	540 (92%)	41 (7%)	3 (0%)	34 69
1	C	581/600 (97%)	537 (92%)	42 (7%)	2 (0%)	46 79
2	D	443/465 (95%)	407 (92%)	31 (7%)	5 (1%)	17 50
2	E	445/465 (96%)	411 (92%)	33 (7%)	1 (0%)	52 84
2	F	449/465 (97%)	407 (91%)	39 (9%)	3 (1%)	26 62
All	All	3086/3195 (97%)	2858 (93%)	213 (7%)	15 (0%)	34 69

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
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%)	476 (95%)	25 (5%)	30 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	500/487 (103%)	476 (95%)	24 (5%)	31 66
1	C	489/487 (100%)	451 (92%)	38 (8%)	16 41
2	D	358/372 (96%)	322 (90%)	36 (10%)	9 27
2	E	355/372 (95%)	329 (93%)	26 (7%)	17 44
2	F	356/372 (96%)	336 (94%)	20 (6%)	26 59
All	All	2559/2577 (99%)	2390 (93%)	169 (7%)	21 51

All (169) 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	125	GLU
1	A	146	GLN
1	A	160	GLN
1	A	173	ILE
1	A	267	THR
1	A	268	ASP
1	A	285	LEU
1	A	330	SER
1	A	338	LEU
1	A	397	ILE
1	A	445	MSE
1	A	454	SER
1	A	458	THR
1	A	465	GLN
1	A	466	GLU
1	A	485	ASN
1	A	488	LEU
1	A	534	LYS
1	A	569	LYS
1	A	571	SER
1	A	575	GLU
1	B	2	GLN
1	B	29	LEU
1	B	40	ILE
1	B	73	VAL
1	B	92	ASP

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Mol	Chain	Res	Type
1	B	103	LEU
1	B	129	GLU
1	B	161	LYS
1	B	188	MSE
1	B	195	ARG
1	B	253	LEU
1	B	273	PHE
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	481	SER
1	B	559	SER
1	B	569	LYS
1	B	571	SER
1	B	575	GLU
1	C	36	ILE
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	201	GLN
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	407	ARG
1	C	445	MSE

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Mol	Chain	Res	Type
1	C	448	ILE
1	C	450	GLN
1	C	451	GLN
1	C	473	ILE
1	C	476	LEU
1	C	486	ASP
1	C	494	LYS
1	C	506	PHE
1	C	509	VAL
1	C	514	SER
1	C	541	TYR
1	C	547	GLU
1	C	553	ARG
1	C	555	ARG
1	C	580	THR
2	D	9	LYS
2	D	22	SER
2	D	39	ILE
2	D	45	LEU
2	D	51	LYS
2	D	60	THR
2	D	61	SER
2	D	73	LEU
2	D	82	SER
2	D	115	VAL
2	D	122	ASP
2	D	143	ARG
2	D	158	LYS
2	D	170	VAL
2	D	188	PHE
2	D	215	ASN
2	D	248	THR
2	D	280	ASN
2	D	305	THR
2	D	308	GLU
2	D	329	LEU
2	D	353	ASP
2	D	354	LYS
2	D	360	LYS
2	D	361	THR
2	D	368	THR
2	D	385	LEU

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Mol	Chain	Res	Type
2	D	395	SER
2	D	397	ILE
2	D	398	ASP
2	D	399	LYS
2	D	403	LYS
2	D	433	LEU
2	D	439	ARG
2	D	440	THR
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	73	LEU
2	E	104	LEU
2	E	110	ASP
2	E	146	LYS
2	E	170	VAL
2	E	171	LEU
2	E	172	ASP
2	E	248	THR
2	E	264	ARG
2	E	278	TYR
2	E	279	THR
2	E	295	LYS
2	E	321	TYR
2	E	352	LYS
2	E	354	LYS
2	E	360	LYS
2	E	363	GLU
2	E	384	GLU
2	E	391	GLU
2	E	397	ILE
2	E	403	LYS
2	F	15	LEU
2	F	19	GLU
2	F	20	LYS
2	F	22	SER
2	F	29	LEU
2	F	33	ARG
2	F	53	MSE

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Mol	Chain	Res	Type
2	F	77	LEU
2	F	119	ILE
2	F	138	LEU
2	F	146	LYS
2	F	204	ILE
2	F	219	ILE
2	F	265	ARG
2	F	267	VAL
2	F	352	LYS
2	F	362	ARG
2	F	380	LYS
2	F	439	ARG
2	F	441	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	153	ASN
1	A	160	GLN
1	A	294	ASN
1	A	404	ASN
1	A	450	GLN
1	A	465	GLN
1	B	25	GLN
1	B	108	GLN
1	B	153	ASN
1	B	160	GLN
1	B	189	GLN
1	B	204	ASN
1	B	264	ASN
1	B	294	ASN
1	B	471	ASN
1	B	485	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

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Mol	Chain	Res	Type
1	C	485	ASN
1	C	502	GLN
1	C	504	ASN
1	C	520	ASN
2	D	67	ASN
2	D	99	ASN
2	D	112	ASN
2	D	137	HIS
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	48	GLN
2	E	67	ASN
2	E	112	ASN
2	E	167	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	F	43	GLN
2	F	55	GLN
2	F	112	ASN
2	F	137	HIS
2	F	157	HIS
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

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^{th} 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%)	-0.18	3 (0%) 91 88	24, 41, 83, 117	0
1	B	563/600 (93%)	0.14	26 (4%) 36 25	38, 71, 129, 155	0
1	C	561/600 (93%)	0.35	47 (8%) 14 6	38, 76, 175, 198	0
2	D	433/465 (93%)	-0.09	13 (3%) 54 41	34, 60, 133, 196	0
2	E	435/465 (93%)	0.15	30 (6%) 20 11	32, 66, 167, 221	0
2	F	437/465 (93%)	0.58	61 (13%) 4 2	42, 91, 191, 212	0
All	All	2992/3195 (93%)	0.15	180 (6%) 25 15	24, 66, 169, 221	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	581	ILE	9.4
2	F	388	VAL	8.0
1	C	565	GLU	7.1
2	F	447	ASP	7.0
2	D	397	ILE	6.7
2	F	398	ASP	6.5
2	F	440	THR	5.9
2	E	393	ALA	5.7
2	E	385	LEU	5.7
2	D	388	VAL	5.7
1	C	489	THR	5.6
2	F	175	ASP	5.6
2	F	387	VAL	5.6
2	F	397	ILE	5.5
1	C	477	VAL	5.3
2	F	431	TRP	5.3
1	C	537	SER	5.3
2	F	392	SER	5.1
1	C	579	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
2	F	174	SER	5.1
2	E	401	TYR	4.9
2	F	393	ALA	4.8
2	F	412	TYR	4.7
2	D	393	ALA	4.7
2	D	387	VAL	4.7
1	C	476	LEU	4.6
2	E	392	SER	4.6
2	F	389	LEU	4.6
2	F	433	LEU	4.6
2	F	435	ALA	4.5
2	E	434	LEU	4.5
2	F	401	TYR	4.3
1	B	482	LEU	4.3
1	B	538	LEU	4.2
2	F	382	ALA	4.2
2	F	385	LEU	4.2
2	D	396	ASP	4.1
2	F	432	GLU	4.1
2	F	391	GLU	4.0
2	F	386	ALA	4.0
2	F	424	THR	4.0
1	B	541	TYR	4.0
1	B	130	VAL	3.9
1	C	535	ALA	3.8
2	E	376	TYR	3.8
1	C	538	LEU	3.8
2	F	429	LEU	3.7
2	F	451	ASP	3.7
2	F	400	ILE	3.7
1	C	541	TYR	3.7
2	F	404	PHE	3.6
2	E	386	ALA	3.6
2	F	375	ALA	3.6
2	F	442	LEU	3.6
1	C	577	ILE	3.6
2	F	452	LYS	3.6
1	B	484	ASP	3.5
2	F	205	ASP	3.5
2	D	390	GLY	3.5
2	E	388	VAL	3.5
2	F	446	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	173	SER	3.4
2	E	387	VAL	3.4
2	F	438	PRO	3.3
2	E	431	TRP	3.3
1	C	280	ASN	3.3
1	C	539	GLY	3.3
2	E	389	LEU	3.3
2	F	390	GLY	3.3
2	F	337	GLY	3.2
2	F	408	PHE	3.2
1	C	473	ILE	3.2
1	C	563	PRO	3.2
1	B	162	ILE	3.2
1	B	393	SER	3.2
2	E	438	PRO	3.1
2	F	395	SER	3.1
2	F	437	LEU	3.1
1	B	542	PHE	3.1
1	C	533	ARG	3.1
1	C	484	ASP	3.0
2	F	449	LEU	3.0
1	C	576	GLU	3.0
1	C	480	ASP	3.0
2	F	371	GLN	3.0
1	C	572	SER	3.0
2	E	394	LEU	3.0
2	E	374	ALA	2.9
2	F	448	ASP	2.9
1	C	528	PHE	2.9
2	E	381	GLN	2.9
2	F	428	ASP	2.9
2	E	270	ARG	2.9
1	C	567	LEU	2.9
1	B	124	ILE	2.8
1	C	481	SER	2.8
2	D	394	LEU	2.8
1	C	561	TYR	2.8
2	E	395	SER	2.8
1	C	578	LYS	2.8
1	C	574	ASN	2.8
2	D	385	LEU	2.7
1	B	478	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	475	ARG	2.7
1	C	522	LEU	2.7
2	E	380	LYS	2.6
2	E	437	LEU	2.6
2	F	102	GLU	2.6
1	C	472	GLU	2.6
1	B	470	LEU	2.6
1	B	581	ILE	2.6
1	C	279	PRO	2.6
1	C	545	ILE	2.6
1	C	547	GLU	2.6
2	F	434	LEU	2.6
2	F	338	ILE	2.6
1	C	160	GLN	2.6
1	C	558	ARG	2.5
1	B	534	LYS	2.5
2	D	395	SER	2.5
2	E	400	ILE	2.5
2	D	392	SER	2.5
1	C	478	GLY	2.5
2	E	310	ASP	2.5
1	C	553	ARG	2.5
1	C	182	LEU	2.5
1	C	582	GLN	2.4
1	B	479	ILE	2.4
1	B	172	PRO	2.4
1	B	540	ALA	2.4
2	E	390	GLY	2.4
2	F	414	ASN	2.4
1	B	452	ASP	2.4
1	A	477	VAL	2.4
2	F	362	ARG	2.4
1	B	123	THR	2.4
1	C	482	LEU	2.4
2	E	101	PRO	2.3
2	E	312	THR	2.3
2	E	384	GLU	2.3
1	C	556	ILE	2.3
1	B	536	LEU	2.3
2	F	396	ASP	2.3
2	F	308	GLU	2.2
2	D	386	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	370	ASN	2.2
2	F	413	VAL	2.2
1	C	119	TRP	2.2
1	A	475	ARG	2.2
1	C	536	LEU	2.2
2	F	407	ARG	2.2
2	F	364	ASP	2.2
2	F	101	PRO	2.2
1	B	485	ASN	2.2
1	B	531	GLU	2.2
1	C	505	ALA	2.2
1	C	580	THR	2.2
2	E	402	ALA	2.1
2	F	399	LYS	2.1
2	F	384	GLU	2.1
1	B	583	LEU	2.1
2	E	103	ILE	2.1
2	F	350	ARG	2.1
1	C	127	GLY	2.1
2	F	394	LEU	2.1
1	B	481	SER	2.1
1	B	539	GLY	2.1
1	C	559	SER	2.1
1	A	482	LEU	2.1
2	F	348	LEU	2.1
2	F	200	GLN	2.0
2	E	433	LEU	2.0
1	B	127	GLY	2.0
2	E	271	ARG	2.0
2	E	371	GLN	2.0
2	F	381	GLN	2.0
2	D	384	GLU	2.0
2	D	123	TYR	2.0
1	C	583	LEU	2.0
1	B	475	ARG	2.0

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

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

6.3 Carbohydrates

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.