Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 09:21 PM JST

PDB ID	:	7DQC
Title	:	Crystal structure of nucleotide-free mutant A(S23C)3B(N64C)3 complex from Enterococcus hirae V-ATPase
Authors	:	Maruyama, S.; Suzuki, K.; Mizutani, K.; Imai, F.L.; Ishizuka-Katsura, Y.; Shirouzu, M.; Murata, M.
Deposited on	:	2020-12-23
Resolution	:	2.71 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:

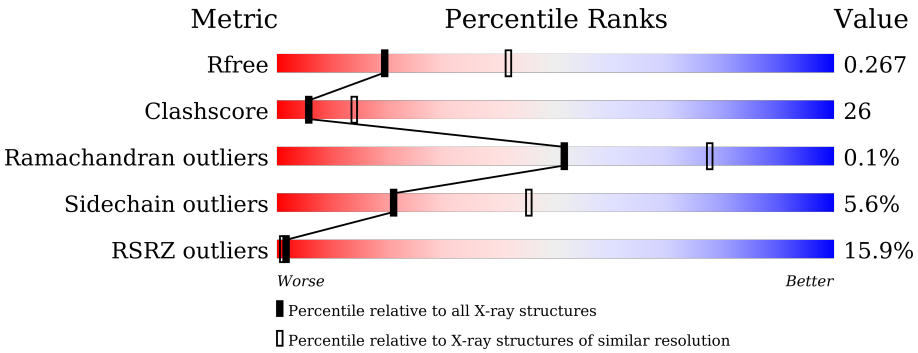
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.71 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	6% 65% 31%
1	B	600	15% 59% 37%
1	C	600	18% 54% 40%
2	D	465	15% 53% 41%
2	E	465	16% 54% 38%
2	F	465	26% 48% 44% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23860 atoms, of which 48 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	0	0	0
			4529	2847	761	895	26			
1	B	586	Total	C	N	O	S	0	0	0
			4501	2827	758	889	27			
1	C	584	Total	C	N	O	S	0	0	0
			4456	2802	746	881	27			

There are 24 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
A	23	CYS	SER	engineered mutation	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
B	23	CYS	SER	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	23	CYS	SER	engineered mutation	UNP Q08636

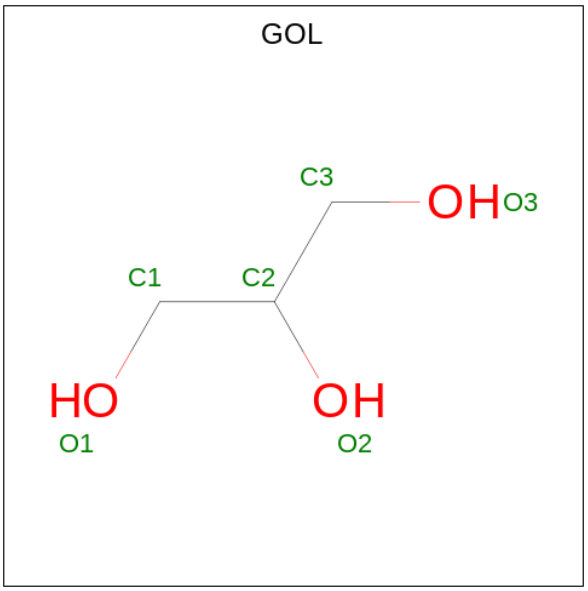
- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	448	Total	C	N	O	S	0	0	0
			3380	2137	590	638	15			
2	E	450	Total	C	N	O	S	0	0	0
			3347	2112	582	640	13			
2	F	450	Total	C	N	O	S	0	0	0
			3277	2068	568	627	14			

There are 24 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
D	64	CYS	ASN	engineered mutation	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
E	64	CYS	ASN	engineered mutation	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
F	64	CYS	ASN	engineered mutation	UNP Q08637

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0

- Molecule 4 is water.

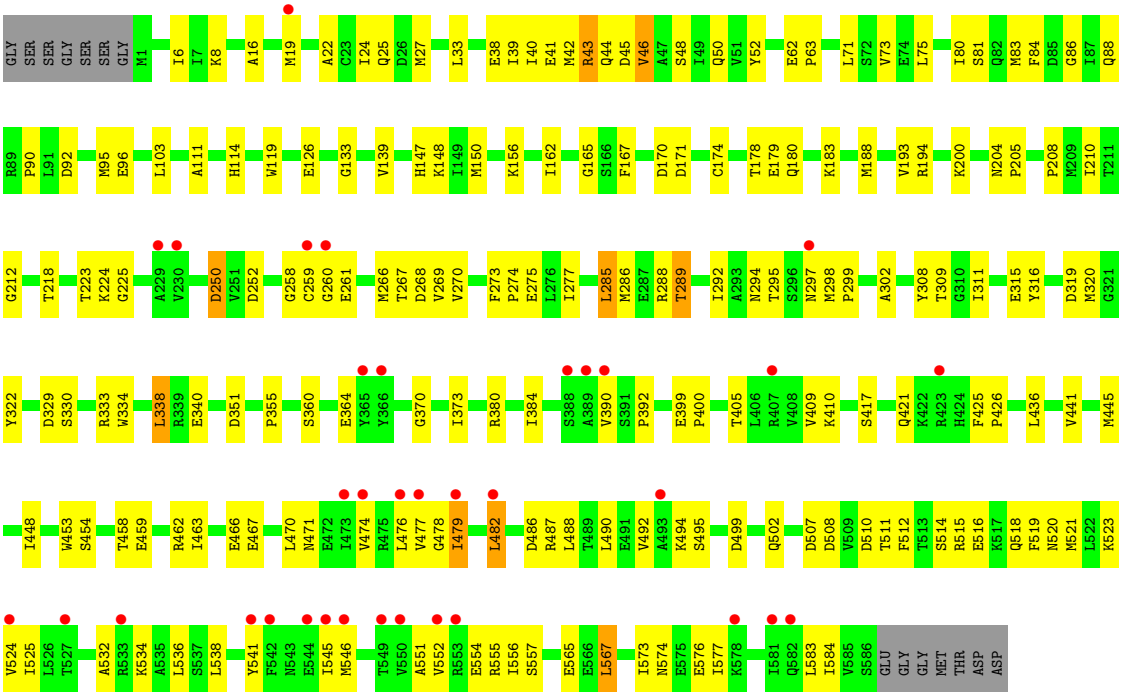
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	103	Total O 103 103	0	0
4	B	45	Total O 45 45	0	0
4	D	34	Total O 34 34	0	0
4	E	42	Total O 42 42	0	0
4	C	43	Total O 43 43	0	0
4	F	19	Total O 19 19	0	0

3 Residue-property plots (i)

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.

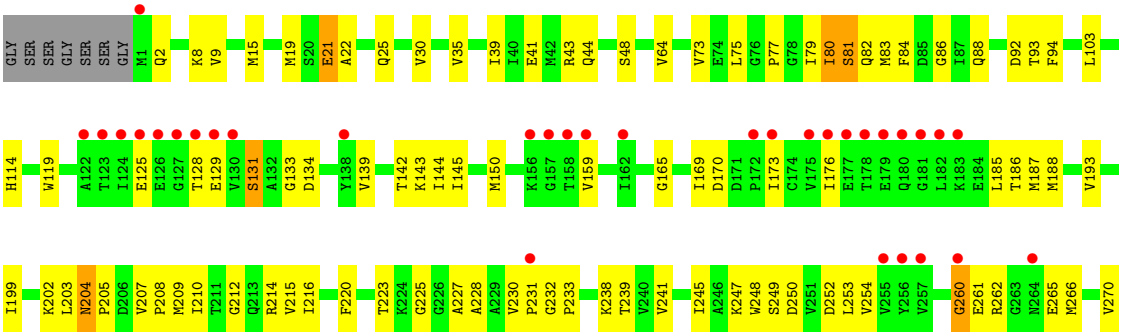
• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain A:



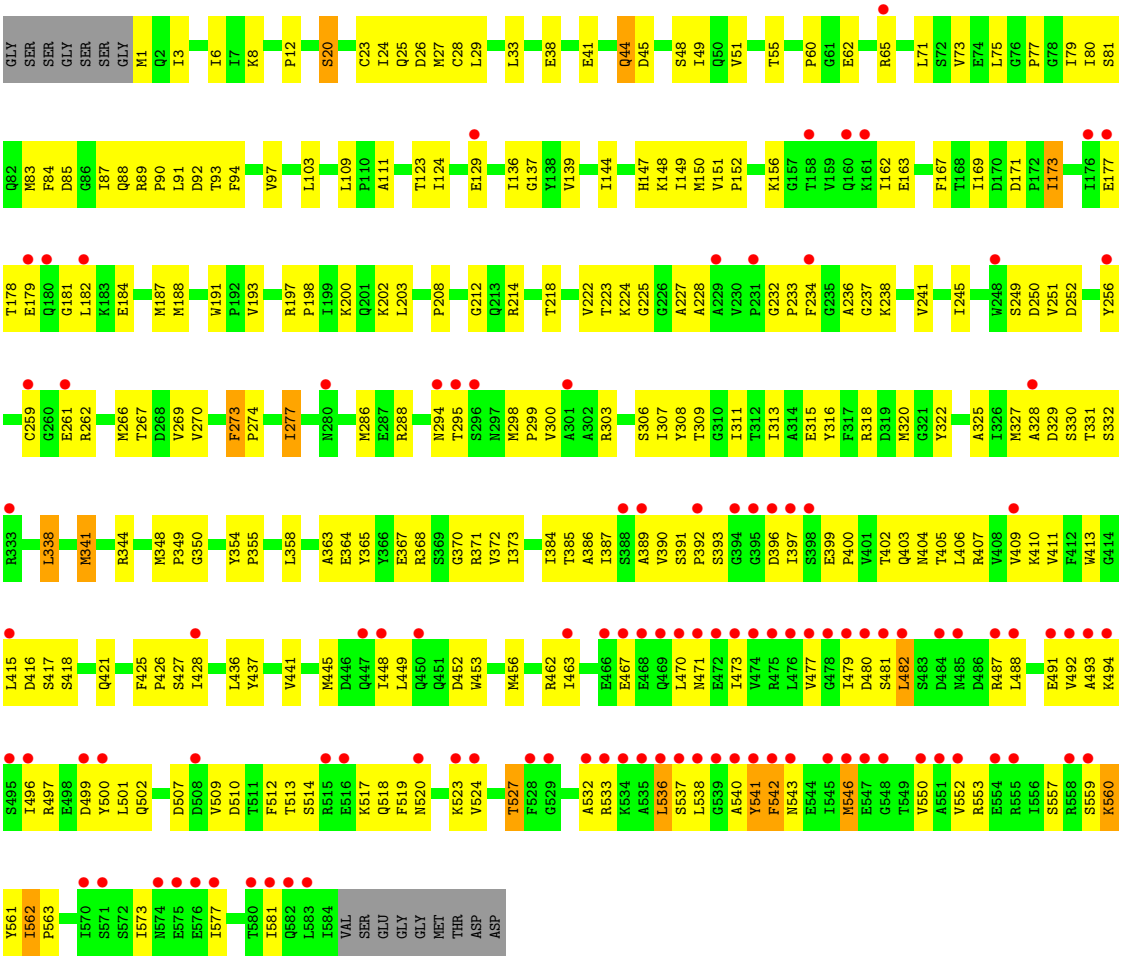
• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain B:



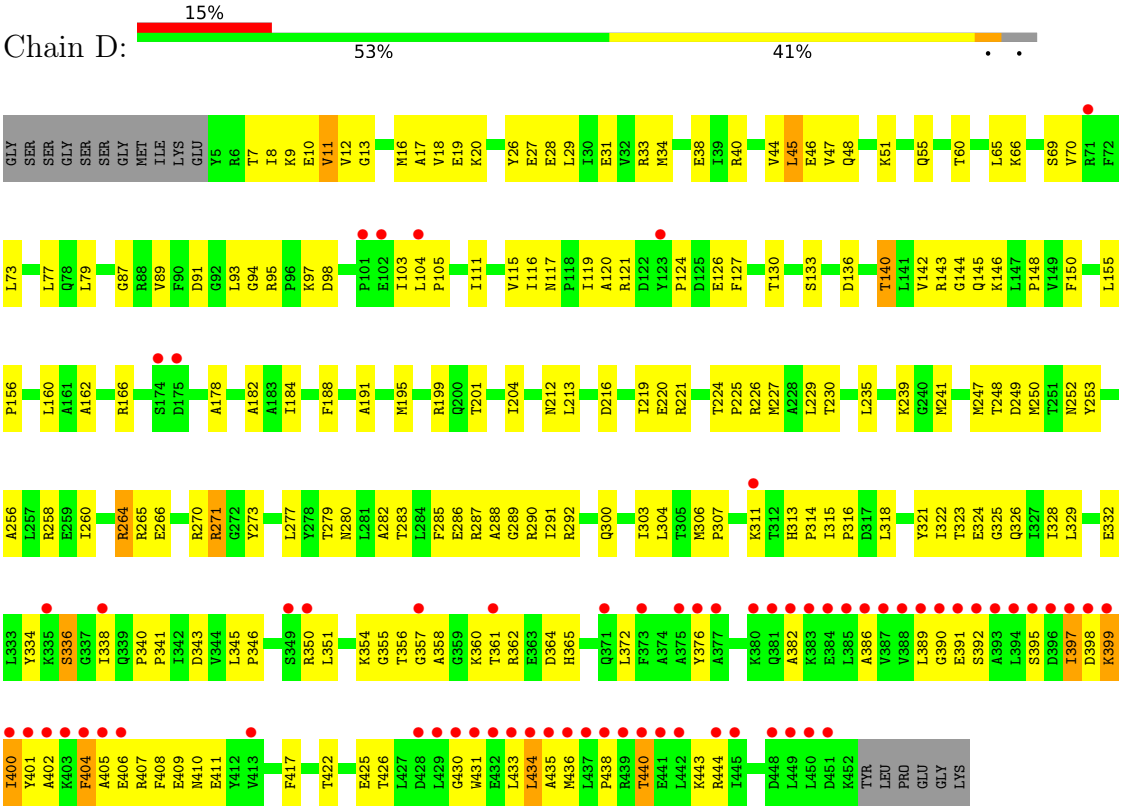
• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain C:



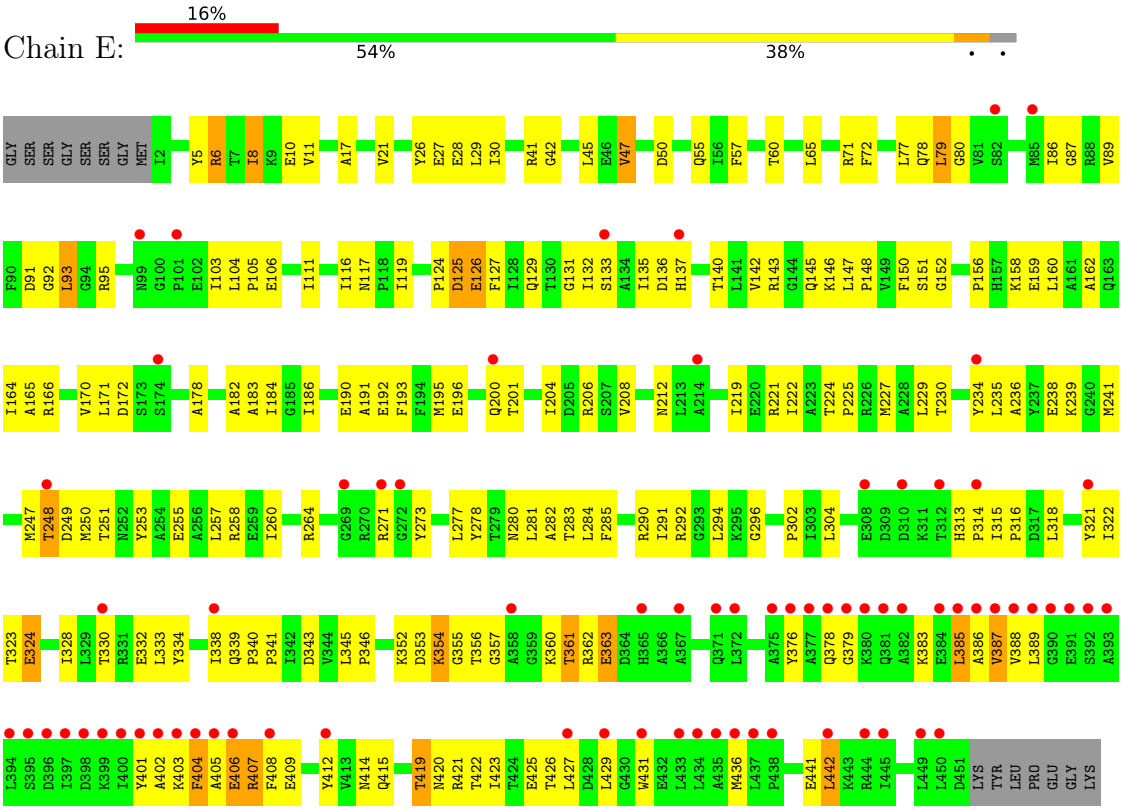
• Molecule 2: V-type sodium ATPase subunit B

Chain D:



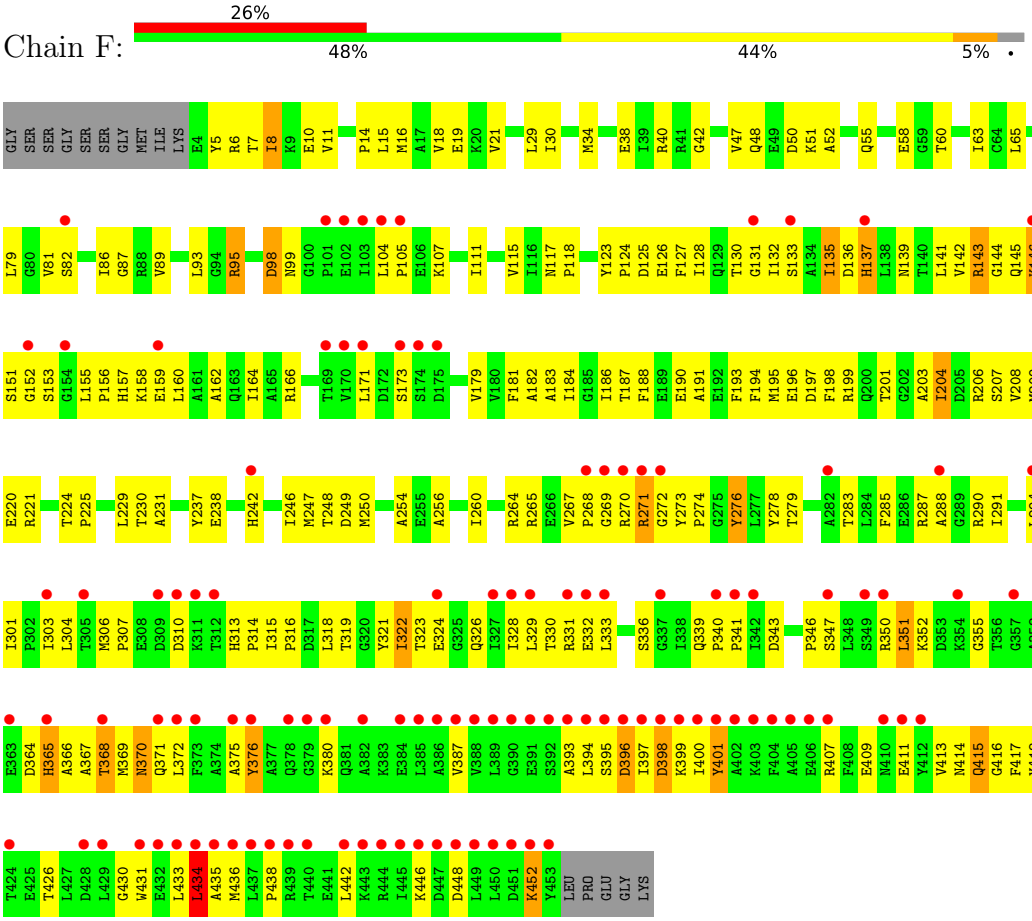
• Molecule 2: V-type sodium ATPase subunit B

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	122.08Å 121.83Å 129.11Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	44.30 – 2.71 44.30 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.30-2.71) 99.8 (44.30-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.266 0.238 , 0.267	Depositor DCC
R_{free} test set	5266 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 72.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.015 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23860	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.20	0/4605	0.38	0/6234
1	B	0.21	0/4577	0.40	1/6199 (0.0%)
1	C	0.21	0/4532	0.38	0/6148
2	D	0.21	0/3441	0.38	0/4658
2	E	0.22	0/3406	0.42	0/4616
2	F	0.23	0/3336	0.43	1/4536 (0.0%)
All	All	0.21	0/23897	0.40	2/32391 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	434	LEU	CB-CG-CD2	5.94	121.10	111.00
1	B	260	GLY	N-CA-C	-5.70	98.86	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4529	0	4462	159	0
1	B	4501	0	4407	221	0
1	C	4456	0	4329	220	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3380	0	3279	188	0
2	E	3347	0	3194	188	0
2	F	3277	0	3037	247	0
3	A	36	48	48	3	0
4	A	103	0	0	6	0
4	B	45	0	0	2	0
4	C	43	0	0	0	0
4	D	34	0	0	5	0
4	E	42	0	0	6	0
4	F	19	0	0	1	0
All	All	23812	48	22756	1180	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 26.

All (1180) 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:F:267:VAL:HG22	2:F:268:PRO:HD2	1.31	1.10
2:F:155:LEU:HD22	2:F:156:PRO:HD2	1.25	1.09
1:C:148:LYS:H	1:C:320:MET:HE3	1.22	1.01
2:D:89:VAL:HG21	2:D:195:MET:HE1	1.39	1.01
1:C:150:MET:HE1	1:C:320:MET:HA	1.41	1.00
1:B:260:GLY:HA3	1:B:261:GLU:HG2	1.39	1.00
2:F:431:TRP:HE3	2:F:434:LEU:HD21	1.27	0.98
2:F:151:SER:HB2	2:F:329:LEU:HD12	1.44	0.97
1:B:540:ALA:HB1	1:B:545:ILE:HD11	1.47	0.96
1:C:251:VAL:HG21	1:C:325:ALA:HB2	1.50	0.93
2:E:278:TYR:HB2	2:E:318:LEU:HD13	1.47	0.93
2:D:390:GLY:N	2:D:391:GLU:HA	1.83	0.93
2:E:148:PRO:HB3	2:E:302:PRO:HG2	1.49	0.92
2:F:135:ILE:O	2:F:139:ASN:N	2.02	0.91
1:C:144:ILE:HG21	1:C:288:ARG:HD3	1.50	0.91
1:B:562:ILE:HB	1:B:570:ILE:HD11	1.52	0.91
2:F:436:MET:O	2:F:438:PRO:HD3	1.71	0.91
2:F:396:ASP:O	2:F:400:ILE:N	2.03	0.91
2:D:402:ALA:O	2:D:406:GLU:N	2.04	0.90
2:E:345:LEU:HG	2:E:376:TYR:HE2	1.37	0.90
2:D:328:ILE:HD12	2:D:346:PRO:HB2	1.55	0.87
1:C:562:ILE:HG22	1:C:563:PRO:HD2	1.55	0.86
2:F:431:TRP:CE3	2:F:434:LEU:HD21	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:267:VAL:CG2	2:F:268:PRO:HD2	2.05	0.86
1:A:338:LEU:HD22	1:A:355:PRO:HG3	1.59	0.85
1:C:27:MET:HE2	1:C:71:LEU:HB2	1.57	0.85
2:F:315:ILE:HB	2:F:316:PRO:HD3	1.60	0.84
2:D:11:VAL:HG11	1:C:24:ILE:HD11	1.60	0.83
2:E:357:GLY:O	2:E:361:THR:N	2.11	0.83
2:D:407:ARG:O	2:D:411:GLU:N	2.11	0.83
1:A:148:LYS:HB2	1:A:320:MET:HE3	1.60	0.83
2:D:401:TYR:O	2:D:405:ALA:N	2.11	0.83
1:B:393:SER:N	1:B:394:GLY:HA3	1.93	0.83
1:B:231:PRO:CG	1:B:414:GLY:HA2	2.09	0.82
1:B:8:LYS:HD3	1:B:15:MET:HE2	1.62	0.82
1:C:410:LYS:HB3	1:C:436:LEU:HB2	1.60	0.82
2:F:201:THR:HG23	2:F:203:ALA:H	1.45	0.81
2:D:399:LYS:HD2	2:D:400:ILE:H	1.46	0.81
2:F:415:GLN:N	2:F:416:GLY:HA2	1.94	0.80
1:A:43:ARG:CB	1:A:46:VAL:HG13	2.12	0.80
2:D:340:PRO:HB3	2:D:417:PHE:HE1	1.45	0.80
1:B:489:THR:HG23	1:B:533:ARG:HH12	1.46	0.80
1:C:51:VAL:HG21	1:C:55:THR:CG2	2.12	0.80
1:B:231:PRO:HG2	1:B:414:GLY:HA2	1.62	0.79
1:C:41:GLU:HG2	1:C:48:SER:HB2	1.65	0.79
1:C:91:LEU:HD13	2:F:118:PRO:HG2	1.64	0.79
2:F:179:VAL:HB	2:F:207:SER:HB3	1.64	0.79
2:F:452:LYS:NZ	2:F:452:LYS:HA	1.98	0.79
2:D:116:ILE:HD13	2:D:291:ILE:HD11	1.64	0.79
2:F:135:ILE:HD12	2:F:136:ASP:H	1.47	0.79
2:F:219:ILE:HD12	2:F:219:ILE:H	1.48	0.79
2:E:219:ILE:HD13	2:E:260:ILE:HD13	1.65	0.79
1:A:333:ARG:NH2	2:D:321:TYR:O	2.16	0.78
2:F:288:ALA:HB2	2:F:300:GLN:HG3	1.65	0.78
2:F:155:LEU:CD2	2:F:156:PRO:HD2	2.11	0.78
2:E:8:ILE:CD1	2:E:65:LEU:HG	2.14	0.77
1:B:445:MET:HE3	1:B:515:ARG:HG3	1.66	0.77
2:D:124:PRO:HG2	2:D:351:LEU:HD13	1.66	0.77
1:B:8:LYS:HD3	1:B:15:MET:CE	2.14	0.76
2:D:166:ARG:HD2	2:D:201:THR:HG21	1.65	0.76
2:E:383:LYS:NZ	2:E:406:GLU:HG3	1.99	0.76
2:F:131:GLY:O	2:F:415:GLN:NE2	2.17	0.76
2:D:362:ARG:HH12	2:D:431:TRP:HE1	1.32	0.76
2:F:124:PRO:HB2	2:F:142:VAL:HG12	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:ASP:HB3	2:D:97:LYS:HE2	1.67	0.76
1:C:463:ILE:HD11	1:C:496:ILE:HD11	1.68	0.75
1:B:232:GLY:HA2	1:B:238:LYS:HD3	1.67	0.75
1:A:44:GLN:CB	1:A:45:ASP:HA	2.17	0.75
1:C:27:MET:CE	1:C:71:LEU:HB2	2.16	0.75
2:F:313:HIS:CE1	2:F:315:ILE:HG12	2.22	0.74
1:B:398:SER:HA	1:B:403:GLN:HE21	1.52	0.74
1:B:19:MET:HE1	1:B:64:VAL:HB	1.70	0.74
2:D:79:LEU:HD13	2:D:227:MET:HE3	1.69	0.74
1:C:232:GLY:HA3	1:C:238:LYS:HD3	1.69	0.74
1:C:129:GLU:N	1:C:129:GLU:OE1	2.20	0.73
2:D:398:ASP:CB	2:D:399:LYS:HB2	2.18	0.73
2:E:89:VAL:HG21	2:E:195:MET:HE1	1.70	0.73
2:D:224:THR:HB	2:D:225:PRO:HD3	1.70	0.73
1:A:103:LEU:HD21	2:D:117:ASN:HA	1.70	0.73
1:B:133:GLY:O	1:B:380:ARG:NH2	2.21	0.73
1:C:139:VAL:HG21	1:C:187:MET:CE	2.19	0.73
1:B:9:VAL:HG13	2:E:47:VAL:HG23	1.70	0.72
2:D:399:LYS:HG3	2:D:401:TYR:H	1.51	0.72
1:A:43:ARG:HB2	1:A:46:VAL:HG13	1.72	0.72
1:B:410:LYS:HB3	1:B:436:LEU:HB2	1.71	0.72
2:D:258:ARG:HD2	2:D:273:TYR:CE1	2.24	0.72
1:C:83:MET:HE2	1:C:270:VAL:HG13	1.71	0.71
2:F:368:THR:O	2:F:372:LEU:HG	1.89	0.71
2:E:132:ILE:HA	2:E:415:GLN:HE22	1.54	0.71
2:F:132:ILE:C	2:F:135:ILE:HD11	2.11	0.71
2:F:224:THR:HB	2:F:225:PRO:HD3	1.73	0.71
1:C:562:ILE:CG2	1:C:563:PRO:HD2	2.20	0.71
2:F:393:ALA:N	2:F:394:LEU:HA	2.04	0.71
2:E:125:ASP:HB2	2:E:126:GLU:HA	1.72	0.70
2:E:222:ILE:HD12	2:E:260:ILE:HD12	1.72	0.70
2:E:10:GLU:HG2	2:E:17:ALA:HB3	1.74	0.70
2:E:314:PRO:O	2:E:318:LEU:HG	1.91	0.70
1:B:260:GLY:HA3	1:B:261:GLU:CG	2.19	0.70
1:C:51:VAL:HG21	1:C:55:THR:HG23	1.73	0.70
2:F:365:HIS:HA	2:F:368:THR:CG2	2.22	0.70
2:F:395:SER:O	2:F:399:LYS:N	2.23	0.69
1:B:81:SER:HB3	1:B:286:MET:O	1.92	0.69
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.74	0.69
1:A:27:MET:CE	1:A:71:LEU:HB2	2.23	0.69
2:F:369:MET:HG3	2:F:370:ASN:N	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:45:LEU:HD13	2:E:264:ARG:HD3	1.73	0.69
2:D:182:ALA:HB3	2:D:247:MET:HG2	1.75	0.69
1:B:579:GLU:O	1:B:583:LEU:HB2	1.91	0.69
2:F:339:GLN:O	2:F:414:ASN:HA	1.93	0.69
2:E:91:ASP:HB2	2:E:95:ARG:H	1.58	0.69
2:F:278:TYR:HB2	2:F:318:LEU:CD1	2.23	0.68
1:B:82:GLN:NE2	1:B:92:ASP:OD2	2.27	0.68
2:E:363:GLU:OE2	2:E:363:GLU:N	2.25	0.68
1:C:559:SER:HA	1:C:562:ILE:HD11	1.76	0.68
1:A:479:ILE:HD11	1:A:487:ARG:CZ	2.24	0.68
1:C:262:ARG:HH21	2:F:324:GLU:HG3	1.59	0.68
2:F:285:PHE:HB2	2:F:322:ILE:HD11	1.75	0.68
1:B:397:ILE:HG23	1:B:402:THR:HG21	1.74	0.68
2:E:222:ILE:CD1	2:E:260:ILE:HD12	2.24	0.67
2:F:155:LEU:HD13	2:F:156:PRO:N	2.08	0.67
2:F:158:LYS:HG3	2:F:159:GLU:OE2	1.94	0.67
2:D:8:ILE:HD11	2:D:70:VAL:HG23	1.74	0.67
1:C:390:VAL:O	1:C:392:PRO:HD3	1.95	0.67
2:E:278:TYR:CB	2:E:318:LEU:HD13	2.22	0.67
2:F:229:LEU:HD13	2:F:287:ARG:HG3	1.76	0.67
2:F:395:SER:HB3	2:F:398:ASP:HB2	1.76	0.67
2:E:407:ARG:HG3	2:E:407:ARG:HH11	1.60	0.66
2:F:155:LEU:HD21	2:F:341:PRO:HG2	1.76	0.66
2:D:399:LYS:HD2	2:D:400:ILE:HG13	1.77	0.66
1:A:260:GLY:H	1:A:294:ASN:HB2	1.61	0.66
1:B:41:GLU:HB2	1:B:48:SER:HB2	1.77	0.66
2:E:345:LEU:HB2	2:E:346:PRO:HD3	1.78	0.66
2:F:137:HIS:CD2	2:F:369:MET:HB3	2.31	0.66
1:B:392:PRO:HG2	1:B:397:ILE:HD13	1.78	0.66
1:C:550:VAL:HG12	1:C:553:ARG:HH12	1.59	0.66
2:F:212:ASN:OD1	2:F:221:ARG:HG2	1.94	0.66
1:C:148:LYS:N	1:C:320:MET:HE3	2.05	0.66
1:A:25:GLN:NE2	1:A:38:GLU:OE2	2.28	0.65
1:A:148:LYS:HE3	3:A:601:GOL:H31	1.76	0.65
1:B:397:ILE:O	1:B:403:GLN:NE2	2.29	0.65
2:D:260:ILE:O	2:D:264:ARG:HG3	1.96	0.65
2:E:136:ASP:O	2:E:137:HIS:ND1	2.29	0.65
1:C:29:LEU:HD12	1:C:65:ARG:HH12	1.60	0.65
1:C:33:LEU:H	1:C:33:LEU:HD12	1.62	0.65
1:B:232:GLY:CA	1:B:238:LYS:HD3	2.26	0.65
1:B:261:GLU:OE1	1:B:330:SER:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:HB2	1:A:180:GLN:NE2	2.12	0.64
2:D:19:GLU:HB3	2:D:20:LYS:HD2	1.79	0.64
2:F:366:ALA:O	2:F:370:ASN:ND2	2.29	0.64
1:A:84:PHE:HB3	1:A:88:GLN:HA	1.79	0.64
2:F:155:LEU:HD11	2:F:329:LEU:HD13	1.78	0.64
2:F:285:PHE:HD2	2:F:322:ILE:HG12	1.61	0.64
2:D:345:LEU:HB2	2:D:346:PRO:HD3	1.79	0.64
2:E:57:PHE:CE2	2:E:219:ILE:HG21	2.32	0.64
2:E:132:ILE:HA	2:E:415:GLN:NE2	2.12	0.64
1:B:392:PRO:HB2	1:B:394:GLY:O	1.97	0.64
1:B:416:ASP:OD1	1:B:418:SER:OG	2.10	0.64
2:D:79:LEU:HD13	2:D:227:MET:CE	2.27	0.64
1:C:218:THR:HG23	1:C:453:TRP:CZ2	2.32	0.64
1:A:150:MET:HE1	1:A:319:ASP:HB3	1.80	0.64
2:F:376:TYR:OH	2:F:409:GLU:HG3	1.97	0.64
1:B:83:MET:CE	2:E:119:ILE:HG22	2.28	0.64
1:B:83:MET:HE1	1:B:270:VAL:HG13	1.81	0.64
1:C:536:LEU:HA	1:C:540:ALA:HB3	1.80	0.64
1:A:476:LEU:N	1:A:477:VAL:HA	2.14	0.63
2:E:79:LEU:HG	2:E:227:MET:HE3	1.79	0.63
1:A:148:LYS:H	1:A:320:MET:CE	2.11	0.63
2:E:129:GLN:OE1	2:E:423:ILE:N	2.29	0.63
2:F:128:ILE:HD11	2:F:143:ARG:HG2	1.79	0.63
2:F:397:ILE:HA	2:F:400:ILE:HG12	1.79	0.63
1:B:555:ARG:NH2	1:B:573:ILE:HA	2.13	0.63
2:D:31:GLU:HG3	2:D:73:LEU:HD11	1.80	0.63
2:E:383:LYS:HG2	2:E:402:ALA:HB1	1.80	0.63
1:C:83:MET:CE	1:C:270:VAL:HG13	2.29	0.63
2:E:156:PRO:HG3	2:E:334:TYR:CE1	2.34	0.63
2:E:280:ASN:O	2:E:283:THR:HG22	1.98	0.63
1:C:12:PRO:O	1:C:51:VAL:HG22	1.98	0.63
2:D:306:MET:CE	2:D:311:LYS:HA	2.29	0.63
1:B:565:GLU:N	1:B:565:GLU:OE1	2.32	0.62
1:C:60:PRO:HD3	2:F:47:VAL:HG13	1.80	0.62
2:F:128:ILE:CD1	2:F:143:ARG:HG2	2.30	0.62
2:F:155:LEU:CD1	2:F:329:LEU:HD13	2.28	0.62
2:F:364:ASP:O	2:F:368:THR:HG22	1.98	0.62
2:E:249:ASP:OD1	2:E:304:LEU:HA	1.98	0.62
1:C:144:ILE:HG21	1:C:288:ARG:CD	2.28	0.62
2:E:258:ARG:NH2	2:E:271:ARG:O	2.31	0.62
2:F:135:ILE:HD13	2:F:136:ASP:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:MET:HE3	1:A:71:LEU:HB2	1.79	0.62
2:F:313:HIS:CG	2:F:314:PRO:HD2	2.34	0.62
1:B:285:LEU:O	1:B:289:THR:HG23	2.00	0.62
1:C:315:GLU:HA	1:C:384:ILE:HD11	1.81	0.62
1:B:412:PHE:HB3	1:B:434:TYR:CE2	2.35	0.62
1:B:541:TYR:O	1:B:545:ILE:HG12	2.00	0.62
2:E:89:VAL:HG21	2:E:195:MET:CE	2.29	0.62
2:E:407:ARG:HG3	2:E:407:ARG:NH1	2.14	0.62
1:C:269:VAL:O	1:C:273:PHE:HB2	2.00	0.62
1:A:148:LYS:HE3	3:A:601:GOL:C3	2.30	0.62
1:B:19:MET:CE	1:B:64:VAL:HB	2.30	0.62
2:E:345:LEU:CG	2:E:376:TYR:HE2	2.10	0.62
2:F:278:TYR:HB2	2:F:318:LEU:HD12	1.80	0.62
2:D:249:ASP:OD2	2:D:304:LEU:HA	2.00	0.62
2:F:184:ILE:N	2:F:248:THR:O	2.30	0.62
2:F:271:ARG:O	2:F:271:ARG:NE	2.31	0.62
1:B:521:MET:HE1	1:B:560:LYS:HB3	1.82	0.61
2:D:252:ASN:OD1	1:C:407:ARG:NH2	2.32	0.61
1:C:214:ARG:HG2	1:C:518:GLN:HG2	1.82	0.61
1:A:19:MET:HG3	1:A:22:ALA:HB2	1.82	0.61
1:B:521:MET:CE	1:B:560:LYS:HB3	2.30	0.61
2:E:282:ALA:CA	2:E:322:ILE:HD13	2.29	0.61
1:C:497:ARG:HA	1:C:501:LEU:HB2	1.83	0.61
1:B:298:MET:HB3	1:B:299:PRO:HD2	1.82	0.61
2:D:66:LYS:HE3	1:C:20:SER:HB2	1.82	0.61
2:E:345:LEU:HG	2:E:376:TYR:CE2	2.28	0.61
1:C:331:THR:HG22	1:C:389:ALA:O	2.01	0.61
2:F:86:ILE:HA	2:F:208:VAL:HG22	1.81	0.61
2:F:184:ILE:HD11	2:F:225:PRO:HG3	1.82	0.61
1:C:123:THR:HG22	1:C:137:GLY:HA2	1.83	0.61
1:B:429:ASN:O	1:B:433:SER:OG	2.18	0.61
2:E:5:TYR:CE2	2:E:21:VAL:HG23	2.35	0.61
1:C:251:VAL:HG11	1:C:325:ALA:N	2.16	0.61
1:C:397:ILE:O	1:C:403:GLN:NE2	2.34	0.61
2:F:166:ARG:NH1	2:F:197:ASP:OD2	2.34	0.61
1:B:202:LYS:HG2	2:F:188:PHE:CE2	2.36	0.60
1:B:274:PRO:HA	1:B:286:MET:HG2	1.83	0.60
1:B:462:ARG:NH1	1:B:466:GLU:OE1	2.33	0.60
2:E:271:ARG:HG3	2:E:314:PRO:HG3	1.84	0.60
2:F:395:SER:CB	2:F:398:ASP:HB2	2.30	0.60
2:E:363:GLU:CD	2:E:363:GLU:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:GLN:OE1	2:F:264:ARG:NH2	2.30	0.60
2:F:135:ILE:CD1	2:F:136:ASP:H	2.13	0.60
2:E:91:ASP:HB3	2:E:93:LEU:H	1.66	0.60
2:E:383:LYS:HZ1	2:E:406:GLU:HG3	1.65	0.60
2:F:187:THR:HG23	2:F:190:GLU:H	1.66	0.60
1:A:546:MET:HA	1:A:546:MET:CE	2.32	0.60
1:C:167:PHE:HB3	1:C:171:ASP:HB2	1.83	0.60
1:C:560:LYS:HD2	1:C:561:TYR:CZ	2.36	0.60
2:F:130:THR:OG1	2:F:136:ASP:OD1	2.18	0.60
1:B:139:VAL:HG21	1:B:187:MET:CE	2.31	0.60
2:D:11:VAL:CG1	1:C:24:ILE:HD11	2.32	0.60
2:E:30:ILE:HD11	2:E:42:GLY:HA3	1.83	0.60
1:C:453:TRP:HZ3	1:C:519:PHE:HA	1.65	0.60
2:F:124:PRO:HB2	2:F:142:VAL:CG1	2.31	0.60
1:B:144:ILE:HD12	1:B:281:THR:HG21	1.84	0.60
1:B:445:MET:CE	1:B:515:ARG:HG3	2.29	0.60
1:C:277:ILE:HD12	1:C:277:ILE:H	1.66	0.60
2:F:186:ILE:CD1	2:F:191:ALA:HB2	2.32	0.60
1:B:300:VAL:HG22	1:B:303:ARG:NH2	2.17	0.60
2:F:166:ARG:NH2	2:F:417:PHE:O	2.35	0.60
2:F:452:LYS:HA	2:F:452:LYS:HZ3	1.65	0.60
2:E:282:ALA:HA	2:E:322:ILE:HD13	1.84	0.60
1:C:75:LEU:HD13	1:C:316:TYR:CD1	2.37	0.60
1:B:398:SER:HA	1:B:403:GLN:NE2	2.16	0.59
2:E:125:ASP:CB	2:E:126:GLU:HA	2.29	0.59
2:E:151:SER:OG	2:E:152:GLY:N	2.35	0.59
1:C:307:ILE:HD11	1:C:328:ALA:HB1	1.84	0.59
1:B:41:GLU:OE2	1:B:43:ARG:NH1	2.23	0.59
1:C:87:ILE:HD11	1:C:89:ARG:NE	2.17	0.59
2:F:407:ARG:O	2:F:411:GLU:N	2.35	0.59
2:D:280:ASN:O	2:D:283:THR:HG22	2.03	0.59
1:C:225:GLY:O	1:C:370:GLY:HA2	2.01	0.59
2:D:126:GLU:HG2	2:D:143:ARG:NH1	2.18	0.59
2:D:315:ILE:HB	2:D:316:PRO:HD3	1.85	0.59
2:F:267:VAL:HG22	2:F:268:PRO:CD	2.20	0.59
2:D:26:TYR:CE2	2:D:27:GLU:HG3	2.37	0.59
2:D:288:ALA:HB2	2:D:300:GLN:HG3	1.84	0.59
2:D:357:GLY:N	2:D:361:THR:HG22	2.18	0.59
2:F:89:VAL:HB	2:F:98:ASP:HB2	1.83	0.59
2:D:166:ARG:CD	2:D:201:THR:HG21	2.32	0.59
2:E:178:ALA:HB2	2:E:241:MET:CE	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASP:HA	2:D:119:ILE:HD11	1.85	0.59
2:F:371:GLN:OE1	2:F:442:LEU:HA	2.02	0.59
1:B:285:LEU:HD21	1:B:288:ARG:NH2	2.18	0.59
2:E:315:ILE:HB	2:E:316:PRO:HD3	1.85	0.59
1:C:29:LEU:HD12	1:C:65:ARG:NH1	2.18	0.59
2:D:398:ASP:HB3	2:D:399:LYS:HB2	1.85	0.59
2:D:438:PRO:HB2	2:D:440:THR:HG23	1.84	0.59
2:E:127:PHE:HB2	2:E:355:GLY:O	2.02	0.59
2:F:137:HIS:CE1	2:F:368:THR:HG23	2.38	0.59
2:F:151:SER:CB	2:F:329:LEU:HD12	2.27	0.59
1:B:260:GLY:CA	1:B:261:GLU:HG2	2.26	0.58
2:D:45:LEU:CD1	2:D:264:ARG:HD3	2.32	0.58
2:E:408:PHE:CE2	2:E:412:TYR:CD2	2.91	0.58
2:F:126:GLU:CB	2:F:143:ARG:HE	2.15	0.58
2:F:330:THR:OG1	2:F:333:LEU:HD13	2.04	0.58
1:A:224:LYS:HE2	1:A:250:ASP:HB3	1.85	0.58
1:B:139:VAL:HG21	1:B:187:MET:HE1	1.85	0.58
2:D:191:ALA:O	2:D:195:MET:HG2	2.03	0.58
1:B:371:ARG:HD2	1:B:381:GLU:OE2	2.03	0.58
2:D:264:ARG:NH1	2:D:266:GLU:OE2	2.35	0.58
2:F:370:ASN:ND2	2:F:370:ASN:H	2.01	0.58
1:A:133:GLY:HA2	1:A:150:MET:HE2	1.84	0.58
2:D:389:LEU:CB	2:D:392:SER:H	2.16	0.58
2:F:125:ASP:OD2	2:F:290:ARG:NH1	2.36	0.58
2:F:153:SER:O	2:F:331:ARG:NH2	2.36	0.58
1:B:199:ILE:HD12	1:B:372:VAL:HB	1.84	0.58
1:B:262:ARG:HB2	1:B:265:GLU:CD	2.24	0.58
1:B:73:VAL:CG1	1:B:309:THR:HG23	2.33	0.58
2:D:91:ASP:OD1	2:D:95:ARG:N	2.20	0.58
2:D:184:ILE:CD1	2:D:225:PRO:HG3	2.34	0.58
1:C:79:ILE:HD11	1:C:313:ILE:HD13	1.84	0.58
1:A:43:ARG:HD3	4:A:761:HOH:O	2.02	0.58
2:E:313:HIS:CG	2:E:314:PRO:HD2	2.39	0.58
2:E:357:GLY:O	2:E:360:LYS:N	2.33	0.58
2:F:332:GLU:N	2:F:332:GLU:OE2	2.36	0.58
1:B:416:ASP:HB3	1:B:419:LEU:HG	1.86	0.58
1:A:225:GLY:O	1:A:370:GLY:HA2	2.03	0.57
1:C:73:VAL:HG11	1:C:309:THR:HG23	1.86	0.57
2:D:328:ILE:CD1	2:D:346:PRO:HB2	2.31	0.57
2:E:116:ILE:HD13	2:E:291:ILE:HD11	1.86	0.57
2:E:250:MET:HB2	2:E:304:LEU:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:ARG:HD2	2:F:201:THR:OG1	2.04	0.57
1:A:320:MET:HE2	1:A:322:TYR:CE2	2.39	0.57
2:F:184:ILE:CD1	2:F:225:PRO:HG3	2.33	0.57
2:F:376:TYR:O	2:F:380:LYS:N	2.30	0.57
2:D:11:VAL:HG12	2:D:65:LEU:HD21	1.87	0.57
2:D:213:LEU:N	2:D:216:ASP:OD2	2.30	0.57
1:C:41:GLU:CG	1:C:48:SER:HB2	2.33	0.57
1:C:124:ILE:HG22	1:C:162:ILE:HD13	1.86	0.57
1:C:523:LYS:O	1:C:527:THR:OG1	2.21	0.57
2:F:19:GLU:OE1	2:F:51:LYS:NZ	2.37	0.57
1:B:391:SER:O	1:B:391:SER:OG	2.22	0.57
2:F:77:LEU:HD12	2:F:77:LEU:O	2.04	0.57
1:A:156:LYS:O	1:A:178:THR:HG22	2.04	0.57
1:A:541:TYR:O	1:A:545:ILE:HG12	2.05	0.57
1:B:230:VAL:CG2	1:B:387:ILE:HD11	2.35	0.57
1:C:298:MET:HB3	1:C:299:PRO:HD2	1.87	0.57
1:C:494:LYS:HA	1:C:497:ARG:NH1	2.20	0.57
2:D:89:VAL:CG2	2:D:195:MET:HE1	2.23	0.56
2:E:79:LEU:HD22	2:E:80:GLY:N	2.20	0.56
1:C:406:LEU:HA	1:C:409:VAL:HG22	1.86	0.56
2:F:409:GLU:O	2:F:413:VAL:HB	2.05	0.56
1:A:148:LYS:CB	1:A:320:MET:HE3	2.32	0.56
1:B:30:VAL:HB	1:B:35:VAL:HG23	1.87	0.56
2:F:271:ARG:HD3	2:F:271:ARG:N	2.20	0.56
1:B:144:ILE:HG12	1:B:287:GLU:HB3	1.86	0.56
2:D:146:LYS:NZ	4:D:501:HOH:O	2.32	0.56
2:E:86:ILE:HD13	2:E:208:VAL:CG2	2.36	0.56
2:F:313:HIS:ND1	2:F:315:ILE:HG12	2.19	0.56
2:F:315:ILE:O	2:F:319:THR:HG23	2.06	0.56
2:F:376:TYR:OH	2:F:409:GLU:N	2.38	0.56
1:B:176:ILE:HD12	1:B:185:LEU:HD11	1.86	0.56
2:F:314:PRO:O	2:F:318:LEU:HD23	2.05	0.56
1:A:298:MET:HB3	1:A:299:PRO:HD2	1.86	0.56
1:C:546:MET:HA	1:C:546:MET:CE	2.36	0.56
2:D:103:ILE:O	2:D:105:PRO:HD3	2.05	0.56
1:B:73:VAL:HG11	1:B:309:THR:HG23	1.88	0.56
2:D:155:LEU:HB3	2:D:156:PRO:HD2	1.87	0.56
2:D:386:ALA:HA	2:D:391:GLU:CB	2.36	0.56
2:E:379:GLY:O	2:E:383:LYS:HG3	2.06	0.56
1:C:90:PRO:HD3	1:C:111:ALA:HA	1.87	0.56
1:A:22:ALA:HB1	1:A:39:ILE:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:GLU:HB3	2:D:350:ARG:HB2	1.88	0.56
2:E:229:LEU:HD21	2:E:247:MET:HE3	1.87	0.56
1:C:232:GLY:CA	1:C:238:LYS:HD3	2.36	0.56
2:D:146:LYS:HD3	2:D:285:PHE:O	2.06	0.56
2:D:354:LYS:HD2	2:D:354:LYS:N	2.21	0.56
2:E:148:PRO:HD3	2:E:323:THR:HB	1.87	0.56
1:C:513:THR:HG23	1:C:517:LYS:HE3	1.87	0.56
2:F:11:VAL:HG22	2:F:16:MET:HG3	1.88	0.56
1:B:212:GLY:HA3	1:B:512:PHE:CD1	2.42	0.55
1:B:489:THR:CG2	1:B:533:ARG:HH12	2.17	0.55
2:D:136:ASP:O	2:D:140:THR:HG23	2.05	0.55
2:E:405:ALA:O	2:E:408:PHE:HB3	2.07	0.55
1:B:397:ILE:O	1:B:397:ILE:HG22	2.07	0.55
2:D:332:GLU:O	2:D:336:SER:HB2	2.07	0.55
2:E:143:ARG:NH2	2:E:170:VAL:HB	2.21	0.55
2:E:345:LEU:HB2	2:E:346:PRO:CD	2.35	0.55
2:E:352:LYS:O	2:E:356:THR:HG23	2.06	0.55
2:E:26:TYR:CE2	2:E:27:GLU:HG3	2.42	0.55
1:C:550:VAL:HA	1:C:553:ARG:NH1	2.21	0.55
2:D:399:LYS:HG3	2:D:401:TYR:N	2.22	0.55
2:E:106:GLU:OE1	2:E:234:TYR:OH	2.21	0.55
1:C:212:GLY:HA3	1:C:512:PHE:CD1	2.42	0.55
2:F:149:VAL:HB	2:F:303:ILE:HD13	1.88	0.55
1:A:523:LYS:HD2	1:A:574:ASN:HD21	1.72	0.55
2:E:150:PHE:HB2	2:E:328:ILE:HD13	1.89	0.55
1:C:191:TRP:CZ2	1:C:198:PRO:HD3	2.42	0.55
1:A:95:MET:CE	2:D:120:ALA:HB2	2.37	0.55
1:A:183:LYS:NZ	4:A:702:HOH:O	2.32	0.55
1:B:262:ARG:HB2	1:B:265:GLU:OE1	2.07	0.55
2:E:55:GLN:OE1	2:E:264:ARG:NH1	2.39	0.55
1:B:209:MET:SD	1:B:249:SER:HB3	2.46	0.55
2:D:292:ARG:HD2	4:D:502:HOH:O	2.06	0.55
2:F:123:TYR:O	2:F:290:ARG:NH1	2.40	0.55
2:D:282:ALA:HB2	2:D:322:ILE:HD13	1.89	0.55
2:F:340:PRO:HB3	2:F:417:PHE:HE1	1.71	0.55
2:F:343:ASP:OD2	2:F:346:PRO:HD3	2.06	0.55
1:C:307:ILE:HG13	1:C:365:TYR:CE1	2.42	0.54
1:C:392:PRO:O	2:F:321:TYR:OH	2.25	0.54
1:B:83:MET:CE	1:B:270:VAL:HG13	2.37	0.54
1:B:210:ILE:HD11	1:B:515:ARG:HE	1.73	0.54
1:B:445:MET:HG2	1:B:453:TRP:CE3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:357:GLY:H	2:D:361:THR:HG22	1.71	0.54
2:E:379:GLY:HA2	2:E:401:TYR:C	2.27	0.54
1:C:562:ILE:HD12	1:C:562:ILE:H	1.73	0.54
2:F:149:VAL:HB	2:F:303:ILE:CD1	2.37	0.54
1:A:462:ARG:O	1:A:466:GLU:HB2	2.07	0.54
1:C:97:VAL:HG11	1:C:109:LEU:CD2	2.38	0.54
1:A:425:PHE:HA	1:A:426:PRO:C	2.28	0.54
1:B:262:ARG:NH2	2:E:323:THR:O	2.40	0.54
2:D:184:ILE:N	2:D:248:THR:O	2.35	0.54
2:F:237:TYR:CZ	2:F:291:ILE:HD13	2.43	0.54
2:F:269:GLY:H	2:F:270:ARG:HA	1.72	0.54
1:A:83:MET:SD	1:A:270:VAL:HG13	2.48	0.54
1:A:95:MET:HE2	2:D:120:ALA:HB2	1.90	0.54
1:A:285:LEU:O	1:A:289:THR:HG23	2.06	0.54
2:D:345:LEU:HG	2:D:376:TYR:HE2	1.71	0.54
2:D:356:THR:HG21	2:D:365:HIS:CE1	2.43	0.54
1:C:400:PRO:O	1:C:404:ASN:ND2	2.26	0.54
1:B:231:PRO:HG2	1:B:415:LEU:H	1.73	0.54
2:D:111:ILE:HA	2:D:230:THR:OG1	2.08	0.54
2:E:8:ILE:HD11	2:E:11:VAL:HG23	1.90	0.54
1:C:462:ARG:HH21	1:C:463:ILE:HG22	1.71	0.54
1:C:559:SER:CA	1:C:562:ILE:HD11	2.36	0.54
2:F:135:ILE:HD12	2:F:136:ASP:N	2.20	0.54
2:F:137:HIS:NE2	2:F:368:THR:HG23	2.23	0.54
2:F:340:PRO:HD3	2:F:416:GLY:O	2.08	0.54
1:A:126:GLU:HG2	1:A:162:ILE:HG22	1.89	0.54
2:D:10:GLU:HB2	2:D:17:ALA:HB3	1.90	0.54
2:D:398:ASP:CA	2:D:399:LYS:HB2	2.38	0.54
2:E:378:GLN:HA	2:E:378:GLN:OE1	2.07	0.54
1:C:156:LYS:O	1:C:178:THR:HG22	2.08	0.54
1:B:205:PRO:HB2	1:B:223:THR:OG1	2.08	0.54
2:E:184:ILE:N	2:E:248:THR:O	2.31	0.54
2:E:338:ILE:HA	2:E:414:ASN:OD1	2.08	0.54
2:F:306:MET:HG2	2:F:316:PRO:HG3	1.88	0.54
1:B:84:PHE:HB2	1:B:292:ILE:HD13	1.90	0.53
1:B:403:GLN:O	1:B:407:ARG:HG3	2.07	0.53
1:C:273:PHE:N	1:C:274:PRO:HD2	2.23	0.53
1:C:307:ILE:HD11	1:C:328:ALA:CB	2.38	0.53
1:B:529:GLY:O	1:B:533:ARG:HB2	2.08	0.53
2:D:431:TRP:O	2:D:435:ALA:N	2.41	0.53
1:A:27:MET:HE2	1:A:71:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:CG	1:A:46:VAL:HG13	2.39	0.53
1:A:148:LYS:H	1:A:320:MET:HE3	1.73	0.53
1:A:205:PRO:HB2	1:A:223:THR:OG1	2.09	0.53
2:D:33:ARG:O	2:D:33:ARG:HD3	2.08	0.53
1:C:222:VAL:HG22	1:C:411:VAL:HG11	1.90	0.53
2:D:34:MET:HE3	2:D:38:GLU:HB3	1.90	0.53
2:D:55:GLN:CD	2:D:219:ILE:HD11	2.28	0.53
2:D:345:LEU:HB2	2:D:346:PRO:CD	2.39	0.53
2:E:383:LYS:HZ2	2:E:406:GLU:HG3	1.74	0.53
1:C:497:ARG:O	1:C:502:GLN:HG3	2.08	0.53
1:B:266:MET:O	1:B:270:VAL:HG23	2.08	0.53
2:D:9:LYS:HD3	2:D:19:GLU:CD	2.29	0.53
2:D:402:ALA:HA	2:D:405:ALA:HB3	1.91	0.53
2:E:87:GLY:HA2	2:E:204:ILE:O	2.08	0.53
1:C:533:ARG:HA	1:C:536:LEU:HB3	1.90	0.53
2:F:125:ASP:OD2	2:F:125:ASP:N	2.34	0.53
1:A:495:SER:O	1:A:499:ASP:HB2	2.09	0.53
1:B:549:THR:O	1:B:553:ARG:HG3	2.09	0.53
2:D:8:ILE:HD13	2:D:16:MET:CE	2.39	0.53
2:E:41:ARG:HB2	2:E:57:PHE:CD1	2.44	0.53
2:E:129:GLN:HE22	2:E:171:LEU:HD13	1.73	0.53
1:C:262:ARG:NH2	2:F:323:THR:O	2.42	0.53
2:F:126:GLU:O	2:F:142:VAL:HG13	2.09	0.53
2:F:151:SER:OG	2:F:157:HIS:HB3	2.08	0.53
1:B:208:PRO:HG3	1:B:441:VAL:HG22	1.91	0.53
1:C:467:GLU:OE2	1:C:497:ARG:NH1	2.42	0.53
2:F:34:MET:HE2	2:F:40:ARG:HG3	1.90	0.53
1:B:273:PHE:HB3	1:B:274:PRO:HD3	1.91	0.53
1:B:405:THR:O	1:B:409:VAL:HG22	2.09	0.53
1:C:60:PRO:HD3	2:F:47:VAL:CG1	2.39	0.53
1:C:139:VAL:HG21	1:C:187:MET:HE2	1.91	0.53
1:C:386:ALA:C	1:C:387:ILE:HD12	2.29	0.53
1:C:416:ASP:OD2	1:C:418:SER:HB2	2.08	0.53
1:C:480:ASP:OD1	1:C:481:SER:N	2.42	0.53
2:F:5:TYR:HB3	2:F:7:THR:HG22	1.91	0.53
2:F:269:GLY:N	2:F:270:ARG:HA	2.24	0.53
1:B:399:GLU:OE2	1:B:402:THR:OG1	2.22	0.53
2:D:362:ARG:HH11	2:D:364:ASP:CB	2.22	0.53
2:E:111:ILE:HA	2:E:230:THR:OG1	2.09	0.53
1:C:25:GLN:HG3	1:C:38:GLU:OE1	2.09	0.53
2:F:95:ARG:HG3	4:F:518:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:GLU:O	1:B:368:ARG:HG3	2.08	0.52
2:D:248:THR:HG22	2:D:249:ASP:HB2	1.91	0.52
2:E:89:VAL:CG2	2:E:195:MET:HE1	2.38	0.52
2:E:386:ALA:HA	2:E:387:VAL:C	2.29	0.52
1:B:173:ILE:HD13	1:B:187:MET:HG2	1.92	0.52
2:E:71:ARG:HD2	4:E:527:HOH:O	2.08	0.52
2:E:376:TYR:CD1	2:E:408:PHE:HD1	2.27	0.52
1:C:173:ILE:HD13	1:C:173:ILE:H	1.73	0.52
1:C:552:VAL:HG11	1:C:577:ILE:HG12	1.91	0.52
2:F:204:ILE:HD13	2:F:204:ILE:O	2.10	0.52
2:F:307:PRO:HG2	2:F:313:HIS:CD2	2.44	0.52
1:A:40:ILE:HG13	1:A:50:GLN:HG2	1.90	0.52
1:B:507:ASP:HB3	1:B:510:ASP:HB3	1.91	0.52
4:B:601:HOH:O	2:E:322:ILE:HG23	2.08	0.52
2:E:125:ASP:HA	2:E:142:VAL:CG1	2.39	0.52
1:C:532:ALA:HA	1:C:581:ILE:HD11	1.90	0.52
1:A:315:GLU:HA	1:A:384:ILE:HD11	1.92	0.52
1:B:210:ILE:HD11	1:B:515:ARG:HH21	1.75	0.52
2:D:116:ILE:HD13	2:D:291:ILE:CD1	2.36	0.52
2:D:430:GLY:O	2:D:434:LEU:HB2	2.08	0.52
2:E:124:PRO:HA	2:E:290:ARG:HD3	1.92	0.52
1:C:425:PHE:HA	1:C:426:PRO:C	2.28	0.52
2:F:135:ILE:CD1	2:F:136:ASP:N	2.72	0.52
2:F:270:ARG:CB	2:F:271:ARG:CA	2.88	0.52
2:F:319:THR:O	2:F:323:THR:HG23	2.10	0.52
1:A:162:ILE:HD13	1:A:174:CYS:HB2	1.91	0.52
1:A:459:GLU:O	1:A:463:ILE:HG13	2.10	0.52
1:B:380:ARG:HG2	4:B:614:HOH:O	2.09	0.52
1:C:84:PHE:HB3	1:C:88:GLN:HA	1.90	0.52
2:F:270:ARG:CB	2:F:271:ARG:HA	2.40	0.52
2:D:87:GLY:HA2	2:D:204:ILE:O	2.09	0.52
1:A:204:ASN:HD21	2:E:192:GLU:HG2	1.75	0.52
1:A:258:GLY:HA2	1:A:329:ASP:O	2.10	0.52
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.92	0.52
2:E:29:LEU:HD21	2:E:77:LEU:HG	1.91	0.52
2:F:431:TRP:HA	2:F:434:LEU:CD1	2.39	0.52
2:D:12:VAL:HG13	1:C:41:GLU:OE2	2.10	0.52
2:E:404:PHE:CZ	2:E:436:MET:CB	2.93	0.52
1:C:417:SER:O	1:C:421:GLN:HG3	2.10	0.52
1:A:43:ARG:HG2	1:A:46:VAL:HG13	1.91	0.51
1:A:212:GLY:HA3	1:A:512:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:HIS:HB3	1:B:170:ASP:OD2	2.10	0.51
1:B:253:LEU:HD13	1:B:317:PHE:CG	2.45	0.51
1:B:397:ILE:CG2	1:B:402:THR:HG21	2.38	0.51
2:D:124:PRO:HG2	2:D:351:LEU:CD1	2.37	0.51
2:D:148:PRO:HD3	2:D:323:THR:HB	1.92	0.51
2:E:166:ARG:HD2	2:E:201:THR:HG21	1.92	0.51
2:E:182:ALA:HB3	2:E:247:MET:HG2	1.91	0.51
1:A:399:GLU:HB2	1:A:400:PRO:HD2	1.91	0.51
2:E:408:PHE:HE2	2:E:412:TYR:CD2	2.27	0.51
2:F:58:GLU:OE1	2:F:58:GLU:N	2.42	0.51
2:F:237:TYR:CE2	2:F:291:ILE:HD13	2.45	0.51
1:B:461:MET:HA	1:B:461:MET:CE	2.41	0.51
1:B:564:GLU:O	1:B:567:LEU:HD11	2.10	0.51
1:C:234:PHE:CE2	2:F:350:ARG:HG2	2.45	0.51
1:C:245:ILE:O	1:C:249:SER:OG	2.23	0.51
2:F:132:ILE:CB	2:F:135:ILE:HD11	2.40	0.51
1:A:297:ASN:ND2	2:D:115:VAL:HG22	2.25	0.51
1:A:573:ILE:O	1:A:577:ILE:HG13	2.10	0.51
1:B:75:LEU:HD13	1:B:316:TYR:CD1	2.45	0.51
1:B:311:ILE:HD13	1:B:368:ARG:HB2	1.92	0.51
2:D:65:LEU:HD12	2:D:65:LEU:H	1.75	0.51
2:D:126:GLU:OE2	2:D:290:ARG:NH1	2.43	0.51
2:D:271:ARG:HB3	2:D:314:PRO:HG2	1.92	0.51
2:F:285:PHE:HB2	2:F:322:ILE:CD1	2.41	0.51
1:A:351:ASP:OD1	2:E:258:ARG:NH2	2.43	0.51
1:B:271:ASN:OD1	2:E:292:ARG:NH2	2.44	0.51
1:B:396:ASP:OD2	1:B:398:SER:N	2.39	0.51
1:B:497:ARG:O	1:B:502:GLN:HG3	2.11	0.51
2:D:45:LEU:CD1	2:D:264:ARG:CD	2.89	0.51
1:C:415:LEU:HD23	1:C:428:ILE:HG12	1.92	0.51
1:A:474:VAL:O	1:A:478:GLY:N	2.44	0.51
2:D:184:ILE:HD13	2:D:225:PRO:HG3	1.92	0.51
2:D:199:ARG:HD3	4:D:522:HOH:O	2.10	0.51
1:A:38:GLU:OE1	1:A:52:TYR:OH	2.29	0.51
1:A:224:LYS:CE	1:A:250:ASP:HB3	2.41	0.51
2:F:87:GLY:HA2	2:F:204:ILE:HD13	1.92	0.51
1:A:194:ARG:NH1	4:A:704:HOH:O	2.42	0.51
1:A:532:ALA:O	1:A:536:LEU:HG	2.11	0.51
1:A:545:ILE:HD13	1:A:584:ILE:HG21	1.92	0.51
1:C:463:ILE:HD11	1:C:496:ILE:CD1	2.36	0.51
1:B:262:ARG:HB2	1:B:265:GLU:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:VAL:HG21	1:C:55:THR:HG21	1.92	0.51
1:A:266:MET:HE3	1:A:266:MET:HA	1.92	0.51
2:D:13:GLY:O	2:D:60:THR:HG21	2.11	0.51
2:E:376:TYR:CD1	2:E:408:PHE:CD1	2.99	0.51
1:C:492:VAL:O	1:C:496:ILE:HG13	2.11	0.51
1:A:551:ALA:O	1:A:554:GLU:HB3	2.11	0.50
1:B:254:VAL:HB	1:B:289:THR:HG22	1.93	0.50
2:F:328:ILE:N	2:F:347:SER:OG	2.30	0.50
2:F:369:MET:HG3	2:F:370:ASN:H	1.74	0.50
1:B:92:ASP:OD2	1:B:93:THR:N	2.42	0.50
1:B:562:ILE:HG13	1:B:570:ILE:HG12	1.92	0.50
2:F:203:ALA:O	2:F:206:ARG:HG2	2.11	0.50
2:F:396:ASP:O	2:F:400:ILE:HG23	2.11	0.50
1:A:43:ARG:HB2	1:A:46:VAL:O	2.11	0.50
1:A:71:LEU:HD23	1:A:193:VAL:HG21	1.93	0.50
2:D:315:ILE:HB	2:D:316:PRO:CD	2.41	0.50
2:D:328:ILE:HD12	2:D:346:PRO:CB	2.33	0.50
1:B:565:GLU:O	1:B:567:LEU:HD22	2.11	0.50
2:D:399:LYS:HD2	2:D:400:ILE:CG1	2.42	0.50
1:C:139:VAL:HG21	1:C:187:MET:HE3	1.91	0.50
1:C:473:ILE:O	1:C:477:VAL:HG22	2.10	0.50
1:A:126:GLU:CG	1:A:162:ILE:HG22	2.40	0.50
1:A:218:THR:HG23	1:A:453:TRP:CZ2	2.46	0.50
1:B:225:GLY:O	1:B:370:GLY:HA2	2.10	0.50
2:E:315:ILE:HB	2:E:316:PRO:CD	2.41	0.50
2:F:144:GLY:HA2	2:F:298:VAL:O	2.12	0.50
1:A:16:ALA:HB3	1:A:19:MET:CE	2.42	0.50
1:B:311:ILE:CD1	1:B:368:ARG:HB2	2.41	0.50
2:F:8:ILE:O	2:F:8:ILE:HG13	2.11	0.50
2:F:155:LEU:HD21	2:F:341:PRO:CG	2.40	0.50
1:A:40:ILE:HG22	1:A:41:GLU:HG3	1.94	0.50
1:C:338:LEU:HD22	1:C:355:PRO:HG3	1.94	0.50
1:C:493:ALA:O	1:C:497:ARG:HG3	2.11	0.50
1:B:230:VAL:HG21	1:B:387:ILE:HD11	1.94	0.50
2:F:422:THR:O	2:F:426:THR:N	2.39	0.50
1:A:80:ILE:O	1:A:81:SER:HB2	2.12	0.50
1:B:80:ILE:HG22	1:B:81:SER:HB3	1.94	0.50
2:D:399:LYS:HD2	2:D:400:ILE:N	2.22	0.50
2:E:219:ILE:HD13	2:E:260:ILE:CD1	2.39	0.50
2:E:408:PHE:CE2	2:E:412:TYR:HD2	2.30	0.50
1:C:266:MET:HE2	1:C:266:MET:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:ASP:HA	2:F:139:ASN:O	2.11	0.50
1:B:567:LEU:HD13	1:B:567:LEU:N	2.27	0.49
1:B:573:ILE:O	1:B:577:ILE:HG13	2.11	0.49
1:A:22:ALA:HB1	1:A:39:ILE:HD13	1.94	0.49
1:B:119:TRP:CZ3	1:B:165:GLY:HA2	2.47	0.49
2:D:389:LEU:C	2:D:391:GLU:HA	2.32	0.49
1:C:33:LEU:HD12	1:C:33:LEU:N	2.28	0.49
1:C:300:VAL:HG22	1:C:303:ARG:NH2	2.27	0.49
2:F:107:LYS:NZ	2:F:238:GLU:OE2	2.34	0.49
1:B:399:GLU:OE2	1:B:401:VAL:HB	2.12	0.49
2:D:28:GLU:O	2:D:44:VAL:HG23	2.13	0.49
2:D:343:ASP:O	2:D:346:PRO:HD2	2.12	0.49
2:E:191:ALA:O	2:E:195:MET:HG2	2.12	0.49
1:C:150:MET:HE1	1:C:320:MET:CA	2.27	0.49
1:C:499:ASP:O	1:C:560:LYS:NZ	2.41	0.49
1:A:405:THR:O	1:A:409:VAL:HG22	2.12	0.49
1:B:210:ILE:HD11	1:B:515:ARG:NH2	2.27	0.49
2:D:29:LEU:HD11	2:D:77:LEU:HD23	1.94	0.49
2:D:145:GLN:HG2	2:D:146:LYS:N	2.26	0.49
2:E:178:ALA:HB2	2:E:241:MET:HE2	1.93	0.49
1:C:251:VAL:HG12	1:C:252:ASP:N	2.27	0.49
2:F:34:MET:CE	2:F:40:ARG:HG3	2.41	0.49
2:F:132:ILE:O	2:F:135:ILE:HD11	2.11	0.49
2:F:256:ALA:O	2:F:260:ILE:HG12	2.11	0.49
2:D:345:LEU:HG	2:D:376:TYR:CE2	2.47	0.49
1:C:92:ASP:OD1	1:C:93:THR:N	2.46	0.49
1:A:119:TRP:CZ3	1:A:165:GLY:HA2	2.47	0.49
1:A:208:PRO:HB3	1:A:441:VAL:HG13	1.93	0.49
2:D:89:VAL:HG21	2:D:195:MET:CE	2.27	0.49
1:C:12:PRO:HG2	1:C:344:ARG:HD2	1.94	0.49
1:C:177:GLU:HA	1:C:182:LEU:HD12	1.95	0.49
1:C:234:PHE:CD2	2:F:350:ARG:HG2	2.48	0.49
2:F:128:ILE:HB	2:F:141:LEU:HB3	1.94	0.49
1:A:297:ASN:HB2	2:D:286:GLU:CB	2.41	0.49
1:A:453:TRP:CZ3	1:A:519:PHE:HA	2.47	0.49
1:A:507:ASP:O	1:A:511:THR:HB	2.12	0.49
1:A:516:GLU:O	1:A:520:ASN:ND2	2.43	0.49
1:B:82:GLN:HG3	1:B:83:MET:N	2.27	0.49
1:B:186:THR:OG1	1:B:187:MET:N	2.46	0.49
1:B:546:MET:HE3	1:B:553:ARG:HD3	1.95	0.49
2:E:236:ALA:O	2:E:296:GLY:HA3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ILE:HG13	1:C:89:ARG:HG3	1.93	0.49
2:F:254:ALA:CB	2:F:315:ILE:HD12	2.42	0.49
1:A:298:MET:HB3	1:A:299:PRO:CD	2.43	0.49
1:A:425:PHE:O	1:A:502:GLN:HA	2.12	0.49
2:D:45:LEU:HD11	2:D:264:ARG:HD3	1.95	0.49
2:E:125:ASP:HB2	2:E:126:GLU:CA	2.42	0.49
2:F:191:ALA:O	2:F:195:MET:HG2	2.12	0.49
2:D:307:PRO:HG2	2:D:313:HIS:CE1	2.48	0.49
2:F:34:MET:HE3	2:F:38:GLU:HB3	1.95	0.49
2:F:151:SER:OG	2:F:155:LEU:HB3	2.12	0.49
2:F:369:MET:CG	2:F:370:ASN:N	2.76	0.49
1:A:514:SER:O	1:A:518:GLN:HG3	2.13	0.49
1:B:453:TRP:HD1	1:B:519:PHE:HD1	1.60	0.49
2:D:235:LEU:O	2:D:239:LYS:HB2	2.13	0.49
2:D:408:PHE:HA	2:D:433:LEU:HD21	1.95	0.49
1:C:541:TYR:HB3	1:C:543:ASN:OD1	2.13	0.49
1:B:210:ILE:HD11	1:B:515:ARG:NE	2.27	0.48
1:B:562:ILE:HG21	1:B:570:ILE:HG13	1.95	0.48
2:D:249:ASP:HB3	2:D:252:ASN:ND2	2.28	0.48
2:E:135:ILE:O	2:E:140:THR:HA	2.12	0.48
2:E:313:HIS:CE1	2:E:315:ILE:HG13	2.47	0.48
2:E:343:ASP:O	2:E:346:PRO:HD2	2.13	0.48
2:F:14:PRO:HG2	2:F:15:LEU:CD1	2.43	0.48
2:F:365:HIS:HA	2:F:368:THR:HG22	1.94	0.48
1:A:467:GLU:HG2	1:A:471:ASN:ND2	2.29	0.48
2:D:271:ARG:CG	2:D:271:ARG:HH11	2.26	0.48
1:C:77:PRO:HG2	1:C:169:ILE:HG22	1.94	0.48
1:C:390:VAL:CG1	1:C:402:THR:HG22	2.42	0.48
2:F:397:ILE:CA	2:F:400:ILE:HG12	2.42	0.48
2:F:452:LYS:HA	2:F:452:LYS:CE	2.43	0.48
1:A:86:GLY:HA3	1:A:302:ALA:O	2.13	0.48
1:B:549:THR:HB	1:B:552:VAL:CG1	2.43	0.48
2:E:71:ARG:HD3	4:E:521:HOH:O	2.14	0.48
1:C:329:ASP:HA	1:C:330:SER:HA	1.48	0.48
1:A:454:SER:O	1:A:458:THR:HG23	2.13	0.48
1:A:499:ASP:OD2	1:A:557:SER:HA	2.13	0.48
1:B:252:ASP:HB2	1:B:322:TYR:HB3	1.96	0.48
2:E:92:GLY:O	2:E:227:MET:HG3	2.14	0.48
1:C:532:ALA:HA	1:C:581:ILE:CD1	2.43	0.48
1:A:103:LEU:HD23	2:D:115:VAL:HG12	1.96	0.48
2:E:415:GLN:O	2:E:419:THR:OG1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:SER:O	1:C:518:GLN:HG3	2.13	0.48
2:F:395:SER:OG	2:F:398:ASP:HB2	2.13	0.48
1:A:267:THR:OG1	2:D:121:ARG:HD2	2.13	0.48
1:B:209:MET:HG2	1:B:250:ASP:OD2	2.13	0.48
1:B:266:MET:HE2	1:B:293:ALA:HB1	1.96	0.48
2:D:126:GLU:N	2:D:126:GLU:OE1	2.46	0.48
1:C:85:ASP:O	1:C:294:ASN:ND2	2.39	0.48
1:C:393:SER:HA	2:F:321:TYR:OH	2.13	0.48
2:F:270:ARG:CB	2:F:271:ARG:HB3	2.44	0.48
2:F:339:GLN:HA	2:F:340:PRO:C	2.32	0.48
1:B:360:SER:O	1:B:364:GLU:HG3	2.14	0.48
1:B:393:SER:N	1:B:394:GLY:CA	2.73	0.48
1:C:23:CYS:O	1:C:26:ASP:HB2	2.14	0.48
1:C:467:GLU:O	1:C:471:ASN:HB2	2.13	0.48
1:A:392:PRO:HB3	1:A:399:GLU:HG2	1.95	0.48
2:D:18:VAL:O	2:D:51:LYS:HA	2.13	0.48
2:E:255:GLU:OE2	2:E:273:TYR:OH	2.31	0.48
2:F:315:ILE:HB	2:F:316:PRO:CD	2.39	0.48
1:A:482:LEU:HD22	1:A:486:ASP:HB3	1.96	0.48
1:B:9:VAL:CG1	2:E:47:VAL:HG23	2.41	0.48
2:E:278:TYR:CE1	2:E:321:TYR:HD2	2.32	0.48
1:B:577:ILE:O	1:B:581:ILE:HG12	2.14	0.48
2:D:382:ALA:O	2:D:386:ALA:N	2.44	0.48
2:E:282:ALA:HB2	2:E:322:ILE:HD13	1.96	0.48
1:C:224:LYS:HE2	1:C:250:ASP:HB3	1.96	0.48
2:D:8:ILE:HD13	2:D:16:MET:HE1	1.95	0.47
1:C:295:THR:O	1:C:303:ARG:HD3	2.14	0.47
1:C:332:SER:HB2	1:C:391:SER:HB2	1.95	0.47
1:B:2:GLN:OE1	1:B:21:GLU:HB2	2.14	0.47
1:B:298:MET:HB3	1:B:299:PRO:CD	2.44	0.47
1:B:415:LEU:HA	1:B:427:SER:O	2.15	0.47
1:A:150:MET:CE	1:A:319:ASP:HB3	2.44	0.47
1:B:495:SER:O	1:B:499:ASP:N	2.40	0.47
2:D:260:ILE:CG2	2:D:264:ARG:HE	2.27	0.47
2:E:86:ILE:HD13	2:E:208:VAL:HG23	1.96	0.47
1:C:491:GLU:HG3	1:C:542:PHE:CZ	2.49	0.47
2:F:126:GLU:CB	2:F:143:ARG:HG3	2.43	0.47
2:F:285:PHE:CB	2:F:322:ILE:HD11	2.42	0.47
1:B:543:ASN:O	1:B:547:GLU:HG3	2.13	0.47
2:D:162:ALA:O	2:D:166:ARG:HG3	2.14	0.47
2:E:171:LEU:HA	2:E:172:ASP:HA	1.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASP:O	1:A:288:ARG:HG2	2.15	0.47
1:A:334:TRP:CH2	1:A:338:LEU:HD12	2.50	0.47
1:B:488:LEU:O	1:B:492:VAL:HG23	2.15	0.47
1:B:552:VAL:O	1:B:556:ILE:HG13	2.15	0.47
2:E:379:GLY:O	2:E:402:ALA:HA	2.14	0.47
1:C:415:LEU:HA	1:C:427:SER:O	2.15	0.47
1:B:231:PRO:HG2	1:B:415:LEU:N	2.30	0.47
2:E:28:GLU:OE1	2:E:72:PHE:HB3	2.14	0.47
2:E:103:ILE:O	2:E:105:PRO:HD3	2.13	0.47
2:E:412:TYR:O	2:E:421:ARG:NH1	2.47	0.47
1:C:94:PHE:CE2	1:C:103:LEU:HA	2.50	0.47
1:C:392:PRO:HB2	1:C:396:ASP:O	2.14	0.47
1:C:546:MET:HA	1:C:546:MET:HE3	1.97	0.47
2:F:160:LEU:O	2:F:164:ILE:HG13	2.15	0.47
2:F:269:GLY:N	2:F:273:TYR:O	2.47	0.47
1:B:399:GLU:OE2	1:B:402:THR:N	2.41	0.47
2:D:156:PRO:HG3	2:D:334:TYR:CE1	2.50	0.47
2:D:166:ARG:NH2	2:D:417:PHE:O	2.47	0.47
2:D:282:ALA:CA	2:D:322:ILE:HD13	2.44	0.47
1:C:452:ASP:O	1:C:456:MET:HG3	2.14	0.47
2:E:131:GLY:HA3	2:E:420:ASN:OD1	2.15	0.47
2:F:198:PHE:O	2:F:204:ILE:HB	2.15	0.47
2:F:246:ILE:CD1	2:F:301:ILE:HB	2.45	0.47
1:B:145:ILE:HG13	1:B:253:LEU:HD21	1.96	0.47
1:C:482:LEU:HD21	1:C:487:ARG:HD2	1.97	0.47
1:A:210:ILE:HG12	1:A:515:ARG:HH21	1.80	0.46
1:A:410:LYS:HB3	1:A:436:LEU:HB2	1.96	0.46
1:A:261:GLU:O	1:A:295:THR:HA	2.15	0.46
1:B:556:ILE:HG12	1:B:573:ILE:HG21	1.97	0.46
2:D:313:HIS:CG	2:D:314:PRO:HD2	2.50	0.46
2:D:324:GLU:HA	2:D:350:ARG:HD2	1.97	0.46
2:F:285:PHE:CD2	2:F:322:ILE:HG12	2.47	0.46
1:A:133:GLY:O	1:A:380:ARG:NH2	2.27	0.46
1:A:266:MET:CE	1:A:269:VAL:HB	2.46	0.46
1:A:308:TYR:HA	1:A:311:ILE:HG22	1.97	0.46
1:B:209:MET:CE	1:B:385:THR:HG21	2.45	0.46
1:C:44:GLN:HB3	1:C:45:ASP:H	1.51	0.46
2:F:186:ILE:HD12	2:F:186:ILE:O	2.14	0.46
2:F:415:GLN:O	2:F:419:THR:OG1	2.20	0.46
1:B:220:PHE:CZ	1:B:433:SER:HB2	2.50	0.46
1:B:461:MET:HE2	1:B:461:MET:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:45:LEU:CD1	2:E:264:ARG:HD3	2.41	0.46
1:C:274:PRO:HA	1:C:286:MET:HG2	1.97	0.46
2:F:60:THR:HA	2:F:63:ILE:HD12	1.96	0.46
2:F:248:THR:OG1	2:F:303:ILE:HB	2.14	0.46
1:A:266:MET:HE2	1:A:269:VAL:HB	1.98	0.46
1:B:86:GLY:HA2	1:B:294:ASN:HD21	1.80	0.46
1:B:329:ASP:HA	1:B:330:SER:HA	1.52	0.46
1:B:513:THR:HG23	1:B:517:LYS:HD3	1.97	0.46
2:F:137:HIS:O	2:F:369:MET:HE3	2.14	0.46
2:F:279:THR:O	2:F:283:THR:HG23	2.16	0.46
1:B:80:ILE:HA	1:B:81:SER:HA	1.71	0.46
1:B:514:SER:O	1:B:518:GLN:HG3	2.15	0.46
1:A:329:ASP:HA	1:A:330:SER:HA	1.55	0.46
1:B:129:GLU:OE1	1:B:129:GLU:N	2.35	0.46
1:B:214:ARG:NH1	1:B:513:THR:OG1	2.48	0.46
2:D:142:VAL:HG21	2:D:351:LEU:O	2.16	0.46
2:E:333:LEU:O	2:E:338:ILE:HG12	2.16	0.46
1:C:573:ILE:O	1:C:577:ILE:HG13	2.16	0.46
1:B:555:ARG:CZ	1:B:573:ILE:HG12	2.45	0.46
2:D:248:THR:HA	2:D:249:ASP:HA	1.68	0.46
2:E:415:GLN:H	2:E:415:GLN:HG2	1.56	0.46
1:C:123:THR:HG22	1:C:137:GLY:CA	2.46	0.46
1:B:315:GLU:HA	1:B:384:ILE:HD11	1.98	0.46
2:E:8:ILE:HD12	2:E:65:LEU:HG	1.93	0.46
1:C:148:LYS:H	1:C:320:MET:CE	2.10	0.46
1:C:256:TYR:HD1	1:C:327:MET:HE3	1.80	0.46
1:C:410:LYS:HB2	1:C:437:TYR:CE2	2.51	0.46
1:A:417:SER:O	1:A:421:GLN:HG3	2.16	0.46
1:B:103:LEU:HD21	2:E:117:ASN:HA	1.98	0.46
1:B:300:VAL:HG22	1:B:303:ARG:HH22	1.78	0.46
1:C:266:MET:HB2	1:C:266:MET:HE3	1.78	0.46
2:F:186:ILE:HD11	2:F:191:ALA:HB2	1.96	0.46
2:D:306:MET:CE	2:D:311:LYS:HG2	2.47	0.45
1:C:75:LEU:HB3	1:C:316:TYR:CE1	2.51	0.45
1:C:341:MET:HA	1:C:341:MET:CE	2.46	0.45
2:F:179:VAL:HB	2:F:207:SER:CB	2.40	0.45
1:A:43:ARG:H	1:A:44:GLN:HA	1.80	0.45
1:B:176:ILE:CD1	1:B:185:LEU:HD11	2.46	0.45
2:E:224:THR:N	2:E:225:PRO:HD2	2.31	0.45
1:C:208:PRO:HA	1:C:223:THR:HA	1.97	0.45
1:C:259:CYS:HB3	1:C:306:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLN:HE22	1:B:92:ASP:CG	2.20	0.45
1:B:128:THR:O	1:B:159:VAL:HG23	2.16	0.45
1:B:546:MET:CE	1:B:553:ARG:HD3	2.46	0.45
2:E:165:ALA:O	2:E:206:ARG:NH2	2.49	0.45
1:C:295:THR:OG1	1:C:298:MET:HG3	2.16	0.45
1:A:555:ARG:HD3	1:A:576:GLU:OE1	2.16	0.45
1:B:114:HIS:HA	1:B:169:ILE:HG12	1.99	0.45
2:D:250:MET:HB2	2:D:304:LEU:HB3	1.99	0.45
2:D:306:MET:HE3	2:D:311:LYS:HG2	1.98	0.45
2:D:357:GLY:H	2:D:361:THR:CG2	2.30	0.45
2:E:29:LEU:HD11	2:E:77:LEU:HA	1.98	0.45
1:C:363:ALA:O	1:C:367:GLU:HB2	2.16	0.45
2:F:8:ILE:HD11	2:F:65:LEU:HD22	1.99	0.45
2:F:393:ALA:HB3	2:F:394:LEU:HA	1.98	0.45
1:A:33:LEU:HD13	4:A:738:HOH:O	2.16	0.45
1:B:142:THR:HB	1:B:287:GLU:OE2	2.16	0.45
1:B:144:ILE:HD11	1:B:283:GLU:HB2	1.97	0.45
2:E:111:ILE:HG21	2:E:227:MET:SD	2.57	0.45
1:C:222:VAL:HG22	1:C:411:VAL:HG21	1.98	0.45
1:C:354:TYR:HB3	1:C:358:LEU:HD22	1.97	0.45
2:F:145:GLN:HG2	2:F:146:LYS:N	2.32	0.45
1:A:340:GLU:OE1	2:D:279:THR:OG1	2.35	0.45
1:B:173:ILE:HD13	1:B:187:MET:CG	2.46	0.45
1:B:227:ALA:HA	1:B:386:ALA:O	2.16	0.45
1:B:556:ILE:HD11	1:B:577:ILE:HD11	1.98	0.45
2:E:404:PHE:HZ	2:E:436:MET:CB	2.29	0.45
1:C:228:ALA:HA	1:C:411:VAL:O	2.16	0.45
1:C:479:ILE:O	1:C:482:LEU:HD22	2.16	0.45
1:C:562:ILE:HG22	1:C:563:PRO:CD	2.36	0.45
2:F:155:LEU:HD13	2:F:156:PRO:CD	2.47	0.45
1:A:448:ILE:HD13	1:A:515:ARG:HH11	1.79	0.45
2:E:30:ILE:C	2:E:30:ILE:HD12	2.37	0.45
2:E:278:TYR:CA	2:E:318:LEU:HD13	2.45	0.45
1:C:266:MET:HA	1:C:266:MET:CE	2.46	0.45
2:F:430:GLY:O	2:F:434:LEU:HD13	2.17	0.45
1:A:24:ILE:HD13	1:A:42:MET:HG2	1.98	0.45
1:A:84:PHE:HB2	1:A:292:ILE:CD1	2.47	0.45
1:A:274:PRO:HA	1:A:286:MET:HG2	1.97	0.45
1:B:77:PRO:HG2	1:B:187:MET:HE2	1.99	0.45
1:B:425:PHE:HA	1:B:426:PRO:C	2.36	0.45
2:E:271:ARG:CG	2:E:314:PRO:HG3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:ASN:O	1:C:524:VAL:HG23	2.17	0.45
2:F:158:LYS:HA	2:F:194:PHE:HZ	1.81	0.45
1:A:476:LEU:N	1:A:477:VAL:CA	2.79	0.45
1:B:231:PRO:HG2	1:B:414:GLY:CA	2.40	0.45
1:B:416:ASP:OD1	1:B:418:SER:N	2.48	0.45
1:B:532:ALA:O	1:B:536:LEU:HG	2.16	0.45
2:D:148:PRO:HD2	2:D:325:GLY:O	2.17	0.45
2:E:125:ASP:HA	2:E:142:VAL:HG13	1.99	0.45
2:E:162:ALA:O	2:E:166:ARG:HG3	2.17	0.45
1:C:364:GLU:O	1:C:368:ARG:HG3	2.17	0.45
1:A:467:GLU:HG2	1:A:471:ASN:HD21	1.82	0.45
1:B:230:VAL:HA	1:B:231:PRO:HD3	1.70	0.45
1:B:311:ILE:O	1:B:315:GLU:HG3	2.16	0.45
1:C:348:MET:HA	1:C:349:PRO:HD3	1.83	0.45
1:B:133:GLY:HA2	1:B:150:MET:CE	2.47	0.44
2:E:148:PRO:CB	2:E:302:PRO:HG2	2.35	0.44
1:C:227:ALA:HA	1:C:386:ALA:O	2.17	0.44
2:F:313:HIS:O	2:F:316:PRO:HD2	2.17	0.44
2:F:351:LEU:HD12	2:F:351:LEU:O	2.17	0.44
2:D:372:LEU:CD2	2:D:434:LEU:HD23	2.48	0.44
1:C:479:ILE:HD12	1:C:482:LEU:HD13	1.99	0.44
1:A:521:MET:O	1:A:524:VAL:HG22	2.18	0.44
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.98	0.44
1:B:204:ASN:OD1	1:B:204:ASN:N	2.31	0.44
1:B:309:THR:O	1:B:313:ILE:HG13	2.17	0.44
2:D:94:GLY:HA3	2:D:227:MET:HE2	1.99	0.44
2:D:94:GLY:HA3	2:D:227:MET:CE	2.47	0.44
2:D:127:PHE:HB2	2:D:355:GLY:O	2.17	0.44
2:E:29:LEU:HD11	2:E:77:LEU:HD23	1.99	0.44
2:E:183:ALA:HB1	2:E:186:ILE:CD1	2.47	0.44
2:F:274:PRO:HB2	2:F:276:TYR:CE2	2.51	0.44
1:A:24:ILE:CD1	1:A:42:MET:HG2	2.47	0.44
1:A:260:GLY:O	1:A:333:ARG:HD3	2.18	0.44
1:A:268:ASP:HB3	4:A:730:HOH:O	2.15	0.44
1:A:482:LEU:CD2	1:A:486:ASP:HB3	2.48	0.44
2:D:443:LYS:N	2:D:444:ARG:CA	2.79	0.44
2:E:304:LEU:HD12	2:E:304:LEU:O	2.17	0.44
2:E:330:THR:HB	2:E:332:GLU:OE1	2.17	0.44
2:E:429:LEU:O	2:E:429:LEU:HD12	2.17	0.44
1:C:318:ARG:HD2	1:C:372:VAL:CG2	2.48	0.44
2:D:65:LEU:HD12	2:D:65:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:10:GLU:HG2	2:E:17:ALA:CB	2.46	0.44
2:E:221:ARG:NH1	4:E:502:HOH:O	2.30	0.44
1:C:327:MET:HA	1:C:387:ILE:O	2.18	0.44
1:C:538:LEU:HD12	1:C:538:LEU:O	2.18	0.44
2:F:201:THR:HG23	2:F:203:ALA:N	2.24	0.44
2:F:415:GLN:HG2	2:F:419:THR:O	2.16	0.44
1:A:8:LYS:HE3	2:D:46:GLU:OE1	2.18	0.44
2:D:256:ALA:O	2:D:260:ILE:HD13	2.17	0.44
2:E:6:ARG:H	2:E:6:ARG:HG2	1.66	0.44
2:E:277:LEU:O	2:E:281:LEU:HG	2.17	0.44
2:E:291:ILE:HB	2:E:294:LEU:HD12	2.00	0.44
1:C:151:VAL:HA	1:C:152:PRO:HD3	1.89	0.44
2:F:159:GLU:HG3	2:F:193:PHE:HZ	1.81	0.44
1:B:390:VAL:HG11	1:B:402:THR:OG1	2.18	0.44
2:D:150:PHE:HB3	2:D:306:MET:SD	2.57	0.44
2:D:156:PRO:HB2	2:D:417:PHE:CE2	2.52	0.44
2:D:358:ALA:HA	2:D:361:THR:O	2.17	0.44
2:D:395:SER:HA	2:D:398:ASP:O	2.18	0.44
2:E:145:GLN:HG3	2:E:324:GLU:HG3	2.00	0.44
2:E:166:ARG:CD	2:E:201:THR:HG21	2.47	0.44
2:E:212:ASN:OD1	2:E:221:ARG:HG3	2.16	0.44
2:E:313:HIS:CD2	2:E:314:PRO:HD2	2.53	0.44
2:E:334:TYR:HB2	2:E:341:PRO:HG3	1.99	0.44
1:C:507:ASP:HB3	1:C:510:ASP:HB3	1.99	0.44
1:C:560:LYS:HG2	1:C:561:TYR:CD2	2.52	0.44
1:B:73:VAL:HA	1:B:88:GLN:OE1	2.18	0.44
2:E:136:ASP:HB3	2:E:423:ILE:HD13	1.99	0.44
1:C:28:CYS:SG	1:C:49:ILE:HD13	2.57	0.44
1:C:85:ASP:HB3	1:C:91:LEU:HD21	1.98	0.44
1:C:200:LYS:HB3	1:C:373:ILE:O	2.18	0.44
2:F:29:LEU:HD12	2:F:42:GLY:O	2.18	0.44
1:A:92:ASP:O	1:A:96:GLU:HG3	2.18	0.44
1:B:43:ARG:HA	2:F:10:GLU:HB3	1.98	0.44
1:B:228:ALA:HA	1:B:411:VAL:O	2.18	0.44
1:B:408:VAL:HG23	1:B:409:VAL:N	2.33	0.44
2:D:111:ILE:O	2:D:226:ARG:HB3	2.18	0.44
2:E:282:ALA:CB	2:E:322:ILE:HD13	2.48	0.44
2:E:339:GLN:HA	2:E:340:PRO:HA	1.88	0.44
2:F:181:PHE:O	2:F:209:MET:HA	2.18	0.44
2:F:372:LEU:O	2:F:375:ALA:HB3	2.18	0.44
1:A:534:LYS:O	1:A:538:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:ILE:HD11	2:D:225:PRO:HG3	1.99	0.43
2:E:178:ALA:HB2	2:E:241:MET:HE1	1.98	0.43
2:F:143:ARG:HH12	2:F:242:HIS:CE1	2.36	0.43
2:F:152:GLY:HA2	2:F:153:SER:HA	1.68	0.43
1:A:567:LEU:HB2	4:A:753:HOH:O	2.17	0.43
1:B:231:PRO:HG3	1:B:412:PHE:CE1	2.53	0.43
2:D:29:LEU:HD11	2:D:77:LEU:HA	2.01	0.43
2:D:188:PHE:CE2	1:C:202:LYS:HG2	2.54	0.43
1:C:197:ARG:HG3	1:C:315:GLU:HB2	2.00	0.43
2:F:264:ARG:C	2:F:265:ARG:HE	2.20	0.43
2:D:422:THR:OG1	2:D:425:GLU:HG3	2.18	0.43
2:F:128:ILE:HD11	2:F:143:ARG:CG	2.47	0.43
2:F:271:ARG:HA	2:F:272:GLY:HA2	1.64	0.43
2:F:401:TYR:HD2	2:F:401:TYR:HA	1.67	0.43
1:A:43:ARG:HD2	1:A:43:ARG:HA	1.49	0.43
1:A:470:LEU:HB2	1:A:490:LEU:HD21	2.01	0.43
1:A:507:ASP:HB3	1:A:510:ASP:HB3	2.00	0.43
2:F:19:GLU:HA	2:F:51:LYS:HA	2.00	0.43
2:F:201:THR:CG2	2:F:203:ALA:H	2.22	0.43
1:B:30:VAL:HB	1:B:35:VAL:CG2	2.47	0.43
1:B:461:MET:CE	1:B:464:LEU:HB2	2.48	0.43
1:B:461:MET:HE3	1:B:464:LEU:HD12	1.99	0.43
2:D:408:PHE:HA	2:D:433:LEU:CD2	2.49	0.43
2:E:127:PHE:CE2	2:E:129:GLN:HB2	2.53	0.43
2:E:379:GLY:HA3	2:E:405:ALA:HB2	2.01	0.43
1:C:197:ARG:HG3	1:C:315:GLU:CB	2.49	0.43
2:F:127:PHE:HB2	2:F:355:GLY:O	2.18	0.43
2:F:246:ILE:HD13	2:F:301:ILE:HB	2.00	0.43
2:F:271:ARG:HD3	2:F:271:ARG:H	1.82	0.43
2:F:278:TYR:CB	2:F:318:LEU:HD12	2.48	0.43
1:A:75:LEU:HD13	1:A:316:TYR:CD1	2.53	0.43
2:D:288:ALA:HB3	4:D:501:HOH:O	2.17	0.43
2:E:251:THR:O	2:E:255:GLU:HG2	2.18	0.43
1:C:203:LEU:HD11	1:C:373:ILE:HG13	2.00	0.43
1:C:509:VAL:HG11	1:C:561:TYR:O	2.19	0.43
2:F:14:PRO:HG2	2:F:15:LEU:HD12	1.99	0.43
1:A:24:ILE:HG21	2:E:60:THR:HG23	2.00	0.43
1:B:521:MET:HE3	1:B:560:LYS:HB3	2.00	0.43
2:E:318:LEU:O	2:E:322:ILE:HG13	2.18	0.43
1:A:441:VAL:O	1:A:445:MET:HG2	2.19	0.43
1:B:86:GLY:HA3	1:B:302:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:PRO:CD	1:B:414:GLY:HA2	2.49	0.43
2:D:126:GLU:HG2	2:D:143:ARG:CZ	2.49	0.43
2:D:229:LEU:HD13	2:D:287:ARG:HD3	2.01	0.43
1:C:222:VAL:HG23	1:C:413:TRP:CZ2	2.53	0.43
1:C:237:GLY:O	1:C:241:VAL:HG23	2.19	0.43
2:F:124:PRO:O	2:F:142:VAL:HG11	2.18	0.43
2:F:141:LEU:HD12	2:F:141:LEU:HA	1.86	0.43
2:F:269:GLY:HA3	2:F:273:TYR:O	2.18	0.43
2:D:362:ARG:NH1	2:D:431:TRP:HE1	2.08	0.43
2:D:404:PHE:HB2	2:D:436:MET:SD	2.59	0.43
2:E:30:ILE:CD1	2:E:42:GLY:HA3	2.47	0.43
2:F:21:VAL:HG22	2:F:50:ASP:O	2.19	0.43
2:F:183:ALA:O	2:F:212:ASN:HB3	2.18	0.43
1:B:552:VAL:HG21	1:B:577:ILE:HG12	2.01	0.43
1:C:193:VAL:HG22	1:C:308:TYR:HB3	2.01	0.43
1:C:445:MET:O	1:C:449:LEU:HB2	2.18	0.43
1:B:231:PRO:HB2	1:B:233:PRO:HD3	2.01	0.42
2:D:178:ALA:HB2	2:D:241:MET:HE2	2.01	0.42
2:D:397:ILE:H	2:D:397:ILE:HG13	1.50	0.42
2:E:352:LYS:HD3	4:E:501:HOH:O	2.18	0.42
1:C:97:VAL:HG11	1:C:109:LEU:HD23	2.01	0.42
1:C:214:ARG:HD2	1:C:500:TYR:CE1	2.53	0.42
1:A:266:MET:HA	1:A:266:MET:CE	2.49	0.42
2:D:66:LYS:CE	1:C:20:SER:HB2	2.47	0.42
2:E:146:LYS:NZ	4:E:506:HOH:O	2.47	0.42
2:E:385:LEU:O	2:E:388:VAL:N	2.52	0.42
1:C:273:PHE:H	1:C:274:PRO:HD2	1.84	0.42
2:F:98:ASP:OD1	2:F:199:ARG:NH1	2.51	0.42
1:A:6:ILE:HD12	1:A:62:GLU:HB2	2.00	0.42
1:B:486:ASP:O	1:B:490:LEU:HG	2.19	0.42
1:C:203:LEU:HB2	1:C:371:ARG:HG2	2.02	0.42
2:F:132:ILE:C	2:F:415:GLN:HE22	2.22	0.42
1:A:62:GLU:HB3	1:A:63:PRO:HD2	2.02	0.42
1:B:459:GLU:O	1:B:463:ILE:HG13	2.19	0.42
1:C:6:ILE:HD12	1:C:62:GLU:HB2	2.01	0.42
1:C:93:THR:O	1:C:97:VAL:HG12	2.19	0.42
1:C:405:THR:O	1:C:409:VAL:HG22	2.19	0.42
2:F:30:ILE:HG22	2:F:72:PHE:CD2	2.54	0.42
2:F:182:ALA:HB3	2:F:247:MET:HG2	2.02	0.42
2:F:250:MET:HB2	2:F:304:LEU:HB3	2.01	0.42
2:F:369:MET:CG	2:F:370:ASN:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:CG1	1:A:309:THR:HG23	2.49	0.42
1:B:247:LYS:HE3	1:B:248:TRP:NE1	2.35	0.42
1:B:445:MET:O	1:B:448:ILE:HG22	2.19	0.42
2:D:45:LEU:N	2:D:45:LEU:HD23	2.34	0.42
1:C:147:HIS:HD2	1:C:149:ILE:HD12	1.85	0.42
2:F:153:SER:H	2:F:331:ARG:NH2	2.18	0.42
1:B:463:ILE:HG22	1:B:493:ALA:HB2	2.01	0.42
1:B:565:GLU:C	1:B:567:LEU:HD13	2.39	0.42
2:E:133:SER:HB3	2:E:426:THR:HG23	2.02	0.42
2:E:190:GLU:O	2:E:193:PHE:HB3	2.20	0.42
1:C:144:ILE:CG2	1:C:288:ARG:HD3	2.37	0.42
1:C:318:ARG:HD3	1:C:384:ILE:HG13	2.01	0.42
1:C:482:LEU:HD23	1:C:482:LEU:O	2.19	0.42
2:F:162:ALA:O	2:F:166:ARG:HB2	2.20	0.42
1:A:567:LEU:HD12	1:A:567:LEU:HA	1.89	0.42
2:E:143:ARG:HH21	2:E:170:VAL:HB	1.85	0.42
2:E:219:ILE:HG12	4:E:522:HOH:O	2.20	0.42
2:F:77:LEU:HD13	2:F:111:ILE:CD1	2.49	0.42
1:A:84:PHE:HB2	1:A:292:ILE:HD13	2.00	0.42
1:B:131:SER:N	1:B:134:ASP:OD2	2.37	0.42
2:D:133:SER:HB3	2:D:426:THR:HG23	2.01	0.42
2:D:248:THR:OG1	2:D:303:ILE:HB	2.20	0.42
2:D:338:ILE:HD12	2:D:409:GLU:O	2.20	0.42
2:E:271:ARG:HG3	2:E:314:PRO:CG	2.49	0.42
1:C:318:ARG:HD2	1:C:372:VAL:HG22	2.01	0.42
2:F:159:GLU:HG3	2:F:193:PHE:CZ	2.55	0.42
2:D:130:THR:OG1	2:D:136:ASP:OD1	2.21	0.42
2:E:235:LEU:O	2:E:239:LYS:HB2	2.18	0.42
2:E:441:GLU:O	2:E:442:LEU:HD12	2.19	0.42
1:C:80:ILE:O	1:C:81:SER:OG	2.28	0.42
1:C:233:PRO:HG2	1:C:236:ALA:HB2	2.01	0.42
1:C:266:MET:O	1:C:270:VAL:HG23	2.20	0.42
2:F:306:MET:HG2	2:F:316:PRO:CG	2.49	0.42
1:A:261:GLU:OE2	1:A:330:SER:N	2.47	0.42
1:A:546:MET:HA	1:A:546:MET:HE2	2.02	0.42
1:A:583:LEU:C	1:A:583:LEU:HD23	2.40	0.42
1:B:207:VAL:HA	1:B:208:PRO:HD3	1.90	0.42
2:E:158:LYS:HG3	2:E:159:GLU:N	2.34	0.42
2:E:345:LEU:CG	2:E:376:TYR:CE2	2.98	0.42
2:E:362:ARG:CB	2:E:427:LEU:CD1	2.98	0.42
1:C:298:MET:HG2	2:F:115:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:TYR:O	1:C:311:ILE:HG22	2.20	0.42
1:C:533:ARG:O	1:C:537:SER:N	2.53	0.42
1:A:488:LEU:O	1:A:492:VAL:HG23	2.20	0.41
1:B:348:MET:HA	1:B:349:PRO:HD3	1.86	0.41
2:E:8:ILE:HD13	2:E:8:ILE:O	2.20	0.41
2:E:257:LEU:HD11	2:E:280:ASN:CG	2.40	0.41
2:F:86:ILE:HA	2:F:208:VAL:CG2	2.49	0.41
2:F:93:LEU:HD13	2:F:220:GLU:HG2	2.01	0.41
2:F:431:TRP:HA	2:F:434:LEU:HD13	2.02	0.41
1:B:44:GLN:HA	1:B:44:GLN:OE1	2.20	0.41
1:B:266:MET:CE	1:B:293:ALA:HB1	2.51	0.41
1:B:390:VAL:HG12	1:B:392:PRO:HD3	2.02	0.41
2:D:304:LEU:O	2:D:304:LEU:HD12	2.21	0.41
1:C:124:ILE:HB	1:C:136:ILE:HA	2.03	0.41
1:C:341:MET:HA	1:C:341:MET:HE3	2.02	0.41
1:C:399:GLU:O	1:C:403:GLN:HG2	2.20	0.41
1:C:470:LEU:HD23	1:C:473:ILE:HD12	2.02	0.41
2:F:431:TRP:O	2:F:434:LEU:HD22	2.20	0.41
1:A:508:ASP:OD1	3:A:605:GOL:O2	2.37	0.41
1:B:81:SER:HB2	1:B:286:MET:HB3	2.02	0.41
1:B:516:GLU:OE1	1:B:516:GLU:N	2.47	0.41
2:D:34:MET:HE2	2:D:40:ARG:HG3	2.02	0.41
2:D:144:GLY:CA	2:D:289:GLY:HA2	2.50	0.41
2:E:196:GLU:O	2:E:200:GLN:HB2	2.20	0.41
1:C:256:TYR:CD1	1:C:327:MET:HE3	2.55	0.41
1:C:261:GLU:O	1:C:295:THR:HA	2.20	0.41
1:A:167:PHE:HB3	1:A:171:ASP:HB2	2.03	0.41
1:A:225:GLY:CA	1:A:370:GLY:HA2	2.49	0.41
1:B:523:LYS:O	1:B:527:THR:OG1	2.33	0.41
2:D:406:GLU:O	2:D:410:ASN:N	2.47	0.41
2:E:253:TYR:CZ	2:E:284:LEU:HD11	2.56	0.41
1:C:224:LYS:CE	1:C:250:ASP:HB3	2.50	0.41
1:B:203:LEU:HD11	1:B:373:ILE:HG13	2.02	0.41
2:D:178:ALA:HB2	2:D:241:MET:CE	2.50	0.41
1:C:73:VAL:CG1	1:C:309:THR:HG23	2.49	0.41
1:C:320:MET:HE2	1:C:322:TYR:HE2	1.86	0.41
1:C:385:THR:HG22	1:C:387:ILE:CD1	2.51	0.41
2:F:396:ASP:O	2:F:400:ILE:HG12	2.19	0.41
1:A:521:MET:O	1:A:525:ILE:HG13	2.21	0.41
1:B:8:LYS:HD3	1:B:15:MET:HE1	1.97	0.41
2:D:282:ALA:CB	2:D:322:ILE:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:285:PHE:HB2	2:E:322:ILE:HG21	2.02	0.41
2:E:353:ASP:HB2	2:E:354:LYS:HE3	2.02	0.41
1:C:488:LEU:HD21	1:C:532:ALA:HB3	2.02	0.41
2:F:304:LEU:CD2	2:F:319:THR:HG21	2.51	0.41
1:A:40:ILE:HG13	1:A:50:GLN:CG	2.49	0.41
1:A:200:LYS:HB3	1:A:373:ILE:O	2.21	0.41
1:A:552:VAL:O	1:A:556:ILE:HG13	2.21	0.41
1:B:22:ALA:HB1	1:B:39:ILE:CD1	2.51	0.41
1:B:75:LEU:HB3	1:B:316:TYR:CE1	2.56	0.41
1:B:413:TRP:O	1:B:428:ILE:HG23	2.20	0.41
2:D:329:LEU:HG	2:D:341:PRO:O	2.21	0.41
2:F:18:VAL:O	2:F:52:ALA:N	2.43	0.41
2:F:111:ILE:HA	2:F:230:THR:OG1	2.21	0.41
2:F:117:ASN:HA	2:F:118:PRO:HD2	1.93	0.41
2:F:248:THR:HA	2:F:249:ASP:HA	1.69	0.41
2:F:333:LEU:O	2:F:336:SER:HB2	2.21	0.41
2:F:446:LYS:C	2:F:448:ASP:H	2.23	0.41
1:B:562:ILE:CB	1:B:570:ILE:HD11	2.38	0.41
1:B:583:LEU:HD22	1:B:583:LEU:HA	1.82	0.41
1:C:8:LYS:HG3	2:F:48:GLN:HB2	2.01	0.41
1:C:274:PRO:HB3	1:C:286:MET:HG3	2.03	0.41
2:F:197:ASP:OD1	2:F:418:TYR:OH	2.16	0.41
1:A:275:GLU:O	1:A:277:ILE:HD12	2.20	0.41
1:A:445:MET:HE1	1:A:515:ARG:HG3	2.03	0.41
1:B:73:VAL:HG13	1:B:193:VAL:CG1	2.51	0.41
1:B:460:GLY:O	1:B:464:LEU:HG	2.21	0.41
1:B:513:THR:HG22	1:B:518:GLN:HG3	2.03	0.41
2:D:33:ARG:HB3	2:D:69:SER:OG	2.21	0.41
2:D:34:MET:CE	2:D:40:ARG:HG3	2.51	0.41
2:D:98:ASP:N	2:D:98:ASP:OD1	2.53	0.41
2:D:160:LEU:HD12	2:D:160:LEU:O	2.21	0.41
2:D:212:ASN:OD1	2:D:221:ARG:HG3	2.21	0.41
2:E:26:TYR:CZ	2:E:27:GLU:HG3	2.55	0.41
2:E:93:LEU:HD12	2:E:93:LEU:HA	1.90	0.41
2:E:234:TYR:O	2:E:238:GLU:HB2	2.21	0.41
2:E:412:TYR:HA	2:E:429:LEU:HD21	2.02	0.41
1:C:109:LEU:HD12	1:C:109:LEU:O	2.21	0.41
1:C:178:THR:N	1:C:181:GLY:O	2.48	0.41
1:C:488:LEU:O	1:C:492:VAL:HG22	2.21	0.41
2:F:30:ILE:C	2:F:30:ILE:HD12	2.41	0.41
2:F:104:LEU:HA	2:F:105:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:HIS:HD2	2:F:369:MET:HB3	1.84	0.41
2:F:264:ARG:HG2	2:F:265:ARG:HH21	1.86	0.41
2:F:270:ARG:CB	2:F:271:ARG:CB	2.99	0.41
2:F:367:ALA:C	2:F:370:ASN:HD22	2.23	0.41
2:F:400:ILE:HG13	2:F:401:TYR:N	2.35	0.41
1:B:260:GLY:CA	1:B:261:GLU:CG	2.94	0.41
2:D:277:LEU:HD23	2:D:318:LEU:HD12	2.02	0.41
1:C:222:VAL:CG2	1:C:411:VAL:HG11	2.51	0.41
1:A:360:SER:O	1:A:364:GLU:HG3	2.20	0.40
1:A:520:ASN:O	1:A:524:VAL:HG13	2.21	0.40
1:B:73:VAL:HG13	1:B:193:VAL:HG12	2.03	0.40
1:B:215:VAL:HG13	1:B:216:ILE:N	2.37	0.40
2:D:225:PRO:HG2	2:D:253:TYR:CD1	2.56	0.40
2:F:81:VAL:HG22	2:F:107:LYS:O	2.22	0.40
2:F:362:ARG:O	2:F:365:HIS:ND1	2.54	0.40
2:D:93:LEU:HD21	2:D:220:GLU:HG2	2.04	0.40
2:D:136:ASP:HA	4:D:519:HOH:O	2.21	0.40
2:E:183:ALA:HB1	2:E:186:ILE:HD13	2.02	0.40
1:C:350:GLY:N	1:C:354:TYR:O	2.53	0.40
1:C:437:TYR:O	1:C:441:VAL:HG23	2.21	0.40
2:F:219:ILE:HD12	2:F:219:ILE:N	2.27	0.40
1:A:24:ILE:O	1:A:25:GLN:HB2	2.21	0.40
1:A:90:PRO:HD3	1:A:111:ALA:HA	2.02	0.40
1:A:139:VAL:O	1:A:147:HIS:N	2.52	0.40
1:A:148:LYS:H	1:A:320:MET:HE1	1.85	0.40
1:B:143:LYS:C	1:B:144:ILE:HD13	2.41	0.40
2:D:104:LEU:HD12	2:D:104:LEU:N	2.36	0.40
2:E:160:LEU:O	2:E:164:ILE:HG13	2.22	0.40
1:C:91:LEU:CD1	2:F:118:PRO:HG2	2.43	0.40
2:F:30:ILE:HG13	2:F:42:GLY:C	2.41	0.40
2:F:79:LEU:HD21	2:F:231:ALA:HB2	2.04	0.40
2:F:132:ILE:CB	2:F:135:ILE:CG1	2.99	0.40
1:A:114:HIS:HD1	1:A:170:ASP:CG	2.25	0.40
1:B:133:GLY:HA2	1:B:150:MET:HE3	2.04	0.40
1:B:241:VAL:O	1:B:245:ILE:HG12	2.22	0.40
1:B:369:SER:HB2	1:B:384:ILE:O	2.21	0.40
2:E:386:ALA:HB1	2:E:389:LEU:O	2.22	0.40
1:C:3:ILE:CD1	1:C:65:ARG:HG2	2.52	0.40
2:F:330:THR:HB	2:F:332:GLU:OE2	2.21	0.40
2:F:396:ASP:OD2	2:F:396:ASP:N	2.51	0.40
1:A:92:ASP:HA	2:D:119:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:CD2	2:D:117:ASN:HA	2.45	0.40
1:B:94:PHE:CE2	1:B:103:LEU:HA	2.56	0.40
1:B:103:LEU:N	1:B:103:LEU:HD22	2.36	0.40
1:B:324:VAL:O	1:B:384:ILE:HA	2.22	0.40
2:E:45:LEU:HD21	2:E:264:ARG:NH1	2.36	0.40
2:E:408:PHE:O	2:E:412:TYR:HB3	2.22	0.40
2:E:422:THR:OG1	2:E:425:GLU:HG3	2.22	0.40
1:C:203:LEU:HD11	1:C:373:ILE:CG1	2.51	0.40
2:F:433:LEU:O	2:F:435:ALA:N	2.50	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%)	576 (99%)	8 (1%)	0	100	100
1	B	584/600 (97%)	573 (98%)	10 (2%)	1 (0%)	47	73
1	C	582/600 (97%)	569 (98%)	13 (2%)	0	100	100
2	D	446/465 (96%)	431 (97%)	15 (3%)	0	100	100
2	E	448/465 (96%)	427 (95%)	20 (4%)	1 (0%)	47	73
2	F	448/465 (96%)	431 (96%)	16 (4%)	1 (0%)	47	73
All	All	3092/3195 (97%)	3007 (97%)	82 (3%)	3 (0%)	51	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	387	VAL
1	B	287	GLU
2	E	387	VAL

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	491/511 (96%)	476 (97%)	15 (3%)	40	69
1	B	484/511 (95%)	466 (96%)	18 (4%)	34	63
1	C	474/511 (93%)	451 (95%)	23 (5%)	25	52
2	D	335/387 (87%)	316 (94%)	19 (6%)	20	44
2	E	325/387 (84%)	300 (92%)	25 (8%)	13	30
2	F	304/387 (79%)	270 (89%)	34 (11%)	6	13
All	All	2413/2694 (90%)	2279 (94%)	134 (6%)	21	45

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	46	VAL
1	A	188	MET
1	A	250	ASP
1	A	259	CYS
1	A	273	PHE
1	A	285	LEU
1	A	289	THR
1	A	338	LEU
1	A	390	VAL
1	A	479	ILE
1	A	482	LEU
1	A	494	LYS
1	A	565	GLU
1	A	567	LEU
1	B	21	GLU
1	B	25	GLN
1	B	79	ILE
1	B	80	ILE
1	B	81	SER
1	B	125	GLU
1	B	131	SER

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Mol	Chain	Res	Type
1	B	188	MET
1	B	204	ASN
1	B	239	THR
1	B	285	LEU
1	B	338	LEU
1	B	387	ILE
1	B	489	THR
1	B	541	TYR
1	B	567	LEU
1	B	582	GLN
1	B	583	LEU
2	D	7	THR
2	D	11	VAL
2	D	45	LEU
2	D	47	VAL
2	D	48	GLN
2	D	140	THR
2	D	264	ARG
2	D	265	ARG
2	D	270	ARG
2	D	271	ARG
2	D	326	GLN
2	D	336	SER
2	D	360	LYS
2	D	397	ILE
2	D	399	LYS
2	D	400	ILE
2	D	404	PHE
2	D	434	LEU
2	D	440	THR
2	E	6	ARG
2	E	8	ILE
2	E	47	VAL
2	E	50	ASP
2	E	78	GLN
2	E	79	LEU
2	E	93	LEU
2	E	104	LEU
2	E	125	ASP
2	E	126	GLU
2	E	147	LEU
2	E	248	THR

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Mol	Chain	Res	Type
2	E	324	GLU
2	E	354	LYS
2	E	361	THR
2	E	363	GLU
2	E	385	LEU
2	E	403	LYS
2	E	404	PHE
2	E	406	GLU
2	E	407	ARG
2	E	409	GLU
2	E	419	THR
2	E	431	TRP
2	E	442	LEU
1	C	1	MET
1	C	20	SER
1	C	44	GLN
1	C	163	GLU
1	C	173	ILE
1	C	179	GLU
1	C	184	GLU
1	C	188	MET
1	C	267	THR
1	C	273	PHE
1	C	277	ILE
1	C	338	LEU
1	C	341	MET
1	C	448	ILE
1	C	482	LEU
1	C	527	THR
1	C	536	LEU
1	C	541	TYR
1	C	542	PHE
1	C	546	MET
1	C	557	SER
1	C	560	LYS
1	C	562	ILE
2	F	6	ARG
2	F	8	ILE
2	F	82	SER
2	F	95	ARG
2	F	98	ASP
2	F	99	ASN

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Mol	Chain	Res	Type
2	F	133	SER
2	F	135	ILE
2	F	137	HIS
2	F	143	ARG
2	F	146	LYS
2	F	171	LEU
2	F	173	SER
2	F	196	GLU
2	F	204	ILE
2	F	271	ARG
2	F	276	TYR
2	F	294	LEU
2	F	310	ASP
2	F	322	ILE
2	F	326	GLN
2	F	351	LEU
2	F	352	LYS
2	F	365	HIS
2	F	368	THR
2	F	370	ASN
2	F	376	TYR
2	F	396	ASP
2	F	398	ASP
2	F	401	TYR
2	F	415	GLN
2	F	419	THR
2	F	434	LEU
2	F	452	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	B	82	GLN
1	B	403	GLN
2	F	137	HIS
2	F	167	GLN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	603	-	5,5,5	0.37	0	5,5,5	0.15	0
3	GOL	A	605	-	5,5,5	0.37	0	5,5,5	0.20	0
3	GOL	A	601	-	5,5,5	0.39	0	5,5,5	0.18	0
3	GOL	A	602	-	5,5,5	0.36	0	5,5,5	0.25	0
3	GOL	A	604	-	5,5,5	0.37	0	5,5,5	0.18	0
3	GOL	A	606	-	5,5,5	0.37	0	5,5,5	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	A	605	-	-	2/4/4/4	-
3	GOL	A	601	-	-	2/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	A	604	-	-	2/4/4/4	-
3	GOL	A	606	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	GOL	O1-C1-C2-C3
3	A	606	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-C3
3	A	605	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-O2
3	A	603	GOL	O1-C1-C2-O2
3	A	606	GOL	O1-C1-C2-O2
3	A	604	GOL	O1-C1-C2-O2
3	A	606	GOL	O2-C2-C3-O3
3	A	601	GOL	O1-C1-C2-O2
3	A	605	GOL	O1-C1-C2-O2
3	A	601	GOL	O1-C1-C2-C3
3	A	604	GOL	O1-C1-C2-C3
3	A	606	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	GOL	1	0
3	A	601	GOL	2	0

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, 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	586/600 (97%)	0.61	35 (5%) 21 20	32, 52, 104, 139	0
1	B	586/600 (97%)	0.98	88 (15%) 2 1	42, 82, 137, 164	0
1	C	584/600 (97%)	1.21	109 (18%) 1 0	54, 87, 139, 158	0
2	D	448/465 (96%)	1.03	68 (15%) 2 1	48, 80, 152, 202	0
2	E	450/465 (96%)	1.08	73 (16%) 1 1	37, 72, 158, 209	0
2	F	450/465 (96%)	1.63	120 (26%) 0 0	51, 95, 172, 201	0
All	All	3104/3195 (97%)	1.07	493 (15%) 1 1	32, 77, 149, 209	0

All (493) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	435	ALA	11.0
2	F	449	LEU	9.5
2	F	385	LEU	9.2
2	E	394	LEU	9.1
1	C	476	LEU	9.0
2	F	386	ALA	9.0
2	F	394	LEU	8.6
1	C	473	ILE	8.5
2	F	392	SER	8.4
2	F	436	MET	8.3
1	C	539	GLY	8.3
2	F	435	ALA	8.1
2	D	373	PHE	8.0
2	D	386	ALA	8.0
2	D	385	LEU	7.9
2	F	453	TYR	7.8
2	F	393	ALA	7.7
1	B	542	PHE	7.6
2	F	412	TYR	7.6

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Mol	Chain	Res	Type	RSRZ
2	D	389	LEU	7.5
2	F	433	LEU	7.3
1	C	480	ASP	7.2
1	C	474	VAL	7.2
2	E	387	VAL	7.2
2	D	392	SER	7.2
1	C	481	SER	7.2
2	D	400	ILE	7.1
2	F	357	GLY	7.1
2	F	402	ALA	7.0
2	D	388	VAL	7.0
2	D	384	GLU	7.0
1	A	542	PHE	6.9
2	F	400	ILE	6.9
1	B	541	TYR	6.9
1	C	396	ASP	6.8
1	C	477	VAL	6.8
2	E	438	PRO	6.8
2	F	440	THR	6.7
2	F	445	ILE	6.7
2	E	389	LEU	6.6
2	F	439	ARG	6.6
2	E	376	TYR	6.6
2	F	382	ALA	6.6
2	F	390	GLY	6.5
2	F	174	SER	6.4
1	A	474	VAL	6.3
2	F	401	TYR	6.2
2	F	431	TRP	6.2
2	F	411	GLU	6.2
2	F	437	LEU	6.2
1	C	470	LEU	6.2
1	C	471	ASN	6.0
2	E	401	TYR	6.0
2	E	388	VAL	5.8
2	F	397	ILE	5.8
1	C	540	ALA	5.8
2	D	433	LEU	5.7
2	E	436	MET	5.7
2	F	450	LEU	5.7
2	F	395	SER	5.7
1	B	473	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
2	D	437	LEU	5.7
2	E	429	LEU	5.7
1	C	532	ALA	5.7
1	C	583	LEU	5.6
1	C	475	ARG	5.6
2	F	389	LEU	5.6
2	E	382	ALA	5.5
2	E	402	ALA	5.5
2	D	397	ILE	5.5
2	F	404	PHE	5.4
2	E	385	LEU	5.4
1	B	548	GLY	5.4
1	C	485	ASN	5.3
2	F	371	GLN	5.3
2	F	131	GLY	5.3
2	F	403	LYS	5.2
1	B	545	ILE	5.2
1	B	540	ALA	5.2
2	E	390	GLY	5.2
2	F	396	ASP	5.2
1	B	538	LEU	5.2
2	F	365	HIS	5.2
2	E	386	ALA	5.1
1	B	531	GLU	5.1
1	B	476	LEU	5.1
2	D	406	GLU	5.1
1	C	543	ASN	5.1
2	D	436	MET	5.1
1	B	536	LEU	5.0
1	B	586	SER	4.9
1	C	467	GLU	4.9
2	D	395	SER	4.9
1	A	541	TYR	4.8
2	F	451	ASP	4.8
2	F	384	GLU	4.8
2	E	399	LYS	4.8
1	B	162	ILE	4.8
1	B	183	LYS	4.8
2	E	445	ILE	4.8
2	D	391	GLU	4.8
1	C	535	ALA	4.8
1	B	482	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
2	F	373	PHE	4.7
2	F	448	ASP	4.7
2	E	375	ALA	4.7
1	B	479	ILE	4.7
1	C	499	ASP	4.6
1	C	554	GLU	4.6
2	D	396	ASP	4.6
1	C	463	ILE	4.6
2	F	438	PRO	4.6
2	F	375	ALA	4.6
2	E	437	LEU	4.5
2	D	449	LEU	4.5
2	D	387	VAL	4.5
2	F	271	ARG	4.4
1	B	1	MET	4.4
2	E	101	PRO	4.4
2	F	406	GLU	4.3
1	A	581	ILE	4.3
1	C	160	GLN	4.3
2	D	448	ASP	4.2
2	F	310	ASP	4.2
2	F	398	ASP	4.2
2	E	381	GLN	4.2
1	C	450	GLN	4.2
2	E	378	GLN	4.2
1	B	534	LYS	4.2
1	B	173	ILE	4.2
1	C	448	ILE	4.2
1	B	487	ARG	4.2
2	D	438	PRO	4.2
2	F	444	ARG	4.2
1	C	492	VAL	4.2
2	E	395	SER	4.2
1	C	129	GLU	4.1
2	F	342	ILE	4.1
1	C	541	TYR	4.1
1	B	577	ILE	4.1
1	C	546	MET	4.1
2	E	397	ILE	4.1
2	D	399	LYS	4.1
2	F	328	ILE	4.1
2	D	445	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	390	GLY	4.1
2	F	443	LYS	4.1
2	F	269	GLY	4.1
2	F	102	GLU	4.0
2	F	359	GLY	4.0
1	C	536	LEU	4.0
1	C	538	LEU	4.0
2	F	101	PRO	4.0
1	C	555	ARG	4.0
1	A	549	THR	4.0
1	C	529	GLY	4.0
2	D	403	LYS	4.0
2	D	434	LEU	4.0
1	B	481	SER	4.0
2	F	428	ASP	4.0
2	E	404	PHE	4.0
2	D	375	ALA	4.0
1	C	482	LEU	4.0
1	C	552	VAL	3.9
2	D	435	ALA	3.9
2	D	123	TYR	3.9
2	E	396	ASP	3.9
2	E	269	GLY	3.9
1	A	545	ILE	3.9
1	B	581	ILE	3.9
2	E	137	HIS	3.9
1	C	528	PHE	3.9
2	E	380	LYS	3.9
2	F	387	VAL	3.8
1	C	550	VAL	3.8
2	F	372	LEU	3.8
1	C	582	GLN	3.8
2	F	391	GLU	3.8
1	B	579	GLU	3.8
2	F	424	THR	3.8
1	B	124	ILE	3.8
1	C	397	ILE	3.8
1	C	487	ARG	3.8
2	D	444	ARG	3.8
2	E	450	LEU	3.8
1	C	180	GLN	3.8
1	C	559	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	552	VAL	3.7
2	E	391	GLU	3.7
2	D	377	ALA	3.7
2	F	446	LYS	3.7
2	D	404	PHE	3.7
2	F	442	LEU	3.7
2	F	405	ALA	3.7
2	F	432	GLU	3.7
2	F	175	ASP	3.7
1	C	65	ARG	3.7
2	E	434	LEU	3.7
2	F	434	LEU	3.7
1	C	179	GLU	3.6
2	F	268	PRO	3.6
1	B	519	PHE	3.6
2	F	388	VAL	3.6
1	B	129	GLU	3.6
1	C	496	ILE	3.6
1	B	549	THR	3.6
2	F	350	ARG	3.5
1	C	545	ILE	3.5
2	D	451	ASP	3.5
1	B	158	THR	3.5
1	B	156	LYS	3.5
1	B	535	ALA	3.5
2	F	312	THR	3.5
2	F	452	LYS	3.5
2	F	399	LYS	3.4
2	F	429	LEU	3.4
1	B	177	GLU	3.4
2	D	175	ASP	3.4
1	A	550	VAL	3.4
1	B	477	VAL	3.4
1	C	537	SER	3.4
2	D	398	ASP	3.4
1	B	582	GLN	3.4
2	E	444	ARG	3.4
1	C	551	ALA	3.3
2	D	393	ALA	3.3
2	E	371	GLN	3.3
2	D	383	LYS	3.3
1	C	177	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	433	LEU	3.3
1	B	159	VAL	3.3
1	C	398	SER	3.3
1	C	495	SER	3.3
2	D	371	GLN	3.3
2	E	393	ALA	3.3
2	F	378	GLN	3.3
1	C	493	ALA	3.3
2	F	337	GLY	3.3
2	E	398	ASP	3.3
1	B	483	SER	3.3
2	F	133	SER	3.3
2	F	170	VAL	3.3
1	A	544	GLU	3.3
1	B	297	ASN	3.2
2	D	382	ALA	3.2
2	F	152	GLY	3.2
2	F	368	THR	3.2
1	B	447	GLN	3.2
1	B	480	ASP	3.2
2	D	402	ALA	3.2
1	B	537	SER	3.2
1	C	580	THR	3.2
2	E	405	ALA	3.2
1	B	546	MET	3.2
1	C	558	ARG	3.2
2	E	431	TRP	3.1
1	C	491	GLU	3.1
1	C	500	TYR	3.1
1	B	488	LEU	3.1
1	C	542	PHE	3.1
1	C	479	ILE	3.1
2	F	333	LEU	3.1
1	B	468	GLU	3.1
2	E	272	GLY	3.1
2	D	381	GLN	3.1
1	C	484	ASP	3.1
1	C	468	GLU	3.1
2	F	341	PRO	3.1
1	C	447	GLN	3.1
1	C	158	THR	3.0
2	E	392	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	200	GLN	3.0
1	B	178	THR	3.0
2	D	380	LYS	3.0
2	E	379	GLY	3.0
1	B	443	ARG	3.0
1	C	574	ASN	3.0
2	D	174	SER	3.0
2	D	440	THR	3.0
2	D	431	TRP	3.0
2	E	400	ILE	3.0
1	C	494	LYS	3.0
1	C	388	SER	3.0
1	B	127	GLY	2.9
1	A	389	ALA	2.9
1	B	128	THR	2.9
1	C	478	GLY	2.9
2	E	234	TYR	2.9
2	E	412	TYR	2.9
2	D	104	LEU	2.9
2	D	429	LEU	2.9
2	E	442	LEU	2.9
2	E	310	ASP	2.9
1	C	466	GLU	2.9
2	D	376	TYR	2.9
2	F	376	TYR	2.9
1	B	515	ARG	2.9
1	C	395	GLY	2.9
1	C	472	GLU	2.9
2	F	380	LYS	2.9
1	A	476	LEU	2.9
2	F	329	LEU	2.9
1	B	157	GLY	2.8
2	E	408	PHE	2.8
1	B	522	LEU	2.8
2	D	441	GLU	2.8
2	D	439	ARG	2.8
2	E	312	THR	2.8
1	C	234	PHE	2.8
1	B	182	LEU	2.8
1	C	488	LEU	2.8
1	A	524	VAL	2.8
2	E	406	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	357	GLY	2.8
1	B	475	ARG	2.8
1	B	179	GLU	2.8
2	D	432	GLU	2.8
1	A	493	ALA	2.8
2	F	360	LYS	2.8
2	F	340	PRO	2.8
2	F	242	HIS	2.8
1	C	161	LYS	2.8
1	C	280	ASN	2.8
1	B	474	VAL	2.7
2	D	413	VAL	2.7
1	C	576	GLU	2.7
1	B	180	GLN	2.7
1	B	176	ILE	2.7
2	F	327	ILE	2.7
2	D	102	GLU	2.7
2	F	147	LEU	2.7
1	B	544	GLU	2.7
1	B	181	GLY	2.7
1	A	259	CYS	2.7
1	C	428	ILE	2.7
2	F	103	ILE	2.7
2	D	394	LEU	2.6
1	B	448	ILE	2.6
2	F	173	SER	2.6
2	F	272	GLY	2.6
1	C	534	LYS	2.6
1	C	575	GLU	2.6
1	B	492	VAL	2.6
1	C	394	GLY	2.6
2	F	137	HIS	2.6
1	C	524	VAL	2.6
1	A	473	ILE	2.6
1	C	176	ILE	2.6
2	E	377	ALA	2.6
1	A	482	LEU	2.6
2	F	363	GLU	2.6
1	A	407	ARG	2.6
2	F	410	ASN	2.5
2	F	282	ALA	2.5
1	C	409	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	508	ASP	2.5
1	A	297	ASN	2.5
2	F	171	LEU	2.5
1	C	295	THR	2.5
1	A	366	TYR	2.5
1	A	533	ARG	2.5
2	F	270	ARG	2.5
1	C	296	SER	2.5
2	D	349	SER	2.5
1	B	122	ALA	2.5
1	C	581	ILE	2.5
1	B	484	ASP	2.5
1	B	123	THR	2.5
2	F	169	THR	2.5
1	C	415	LEU	2.5
1	C	259	CYS	2.5
2	E	133	SER	2.5
1	B	533	ARG	2.5
2	D	101	PRO	2.5
2	F	104	LEU	2.4
1	B	572	SER	2.4
1	C	577	ILE	2.4
2	D	401	TYR	2.4
1	B	172	PRO	2.4
1	C	389	ALA	2.4
2	E	358	ALA	2.4
2	F	288	ALA	2.4
2	E	82	SER	2.4
2	E	403	LYS	2.4
2	F	309	ASP	2.4
2	F	324	GLU	2.4
1	C	469	GLN	2.4
1	B	578	LYS	2.4
1	C	516	GLU	2.4
1	C	392	PRO	2.4
2	D	450	LEU	2.4
2	E	330	THR	2.4
1	A	477	VAL	2.4
2	E	271	ARG	2.4
2	D	405	ALA	2.4
1	C	520	ASN	2.4
1	B	138	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	378	ASP	2.3
2	D	311	LYS	2.3
2	F	154	GLY	2.3
2	E	308	GLU	2.3
2	E	384	GLU	2.3
2	F	82	SER	2.3
2	D	71	ARG	2.3
1	C	248	TRP	2.3
1	C	571	SER	2.3
2	D	430	GLY	2.3
2	F	303	ILE	2.3
1	A	230	VAL	2.3
1	B	231	PRO	2.3
1	B	130	VAL	2.3
2	F	362	ARG	2.3
1	A	546	MET	2.3
2	D	442	LEU	2.3
2	F	354	LYS	2.3
1	B	328	ALA	2.3
1	C	229	ALA	2.3
1	C	261	GLU	2.3
1	A	388	SER	2.3
1	B	125	GLU	2.3
1	A	390	VAL	2.3
1	B	175	VAL	2.3
1	A	423	ARG	2.2
1	C	533	ARG	2.2
2	E	321	TYR	2.2
1	C	547	GLU	2.2
2	E	314	PRO	2.2
1	A	582	GLN	2.2
1	A	229	ALA	2.2
1	B	305	ALA	2.2
1	A	479	ILE	2.2
1	C	570	ILE	2.2
1	C	333	ARG	2.2
2	F	407	ARG	2.2
1	C	328	ALA	2.2
1	C	256	TYR	2.2
2	F	311	LYS	2.2
1	B	550	VAL	2.2
1	B	543	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	349	SER	2.2
1	B	348	MET	2.2
1	B	255	VAL	2.2
2	F	332	GLU	2.2
1	B	264	ASN	2.2
2	E	365	HIS	2.2
2	F	159	GLU	2.2
1	C	301	ALA	2.2
2	E	85	MET	2.2
1	A	365	TYR	2.1
2	E	338	ILE	2.1
1	C	231	PRO	2.1
1	A	260	GLY	2.1
2	D	428	ASP	2.1
2	F	379	GLY	2.1
1	B	580	THR	2.1
1	B	126	GLU	2.1
1	B	463	ILE	2.1
2	F	294	LEU	2.1
1	B	260	GLY	2.1
2	F	447	ASP	2.1
1	A	527	THR	2.1
2	D	361	THR	2.1
2	E	174	SER	2.1
1	B	257	VAL	2.1
1	A	19	MET	2.1
2	E	99	ASN	2.1
1	C	548	GLY	2.1
2	E	248	THR	2.1
2	D	338	ILE	2.1
1	C	523	LYS	2.1
2	D	335	LYS	2.1
1	B	583	LEU	2.1
2	E	372	LEU	2.1
1	B	295	THR	2.1
1	C	294	ASN	2.1
2	D	350	ARG	2.1
2	F	419	THR	2.1
1	B	516	GLU	2.1
1	B	256	TYR	2.1
2	E	214	ALA	2.1
2	E	367	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	553	ARG	2.1
2	F	305	THR	2.1
1	C	182	LEU	2.0
2	F	105	PRO	2.0
1	C	515	ARG	2.0
1	A	578	LYS	2.0
2	E	427	LEU	2.0
2	E	449	LEU	2.0
2	F	149	VAL	2.0
2	F	347	SER	2.0
2	F	146	LYS	2.0
2	F	331	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	603	6/6	0.29	0.39	101,121,125,125	0
3	GOL	A	601	6/6	0.34	0.35	114,136,139,139	0
3	GOL	A	605	6/6	0.50	0.32	113,136,138,138	0
3	GOL	A	602	6/6	0.81	0.27	88,106,108,108	0
3	GOL	A	604	6/6	0.86	0.33	77,93,95,95	0
3	GOL	A	606	6/6	0.88	0.26	91,109,112,112	0

6.5 Other polymers (i)

There are no such residues in this entry.