Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:47 am BST

PDB ID	:	5D98
Title	:	Influenza C Virus RNA-dependent RNA Polymerase - Space group P43212
Authors	:	Hengrung, N.; El Omari, K.; Serna Martin, I.; Vreede, F.T.; Cusack, S.; Rambo, R.P.; Vonrhein, C.; Bricogne, G.; Stuart, D.I.; Grimes, J.M.; Fodor, E.
Deposited on	:	2015-08-18
Resolution	:	3.90 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 following versions of software and data (see references ①) were used in the production of this report:

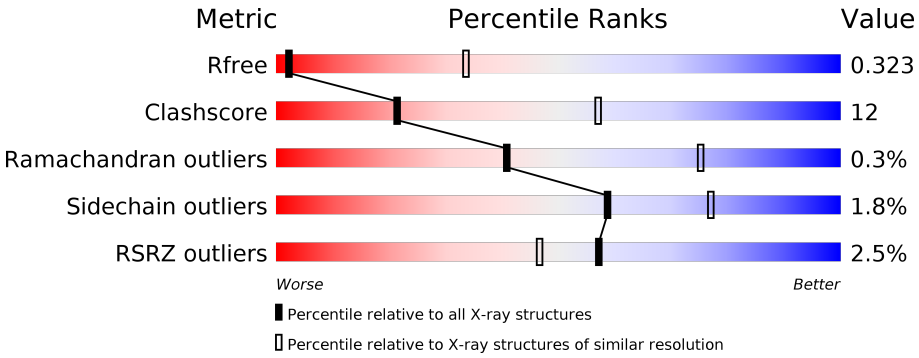
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 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	709	2% 67% 30%
1	D	709	% 68% 29%
2	B	754	2% 74% 19% 6%
2	E	754	3% 73% 20% 6%
3	C	782	3% 70% 26%
3	F	782	3% 67% 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34720 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			
1	D	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			
2	E	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			
3	F	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	775	ALA	-	expression tag	UNP Q9IMP3
C	776	ARG	-	expression tag	UNP Q9IMP3
C	777	GLU	-	expression tag	UNP Q9IMP3
C	778	ASN	-	expression tag	UNP Q9IMP3
C	779	LEU	-	expression tag	UNP Q9IMP3
C	780	TYR	-	expression tag	UNP Q9IMP3
C	781	PHE	-	expression tag	UNP Q9IMP3
C	782	GLN	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	775	ALA	-	expression tag	UNP Q9IMP3
F	776	ARG	-	expression tag	UNP Q9IMP3
F	777	GLU	-	expression tag	UNP Q9IMP3
F	778	ASN	-	expression tag	UNP Q9IMP3
F	779	LEU	-	expression tag	UNP Q9IMP3
F	780	TYR	-	expression tag	UNP Q9IMP3
F	781	PHE	-	expression tag	UNP Q9IMP3
F	782	GLN	-	expression tag	UNP Q9IMP3

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

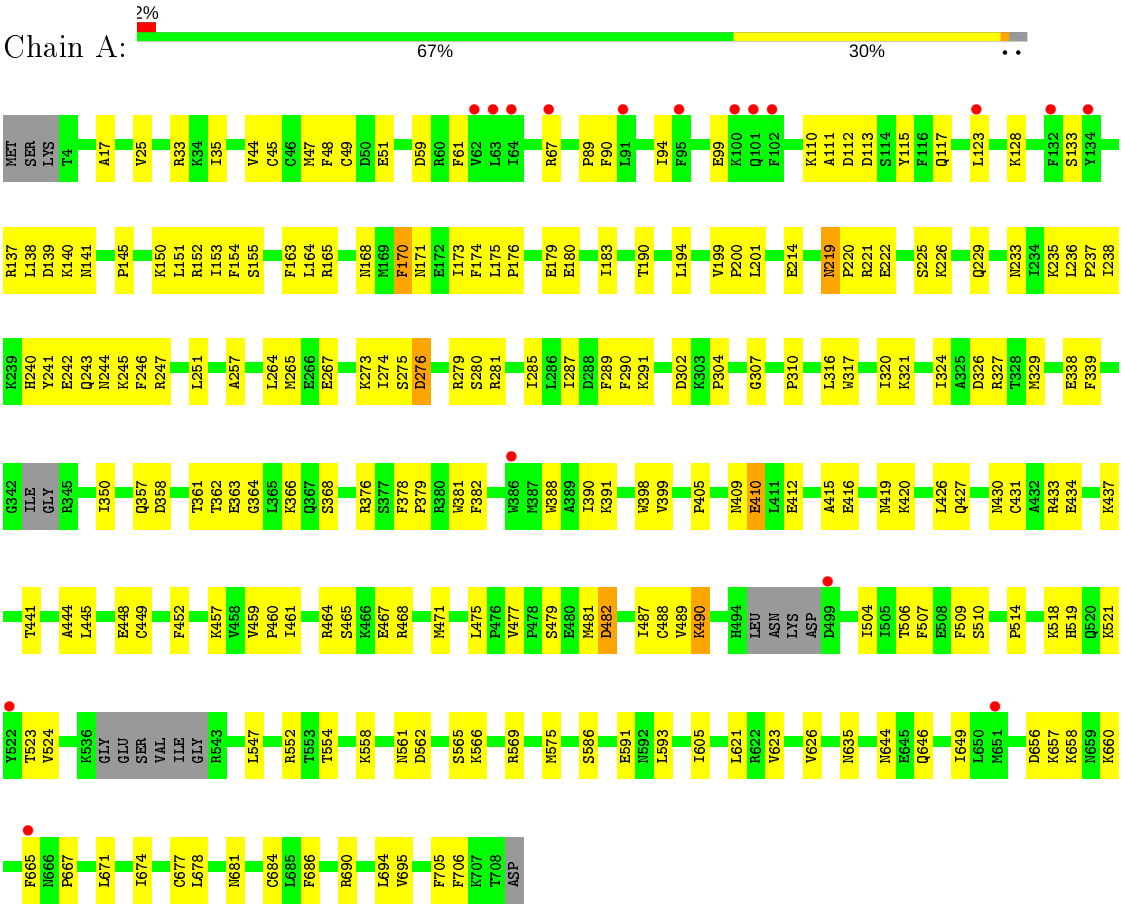
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

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 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.

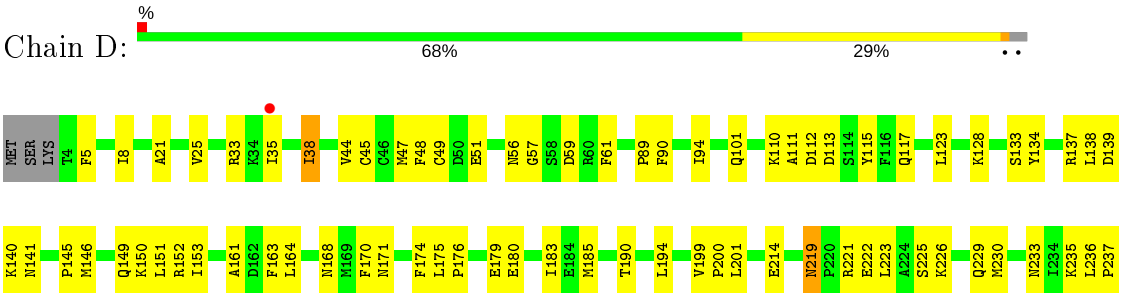
- Molecule 1: Polymerase acidic protein

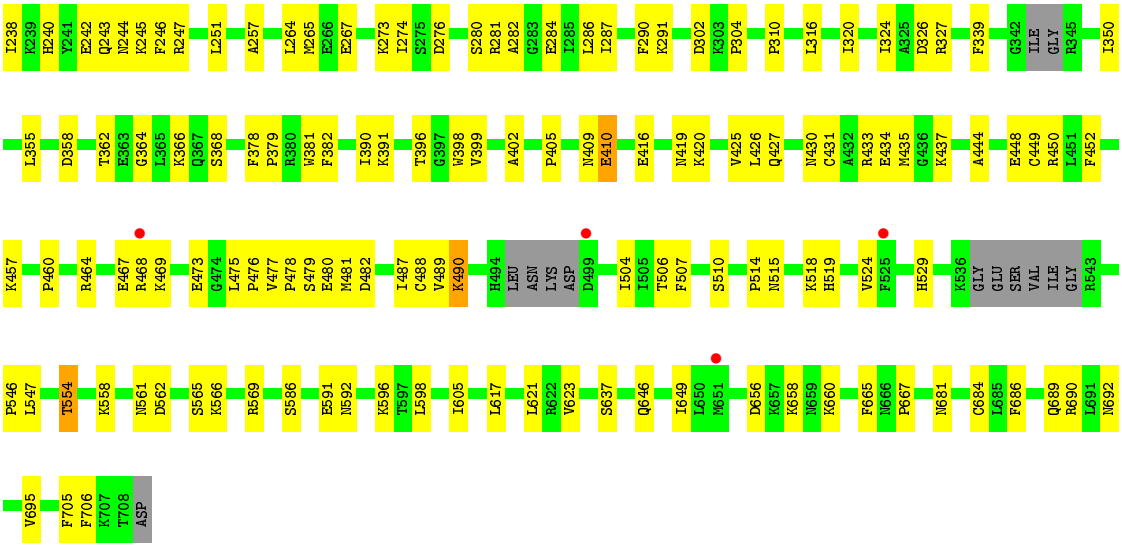
Chain A:



- Molecule 1: Polymerase acidic protein

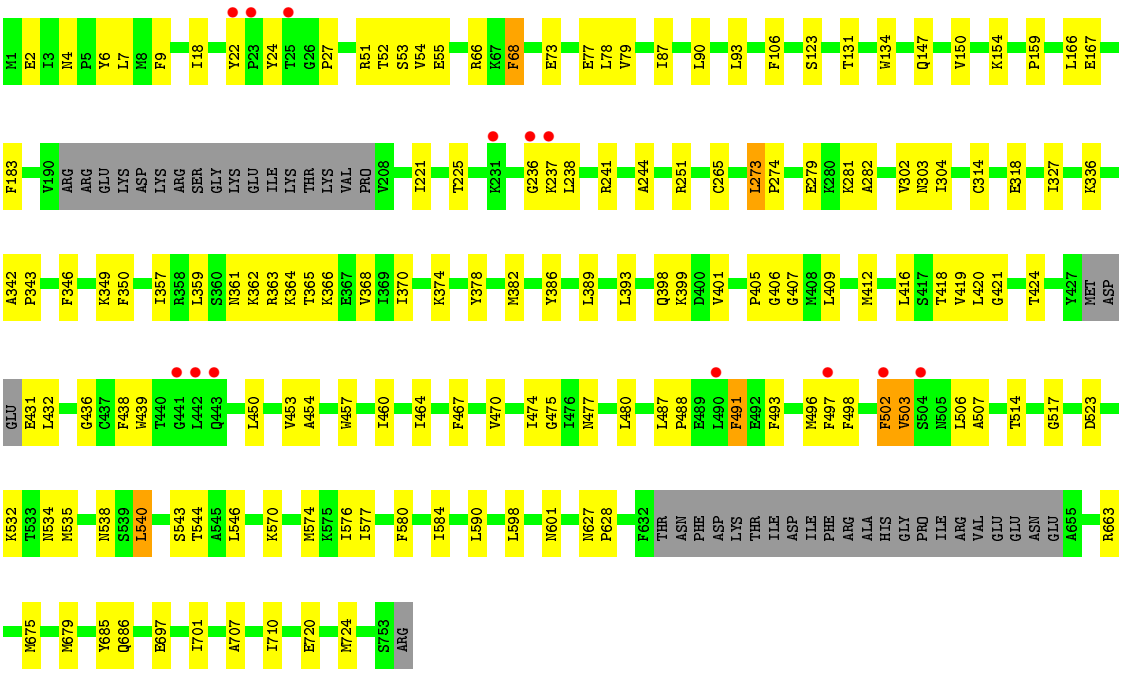
Chain D:





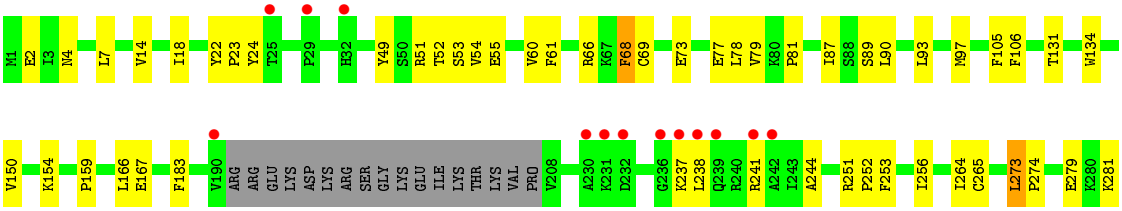
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

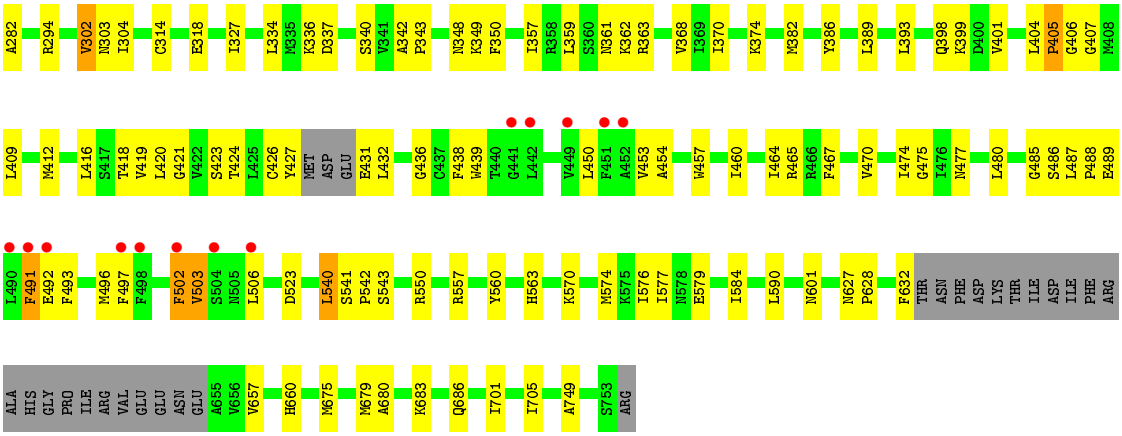
Chain B:



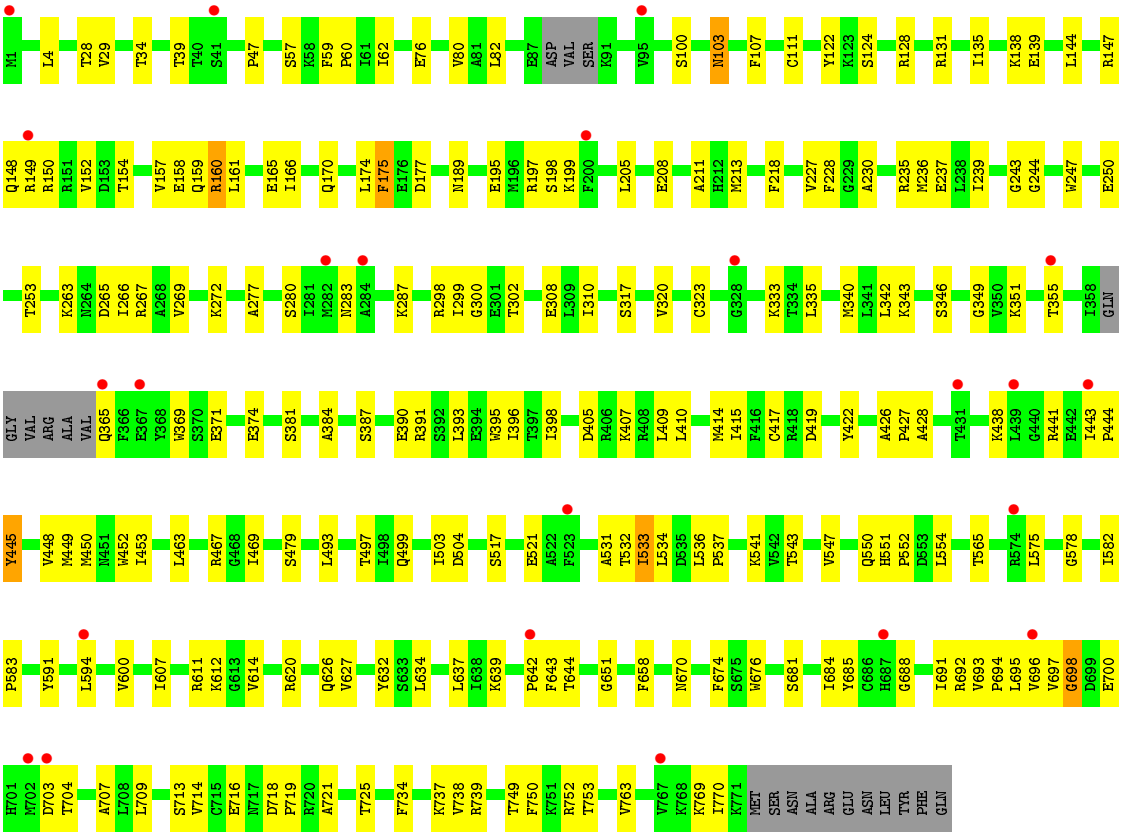
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain E:

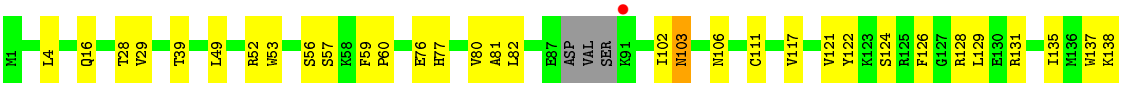


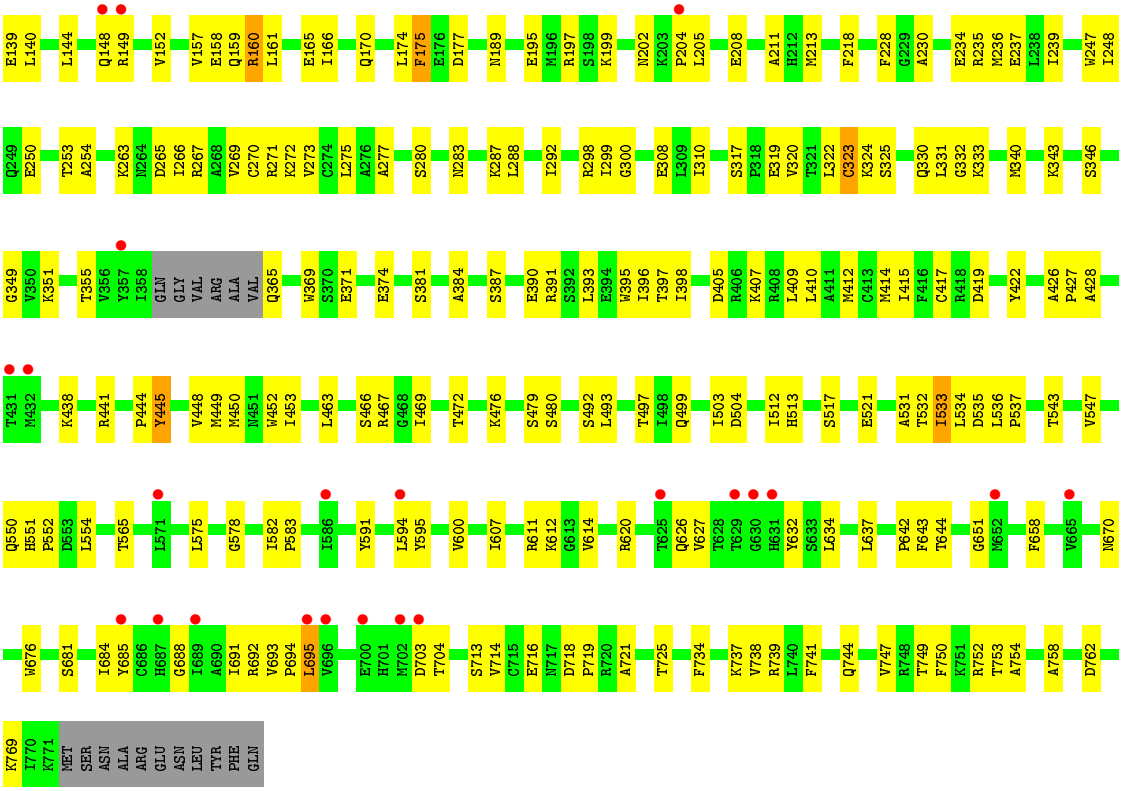


• Molecule 3: Polymerase basic protein 2



• Molecule 3: Polymerase basic protein 2




E139 L140 L144 Q148 R149 V152 V157 E158 Q159 R160 L161 E165 I166 Q170 L174 F175 E176 D177 N189 E195 M196 R197 S198 K199 N202 K203 P204 L205 E208 A211 H212 M213 F218 F228 G229 A230 E234 R235 M236 E237 L238 I239 W247 I248
Q249 E250 T253 A254 K263 N264 D265 I266 R267 A268 V269 C270 R271 K272 V273 C274 L275 A276 A277 S280 N283 K287 L288 I292 R298 I299 G300 E308 L309 I310 S317 P318 E319 V320 T321 L322 C323 K324 S325 Q330 L331 G332 K333 M340 K343 S346
G349 V350 K351 T355 V356 Y357 I358 GLN GLY VAL ARG ALA VAL Q365 W369 S370 E371 E374 S381 A384 S387 E390 R391 S392 L393 E394 W395 I396 T397 I398 D405 R406 K407 R408 L409 L410 A411 M412 C413 M414 I415 F416 C417 R418 D419 Y422 A426 P427 A428
T431 M432 K438 R441 P444 Y445 V448 M449 M450 N451 W452 I453 L463 S466 R467 G468 I469 T472 K476 S479 S480 S492 L493 T497 I498 Q499 I503 D504 I512 H513 S517 E521 A531 T532 I533 L534 D535 L536 P537 T543 V547
Q550 H551 P552 D553 L554 T565 L571 L575 G578 I582 P583 I586 Y591 L594 Y595 V600 I607 R611 K612 G613 V614 R620 T625 Q626 V627 T628 T629 G630 H631 Y632 S633 L634 L637 P642 F643 T644 G651 M652 F658 V665 N670
W676 S681 I684 Y685 G686 H687 G688 I689 A690 I691 R692 V693 P694 L695 V696 E700 H701 M702 D703 T704 S713 V714 C715 E716 W717 D718 P719 R720 A721 T725 F734 K737 V738 R739 L740 F741 Q744 V747 R748 T749 F750 K751 R752 T753 A754 A758 D762
K769 I770 K771 MET SER ASN ALA ARG GLU ASN LEU TYR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	185.66Å 185.66Å 598.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.90 100.57 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.01-3.90) 98.8 (100.57-3.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.89Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.286 , 0.326 0.286 , 0.323	Depositor DCC
R_{free} test set	4772 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	161.2	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 132.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	34720	wwPDB-VP
Average B, all atoms (Å^2)	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: MG

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	0.41	0/5746	0.57	1/7717 (0.0%)
1	D	0.43	0/5746	0.57	1/7717 (0.0%)
2	B	0.40	0/5749	0.56	0/7723
2	E	0.41	0/5749	0.57	0/7723
3	C	0.41	0/6185	0.59	0/8322
3	F	0.42	0/6185	0.59	0/8322
All	All	0.41	0/35360	0.58	2/47524 (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})
1	A	219	ASN	C-N-CD	5.11	139.14	128.40
1	D	219	ASN	C-N-CD	5.11	139.12	128.40

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	5630	0	5632	147	0
1	D	5630	0	5632	167	0
2	B	5652	0	5749	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	5652	0	5749	126	0
3	C	6076	0	6183	182	0
3	F	6076	0	6183	198	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
All	All	34720	0	35128	840	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 (840) 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)
3:F:138:LYS:HE2	3:F:250:GLU:CG	1.22	1.59
3:F:138:LYS:CE	3:F:250:GLU:HG2	1.34	1.48
3:F:138:LYS:CE	3:F:250:GLU:CG	1.83	1.46
3:F:138:LYS:CE	3:F:250:GLU:CD	1.86	1.41
3:F:138:LYS:NZ	3:F:250:GLU:HG2	1.33	1.36
3:F:138:LYS:HE3	3:F:250:GLU:CD	1.42	1.33
3:C:718:ASP:CG	3:C:719:PRO:HD3	1.59	1.23
3:F:718:ASP:CG	3:F:719:PRO:HD3	1.60	1.21
1:D:396:THR:HG21	1:D:468:ARG:CD	1.70	1.20
2:E:18:ILE:HD12	2:E:497:PHE:CD1	1.76	1.20
1:D:396:THR:HG21	1:D:468:ARG:HD2	1.22	1.09
3:F:138:LYS:HE2	3:F:250:GLU:CB	1.83	1.09
2:B:724:MET:CG	3:C:725:THR:HG21	1.84	1.07
2:E:18:ILE:CD1	2:E:497:PHE:CD1	2.38	1.06
2:B:724:MET:HG2	3:C:725:THR:HG21	1.37	1.02
2:E:487:LEU:HG	2:E:488:PRO:HD2	1.43	0.98
3:F:138:LYS:HE2	3:F:250:GLU:CD	1.67	0.97
3:C:583:PRO:HG3	3:C:695:LEU:HD12	1.47	0.96
3:F:138:LYS:NZ	3:F:250:GLU:CG	2.15	0.95
1:D:396:THR:CG2	1:D:468:ARG:HD2	1.97	0.94
2:B:487:LEU:HG	2:B:488:PRO:HD2	1.50	0.93
3:F:138:LYS:HB3	3:F:250:GLU:HB2	1.50	0.93
3:F:138:LYS:HZ3	3:F:250:GLU:HG2	1.17	0.92
1:D:469:LYS:HD3	1:D:475:LEU:HD13	1.51	0.91
3:C:583:PRO:CG	3:C:695:LEU:HD12	2.04	0.87
3:C:694:PRO:C	3:C:695:LEU:HD23	1.94	0.87
1:A:176:PRO:HA	1:A:180:GLU:HB3	1.58	0.85
3:C:583:PRO:HB3	3:C:695:LEU:CD1	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:694:PRO:O	3:C:695:LEU:HD23	1.78	0.83
3:F:230:ALA:HB1	3:F:235:ARG:HD2	1.61	0.83
2:B:724:MET:HG3	3:C:725:THR:HG21	1.60	0.83
2:B:686:GLN:NE2	3:C:39:THR:OG1	2.11	0.82
2:E:18:ILE:HD12	2:E:497:PHE:CE1	2.15	0.82
2:E:487:LEU:HG	2:E:488:PRO:CD	2.09	0.82
3:C:583:PRO:CB	3:C:695:LEU:HD12	2.10	0.81
3:F:138:LYS:HE3	3:F:250:GLU:OE2	1.79	0.81
1:A:368:SER:HB2	2:B:359:LEU:HD23	1.60	0.81
3:C:583:PRO:CB	3:C:695:LEU:CD1	2.58	0.81
1:D:44:VAL:HG13	1:D:153:ILE:HD11	1.63	0.80
1:D:176:PRO:HA	1:D:180:GLU:HB3	1.62	0.80
1:D:477:VAL:HG12	1:D:478:PRO:O	1.82	0.79
3:C:583:PRO:HB3	3:C:695:LEU:HD12	1.62	0.79
3:F:138:LYS:CE	3:F:250:GLU:OE2	2.30	0.79
3:F:718:ASP:OD2	3:F:719:PRO:HD3	1.82	0.78
1:D:304:PRO:HG3	1:D:310:PRO:HB3	1.65	0.78
3:C:692:ARG:HG3	3:C:694:PRO:HD2	1.64	0.78
1:A:44:VAL:HG13	1:A:153:ILE:HD11	1.63	0.78
2:E:627:ASN:ND2	3:F:111:CYS:SG	2.57	0.77
2:E:68:PHE:HE1	2:E:406:GLY:HA3	1.48	0.77
2:B:68:PHE:HE1	2:B:406:GLY:HA3	1.50	0.77
1:D:151:LEU:HD13	3:F:753:THR:HG23	1.67	0.77
3:C:583:PRO:HG3	3:C:695:LEU:CD1	2.15	0.77
2:B:363:ARG:HD3	3:F:139:GLU:OE2	1.85	0.77
1:A:464:ARG:HG2	1:A:482:ASP:HB3	1.67	0.76
1:D:138:LEU:HD11	1:D:140:LYS:HE3	1.66	0.76
3:F:721:ALA:HB1	3:F:738:VAL:HA	1.65	0.76
2:B:487:LEU:HG	2:B:488:PRO:CD	2.14	0.76
3:C:533:ILE:HG22	3:C:534:LEU:H	1.49	0.75
1:A:304:PRO:HG3	1:A:310:PRO:HB3	1.69	0.75
2:E:686:GLN:NE2	3:F:39:THR:OG1	2.19	0.75
1:A:138:LEU:HD11	1:A:140:LYS:HE3	1.68	0.75
1:D:171:ASN:ND2	2:E:167:GLU:OE2	2.20	0.75
2:B:363:ARG:CD	3:F:139:GLU:OE2	2.35	0.74
1:A:264:LEU:HD21	1:A:267:GLU:HB2	1.67	0.74
3:C:230:ALA:HB1	3:C:235:ARG:HD2	1.68	0.74
2:E:68:PHE:CE1	2:E:406:GLY:HA3	2.23	0.74
3:F:533:ILE:HG22	3:F:534:LEU:H	1.51	0.74
3:C:533:ILE:HG22	3:C:534:LEU:N	2.02	0.73
1:A:25:VAL:HG21	1:A:35:ILE:HG22	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:LYS:HB2	1:D:475:LEU:HD12	1.71	0.73
1:A:200:PRO:HG3	2:B:318:GLU:HB3	1.69	0.73
1:D:25:VAL:HG21	1:D:35:ILE:HG22	1.71	0.72
2:E:487:LEU:CG	2:E:488:PRO:HD2	2.19	0.72
3:C:531:ALA:O	3:C:532:THR:HG22	1.89	0.72
2:E:349:LYS:NZ	2:E:407:GLY:O	2.21	0.72
3:F:531:ALA:O	3:F:532:THR:HG22	1.90	0.72
3:C:721:ALA:HB1	3:C:738:VAL:HA	1.72	0.72
3:F:533:ILE:HG22	3:F:534:LEU:N	2.04	0.71
3:F:57:SER:HB2	3:F:60:PRO:HG3	1.72	0.71
2:E:350:PHE:HB3	2:E:401:VAL:HG21	1.71	0.71
3:C:718:ASP:OD1	3:C:719:PRO:HD3	1.89	0.71
1:A:171:ASN:ND2	2:B:167:GLU:OE2	2.24	0.70
3:C:57:SER:HB2	3:C:60:PRO:HG3	1.73	0.70
1:D:477:VAL:HG13	1:D:478:PRO:HD2	1.73	0.70
2:B:496:MET:HA	2:B:503:VAL:HG21	1.73	0.70
1:D:476:PRO:O	1:D:477:VAL:HG23	1.91	0.70
2:B:68:PHE:CE1	2:B:406:GLY:HA3	2.25	0.70
1:D:21:ALA:HA	1:D:38:ILE:HD11	1.73	0.70
2:B:147:GLN:NE2	2:B:685:TYR:CE2	2.60	0.70
2:B:349:LYS:NZ	2:B:407:GLY:O	2.20	0.70
3:C:718:ASP:OD2	3:C:719:PRO:HD3	1.90	0.70
1:D:469:LYS:CD	1:D:475:LEU:HD13	2.21	0.69
2:B:576:ILE:HD11	3:C:100:SER:HB2	1.75	0.69
1:D:240:HIS:NE2	1:D:656:ASP:OD2	2.26	0.69
1:A:151:LEU:HD13	3:C:753:THR:HG23	1.73	0.69
1:D:477:VAL:HG11	1:D:480:GLU:OE2	1.91	0.69
2:B:350:PHE:HB3	2:B:401:VAL:HG21	1.73	0.69
3:F:718:ASP:CG	3:F:719:PRO:CD	2.52	0.69
2:E:131:THR:HG21	2:E:251:ARG:HD2	1.74	0.69
3:C:718:ASP:CG	3:C:719:PRO:CD	2.51	0.68
1:D:419:ASN:ND2	2:E:543:SER:OG	2.26	0.68
1:D:396:THR:HG21	1:D:468:ARG:CG	2.23	0.68
2:B:487:LEU:CG	2:B:488:PRO:HD2	2.22	0.68
2:E:421:GLY:O	2:E:424:THR:OG1	2.11	0.68
1:A:399:VAL:HB	1:A:427:GLN:HE22	1.58	0.67
1:D:350:ILE:HB	2:E:368:VAL:HG22	1.75	0.67
1:D:222:GLU:HA	1:D:225:SER:HB3	1.75	0.67
2:B:431:GLU:HG3	2:B:432:LEU:H	1.59	0.67
3:F:138:LYS:HE2	3:F:250:GLU:HB2	1.75	0.67
3:C:174:LEU:C	3:C:174:LEU:HD23	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:431:GLU:HG3	2:E:432:LEU:H	1.59	0.67
2:E:701:ILE:HD11	3:F:208:GLU:HA	1.75	0.67
2:B:90:LEU:HA	2:B:93:LEU:HD12	1.77	0.67
3:F:174:LEU:C	3:F:174:LEU:HD23	2.15	0.67
3:F:235:ARG:NH2	3:F:253:THR:OG1	2.28	0.67
2:B:147:GLN:NE2	2:B:685:TYR:CD2	2.63	0.66
1:D:243:GLN:HG2	1:D:667:PRO:HG2	1.77	0.66
3:C:415:ILE:HD11	3:C:453:ILE:HD13	1.77	0.66
1:D:242:GLU:N	1:D:242:GLU:OE1	2.29	0.66
1:D:264:LEU:HD21	1:D:267:GLU:HB2	1.78	0.66
2:B:147:GLN:HE21	2:B:685:TYR:HE2	1.42	0.66
3:F:138:LYS:HE3	3:F:250:GLU:OE1	1.92	0.66
1:A:240:HIS:NE2	1:A:656:ASP:OD2	2.28	0.65
1:D:200:PRO:HG3	2:E:318:GLU:HB3	1.78	0.65
2:E:14:VAL:O	2:E:18:ILE:HG23	1.96	0.65
3:F:415:ILE:HD11	3:F:453:ILE:HD13	1.77	0.65
1:D:449:CYS:SG	1:D:490:LYS:NZ	2.68	0.65
2:E:420:LEU:O	2:E:423:SER:OG	2.10	0.65
2:E:496:MET:HA	2:E:503:VAL:HG21	1.78	0.65
2:B:265:CYS:HB3	2:B:274:PRO:HG3	1.79	0.65
1:D:473:GLU:OE2	1:D:475:LEU:HD21	1.97	0.64
2:B:421:GLY:O	2:B:424:THR:OG1	2.15	0.64
3:C:694:PRO:O	3:C:709:LEU:O	2.15	0.64
2:E:409:LEU:HD11	2:E:412:MET:HG2	1.79	0.64
3:C:175:PHE:CE1	3:C:177:ASP:HB2	2.33	0.64
3:C:670:ASN:HB3	3:C:676:TRP:H	1.62	0.64
3:C:583:PRO:CG	3:C:695:LEU:CD1	2.74	0.64
1:D:514:PRO:HG3	1:D:524:VAL:HG11	1.79	0.64
2:B:724:MET:HG3	3:C:725:THR:CG2	2.28	0.64
3:F:393:LEU:N	3:F:417:CYS:SG	2.71	0.63
1:D:410:GLU:HG2	3:F:137:TRP:HB3	1.80	0.63
1:D:637:SER:HB2	2:E:238:LEU:HA	1.79	0.63
2:B:724:MET:CG	3:C:725:THR:CG2	2.70	0.63
3:C:693:VAL:N	3:C:694:PRO:CD	2.62	0.63
3:C:583:PRO:CB	3:C:695:LEU:HD13	2.27	0.63
3:F:533:ILE:CG2	3:F:534:LEU:H	2.08	0.63
2:B:282:ALA:HB2	3:C:148:GLN:HG2	1.80	0.63
1:D:399:VAL:HB	1:D:427:GLN:HE22	1.63	0.63
1:A:291:LYS:HD3	1:A:324:ILE:HG22	1.81	0.63
1:A:449:CYS:SG	1:A:490:LYS:NZ	2.72	0.63
3:C:583:PRO:HB3	3:C:695:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:282:ALA:HB3	3:F:149:ARG:HD3	1.80	0.63
3:C:533:ILE:CG2	3:C:534:LEU:H	2.07	0.63
1:D:286:LEU:HD21	1:D:482:ASP:OD2	1.99	0.63
3:F:283:ASN:O	3:F:287:LYS:NZ	2.30	0.63
2:B:627:ASN:ND2	3:C:111:CYS:SG	2.72	0.62
1:D:396:THR:HG21	1:D:468:ARG:NE	2.14	0.62
1:D:219:ASN:HB2	1:D:221:ARG:HH11	1.63	0.62
1:D:477:VAL:CG1	1:D:478:PRO:HD2	2.29	0.62
2:E:18:ILE:CD1	2:E:497:PHE:HD1	2.11	0.62
2:E:303:ASN:ND2	2:E:488:PRO:O	2.33	0.62
3:F:271:ARG:HG2	3:F:319:GLU:HG2	1.81	0.62
1:A:222:GLU:HA	1:A:225:SER:HB3	1.82	0.62
1:A:514:PRO:HG3	1:A:524:VAL:HG11	1.82	0.62
3:C:235:ARG:NH2	3:C:253:THR:OG1	2.32	0.62
3:F:438:LYS:HG3	3:F:441:ARG:HB2	1.80	0.62
3:C:695:LEU:CD1	3:C:734:PHE:HZ	2.11	0.62
1:D:690:ARG:HH12	2:E:2:GLU:HB3	1.63	0.61
1:D:175:LEU:HB3	1:D:176:PRO:HD2	1.83	0.61
2:B:131:THR:HG21	2:B:251:ARG:HD2	1.82	0.61
2:B:281:LYS:HB3	2:B:502:PHE:HE2	1.63	0.61
1:A:405:PRO:HG2	2:B:601:ASN:ND2	2.16	0.61
3:F:189:ASN:ND2	3:F:308:GLU:OE1	2.34	0.61
3:C:438:LYS:HG3	3:C:441:ARG:HB2	1.82	0.61
1:A:233:ASN:HA	2:B:78:LEU:HD12	1.82	0.61
1:A:175:LEU:HB3	1:A:176:PRO:HD2	1.82	0.61
1:A:575:MET:HG2	2:B:544:THR:HA	1.81	0.61
3:F:280:SER:HB3	3:F:287:LYS:HE2	1.83	0.61
1:D:200:PRO:HB3	2:E:69:CYS:HB2	1.83	0.60
1:D:223:LEU:HD22	2:E:432:LEU:HD23	1.83	0.60
3:C:697:VAL:O	3:C:698:GLY:C	2.37	0.60
2:B:357:ILE:O	2:B:370:ILE:HG22	2.01	0.60
1:A:242:GLU:N	1:A:242:GLU:OE1	2.34	0.60
2:B:438:PHE:HB2	2:B:453:VAL:HB	1.83	0.60
1:D:291:LYS:HD3	1:D:324:ILE:HG22	1.82	0.60
2:E:51:ARG:NH2	2:E:77:GLU:O	2.34	0.60
1:A:243:GLN:HG2	1:A:667:PRO:HG2	1.82	0.60
1:A:174:PHE:HB2	1:A:179:GLU:HB2	1.83	0.60
3:C:280:SER:HB3	3:C:287:LYS:HE2	1.83	0.60
3:C:189:ASN:ND2	3:C:308:GLU:OE1	2.35	0.60
3:C:607:ILE:HB	3:C:612:LYS:HE3	1.82	0.60
1:D:476:PRO:O	1:D:477:VAL:CG2	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:138:LYS:CB	3:F:250:GLU:HB2	2.28	0.59
3:C:695:LEU:HD11	3:C:734:PHE:HZ	1.66	0.59
3:F:53:TRP:O	3:F:56:SER:OG	2.15	0.59
3:C:138:LYS:HB3	3:C:250:GLU:HB2	1.85	0.59
3:F:166:ILE:HD12	3:F:218:PHE:HB2	1.84	0.59
3:C:175:PHE:HD1	3:C:177:ASP:H	1.51	0.59
1:D:469:LYS:HD3	1:D:475:LEU:CD1	2.27	0.59
3:C:150:ARG:HB3	3:C:152:VAL:HG23	1.83	0.58
3:C:716:GLU:O	3:C:749:THR:OG1	2.14	0.58
1:D:402:ALA:HB3	2:E:550:ARG:HG2	1.85	0.58
3:F:716:GLU:O	3:F:749:THR:OG1	2.14	0.58
3:F:575:LEU:HD13	3:F:582:ILE:HG13	1.85	0.58
3:F:355:THR:HG22	3:F:365:GLN:HA	1.85	0.58
1:A:214:GLU:OE1	2:B:336:LYS:NZ	2.35	0.58
2:E:154:LYS:HG2	2:E:159:PRO:HA	1.85	0.58
2:E:439:TRP:HB2	2:E:450:LEU:HD11	1.86	0.58
2:E:496:MET:HG2	2:E:503:VAL:HG11	1.84	0.58
2:B:363:ARG:HD2	3:F:139:GLU:OE2	2.03	0.58
1:D:245:LYS:HA	1:D:706:PHE:HB2	1.84	0.58
1:A:245:LYS:HA	1:A:706:PHE:HB2	1.86	0.57
2:B:106:PHE:HB3	2:B:327:ILE:HG23	1.84	0.57
1:A:558:LYS:HA	1:A:561:ASN:HD22	1.69	0.57
3:C:283:ASN:O	3:C:287:LYS:NZ	2.31	0.57
3:C:634:LEU:CD2	3:C:696:VAL:HA	2.34	0.57
1:D:558:LYS:HA	1:D:561:ASN:HD22	1.69	0.57
2:E:265:CYS:HB3	2:E:274:PRO:HG3	1.87	0.57
3:C:393:LEU:HD22	3:C:396:ILE:HD11	1.86	0.57
2:E:134:TRP:HZ3	2:E:183:PHE:CE1	2.22	0.57
3:F:265:ASP:O	3:F:269:VAL:HG23	2.04	0.57
1:A:47:MET:O	1:A:152:ARG:NH1	2.38	0.57
1:A:467:GLU:HB3	1:A:479:SER:HB2	1.86	0.57
2:B:710:ILE:HG13	3:C:29:VAL:HA	1.86	0.57
1:D:274:ILE:HA	1:D:481:MET:HB3	1.86	0.57
2:B:398:GLN:HG3	2:B:399:LYS:H	1.70	0.57
2:B:675:MET:O	2:B:679:MET:HG2	2.05	0.56
2:B:134:TRP:HZ3	2:B:183:PHE:CE1	2.24	0.56
3:C:393:LEU:N	3:C:417:CYS:SG	2.78	0.56
2:E:237:LYS:HE2	2:E:241:ARG:HE	1.70	0.56
2:E:359:LEU:HB2	2:E:368:VAL:HB	1.87	0.56
2:E:357:ILE:O	2:E:370:ILE:HG22	2.04	0.56
2:E:398:GLN:HG3	2:E:399:LYS:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:THR:HG22	2:B:54:VAL:H	1.69	0.56
3:C:277:ALA:HA	3:C:287:LYS:HD3	1.88	0.56
1:D:174:PHE:HB2	1:D:179:GLU:HB2	1.86	0.56
2:E:52:THR:HG22	2:E:54:VAL:H	1.70	0.56
2:B:51:ARG:NH2	2:B:77:GLU:O	2.39	0.56
3:F:174:LEU:O	3:F:174:LEU:HD23	2.06	0.56
3:F:387:SER:HG	3:F:395:TRP:HE3	1.54	0.56
1:D:281:ARG:HD3	2:E:570:LYS:HB3	1.87	0.56
1:D:426:LEU:HD21	1:D:621:LEU:HD22	1.88	0.56
2:E:90:LEU:HA	2:E:93:LEU:HD12	1.87	0.56
3:F:552:PRO:HB2	3:F:554:LEU:HG	1.87	0.56
1:D:47:MET:O	1:D:152:ARG:NH1	2.39	0.56
3:F:634:LEU:HA	3:F:637:LEU:HD12	1.87	0.56
2:B:154:LYS:HG2	2:B:159:PRO:HA	1.86	0.56
1:D:51:GLU:OE1	1:D:51:GLU:N	2.38	0.56
1:D:59:ASP:OD2	3:F:769:LYS:NZ	2.38	0.56
1:D:230:MET:SD	2:E:465:ARG:HB3	2.46	0.55
2:E:281:LYS:HB3	2:E:502:PHE:HE2	1.71	0.55
2:E:574:MET:HA	2:E:577:ILE:HD12	1.88	0.55
1:A:566:LYS:HE3	1:A:569:ARG:HH21	1.71	0.55
2:B:496:MET:HG2	2:B:503:VAL:HG11	1.88	0.55
2:E:53:SER:H	2:E:73:GLU:HG3	1.71	0.55
1:A:690:ARG:HH12	2:B:2:GLU:HB3	1.72	0.55
3:C:148:GLN:HB3	3:C:504:ASP:OD2	2.07	0.55
1:D:286:LEU:HD11	1:D:482:ASP:OD2	2.07	0.55
1:A:338:GLU:HG2	3:F:254:ALA:HB1	1.88	0.55
3:F:681:SER:HB3	3:F:691:ILE:HD11	1.89	0.55
3:C:355:THR:HG22	3:C:365:GLN:HA	1.89	0.55
3:C:697:VAL:O	3:C:698:GLY:O	2.25	0.55
1:A:281:ARG:HD3	2:B:570:LYS:HB3	1.89	0.55
3:C:174:LEU:O	3:C:174:LEU:HD23	2.06	0.55
1:D:112:ASP:HB2	1:D:139:ASP:HB2	1.88	0.55
1:A:238:ILE:HG21	1:A:665:PHE:HA	1.89	0.54
2:B:439:TRP:HB2	2:B:450:LEU:HD11	1.89	0.54
3:C:310:ILE:HD13	3:C:323:CYS:HB3	1.89	0.54
3:F:175:PHE:HD1	3:F:177:ASP:H	1.55	0.54
3:F:643:PHE:CZ	3:F:658:PHE:HB3	2.42	0.54
3:F:670:ASN:HB3	3:F:676:TRP:H	1.71	0.54
1:A:287:ILE:HA	1:A:290:PHE:HB2	1.89	0.54
1:A:382:PHE:HB3	1:A:686:PHE:CE1	2.42	0.54
3:F:565:THR:HG22	3:F:685:TYR:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:ALA:HB3	2:B:409:LEU:HD13	1.90	0.54
1:D:477:VAL:HG12	1:D:478:PRO:N	2.23	0.54
3:F:591:TYR:CD2	3:F:627:VAL:HG21	2.42	0.54
1:A:33:ARG:HH11	1:A:183:ILE:HG21	1.73	0.54
1:A:694:LEU:HD22	2:B:6:TYR:HB3	1.89	0.54
1:D:49:CYS:HB2	1:D:61:PHE:HB2	1.90	0.54
3:F:267:ARG:O	3:F:271:ARG:HG3	2.07	0.54
2:B:314:CYS:SG	2:B:477:ASN:ND2	2.81	0.54
1:D:409:ASN:OD1	1:D:409:ASN:N	2.40	0.54
3:F:536:LEU:HD12	3:F:537:PRO:HD2	1.89	0.54
3:C:272:LYS:HZ2	3:C:543:THR:HG23	1.72	0.53
2:E:438:PHE:HB2	2:E:453:VAL:HB	1.89	0.53
3:C:333:LYS:HE3	3:C:343:LYS:HD3	1.90	0.53
3:F:317:SER:HB3	3:F:320:VAL:HG23	1.91	0.53
1:A:409:ASN:N	1:A:409:ASN:OD1	2.41	0.53
1:A:274:ILE:HA	1:A:481:MET:HB3	1.90	0.53
3:C:387:SER:HG	3:C:395:TRP:HE3	1.55	0.53
3:C:444:PRO:HG2	3:C:533:ILE:HD11	1.91	0.53
3:C:536:LEU:HD12	3:C:537:PRO:HD2	1.91	0.53
3:C:721:ALA:CB	3:C:738:VAL:HA	2.37	0.53
3:F:271:ARG:O	3:F:275:LEU:HG	2.09	0.53
2:E:294:ARG:HG3	3:F:395:TRP:CH2	2.43	0.53
3:C:575:LEU:HD13	3:C:582:ILE:HG13	1.91	0.53
3:C:565:THR:HG22	3:C:685:TYR:HB3	1.90	0.53
1:D:33:ARG:HH11	1:D:183:ILE:HG21	1.73	0.53
1:D:382:PHE:HB3	1:D:686:PHE:CE1	2.42	0.53
1:A:390:ILE:HD11	1:A:623:VAL:HA	1.91	0.53
2:E:51:ARG:HH12	2:E:78:LEU:HA	1.74	0.53
1:D:265:MET:HG2	1:D:434:GLU:HG2	1.91	0.53
3:F:517:SER:N	3:F:521:GLU:O	2.34	0.53
3:C:693:VAL:N	3:C:694:PRO:HD2	2.23	0.53
2:E:314:CYS:SG	2:E:477:ASN:ND2	2.82	0.53
2:E:382:MET:SD	2:E:386:TYR:HB3	2.49	0.53
3:F:277:ALA:HA	3:F:287:LYS:HD3	1.91	0.53
1:D:56:ASN:OD1	1:D:57:GLY:N	2.40	0.52
2:E:628:PRO:HG3	3:F:205:LEU:HD13	1.91	0.52
1:A:398:TRP:CE3	1:A:465:SER:HB2	2.44	0.52
3:F:718:ASP:OD1	3:F:719:PRO:HD3	2.07	0.52
2:B:147:GLN:NE2	2:B:685:TYR:HE2	2.04	0.52
3:F:607:ILE:HB	3:F:612:LYS:HE3	1.90	0.52
1:A:59:ASP:OD2	3:C:769:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:LYS:HE2	2:B:241:ARG:HE	1.74	0.52
3:C:175:PHE:HE1	3:C:177:ASP:HB2	1.72	0.52
3:C:620:ARG:NH2	3:C:644:THR:O	2.42	0.52
2:E:542:PRO:HD3	3:F:247:TRP:CZ2	2.44	0.52
1:D:287:ILE:HA	1:D:290:PHE:HB2	1.90	0.52
1:D:390:ILE:HD11	1:D:623:VAL:HA	1.92	0.52
2:B:382:MET:SD	2:B:386:TYR:HB3	2.50	0.52
1:D:201:LEU:HD21	2:E:87:ILE:HD11	1.92	0.52
3:F:626:GLN:O	3:F:632:TYR:HB3	2.10	0.52
1:A:426:LEU:HD21	1:A:621:LEU:HD22	1.92	0.52
3:C:453:ILE:HG12	3:C:463:LEU:HD22	1.91	0.52
1:D:110:LYS:HG2	1:D:111:ALA:H	1.74	0.52
3:F:124:SER:HB2	3:F:128:ARG:HH21	1.73	0.52
3:F:346:SER:HB2	3:F:374:GLU:H	1.76	0.52
3:C:346:SER:HB2	3:C:374:GLU:H	1.74	0.51
3:F:138:LYS:HB3	3:F:250:GLU:OE2	2.10	0.51
2:B:51:ARG:HH12	2:B:78:LEU:HA	1.74	0.51
3:C:551:HIS:ND1	3:C:551:HIS:O	2.43	0.51
3:F:393:LEU:HD22	3:F:396:ILE:HD11	1.92	0.51
2:B:361:ASN:C	2:B:363:ARG:H	2.14	0.51
2:B:359:LEU:HB2	2:B:368:VAL:HB	1.92	0.51
2:E:244:ALA:HB3	2:E:409:LEU:HD13	1.91	0.51
2:E:79:VAL:HB	2:E:480:LEU:HD11	1.92	0.51
3:F:175:PHE:CE1	3:F:177:ASP:HB2	2.44	0.51
3:F:230:ALA:CB	3:F:235:ARG:HD2	2.37	0.51
3:C:681:SER:HB3	3:C:691:ILE:HD11	1.92	0.51
1:A:657:LYS:HE3	2:B:9:PHE:O	2.10	0.51
3:F:718:ASP:CB	3:F:719:PRO:HD3	2.36	0.51
1:A:112:ASP:HB2	1:A:139:ASP:HB2	1.93	0.51
1:A:398:TRP:CG	1:A:433:ARG:HA	2.45	0.51
2:B:574:MET:HA	2:B:577:ILE:HD12	1.93	0.51
1:A:155:SER:HB3	3:C:713:SER:OG	2.11	0.51
1:A:358:ASP:O	1:A:362:THR:HA	2.11	0.51
1:A:379:PRO:HB3	1:A:381:TRP:NE1	2.26	0.51
2:B:18:ILE:HG12	2:B:497:PHE:CE1	2.46	0.51
2:E:675:MET:O	2:E:679:MET:HG2	2.11	0.51
1:D:690:ARG:NH2	2:E:2:GLU:OE1	2.40	0.51
1:A:51:GLU:N	1:A:51:GLU:OE1	2.43	0.51
2:B:701:ILE:HD11	3:C:208:GLU:HA	1.92	0.51
1:A:49:CYS:HB2	1:A:61:PHE:HB2	1.93	0.50
3:C:349:GLY:HA3	3:C:371:GLU:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:MET:HE2	2:E:337:ASP:HB3	1.93	0.50
3:F:547:VAL:HG13	3:F:688:GLY:HA2	1.92	0.50
3:F:734:PHE:HA	3:F:752:ARG:HG3	1.94	0.50
3:C:547:VAL:HG13	3:C:688:GLY:HA2	1.93	0.50
3:C:578:GLY:HA2	3:C:734:PHE:CD2	2.47	0.50
3:C:591:TYR:CD2	3:C:627:VAL:HG21	2.45	0.50
1:D:467:GLU:HB3	1:D:479:SER:HB2	1.92	0.50
3:F:333:LYS:HE3	3:F:343:LYS:HD3	1.92	0.50
1:A:695:VAL:HG13	1:A:705:PHE:CD1	2.45	0.50
2:B:282:ALA:HB3	3:C:149:ARG:HD3	1.92	0.50
1:D:45:CYS:HB3	1:D:94:ILE:HD11	1.94	0.50
2:E:370:ILE:HD11	2:E:374:LYS:HB2	1.93	0.50
2:B:487:LEU:CD2	2:B:488:PRO:HD2	2.41	0.50
2:B:517:GLY:N	2:B:523:ASP:OD1	2.26	0.50
3:C:531:ALA:O	3:C:532:THR:CG2	2.60	0.50
1:A:235:LYS:HZ3	2:B:464:ILE:HG22	1.75	0.50
1:A:677:CYS:HA	2:B:238:LEU:HD22	1.94	0.50
2:E:389:LEU:O	2:E:393:LEU:HD23	2.12	0.50
2:E:542:PRO:HD3	3:F:247:TRP:CE2	2.46	0.50
1:A:90:PHE:HB2	1:A:123:LEU:HD21	1.94	0.50
1:D:238:ILE:HG21	1:D:665:PHE:HA	1.94	0.50
1:D:244:ASN:O	1:D:705:PHE:HA	2.12	0.49
1:D:368:SER:HB2	2:E:359:LEU:HD23	1.93	0.49
2:B:363:ARG:HD3	3:F:139:GLU:CD	2.32	0.49
3:C:230:ALA:CB	3:C:235:ARG:HD2	2.41	0.49
1:D:464:ARG:HG2	1:D:482:ASP:HB3	1.95	0.49
1:A:674:ILE:O	1:A:678:LEU:HD13	2.11	0.49
2:B:79:VAL:HB	2:B:480:LEU:HD11	1.94	0.49
1:D:405:PRO:HG2	2:E:601:ASN:ND2	2.27	0.49
3:F:158:GLU:HG3	3:F:159:GLN:HG3	1.94	0.49
1:A:416:GLU:HG2	1:A:420:LYS:HE2	1.94	0.49
1:A:287:ILE:CG2	1:A:460:PRO:HB3	2.43	0.49
1:A:488:CYS:SG	1:A:504:ILE:HD11	2.51	0.49
3:C:144:LEU:HD21	3:C:228:PHE:HB3	1.95	0.49
3:C:317:SER:HB3	3:C:320:VAL:HG23	1.93	0.49
3:F:148:GLN:HB3	3:F:504:ASP:OD2	2.11	0.49
1:A:110:LYS:HG2	1:A:111:ALA:H	1.76	0.49
3:C:158:GLU:HG3	3:C:159:GLN:HG3	1.94	0.49
1:D:469:LYS:CE	1:D:475:LEU:HD13	2.43	0.49
2:B:389:LEU:O	2:B:393:LEU:HD23	2.12	0.49
3:C:298:ARG:NH1	3:C:684:ILE:HD11	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:ASP:O	1:D:362:THR:HA	2.13	0.49
1:D:469:LYS:HB2	1:D:475:LEU:CD1	2.40	0.49
2:E:416:LEU:O	2:E:419:VAL:HB	2.13	0.49
3:F:140:LEU:O	3:F:248:ILE:HG22	2.12	0.49
1:D:398:TRP:CG	1:D:433:ARG:HA	2.47	0.49
1:A:586:SER:HA	1:A:593:LEU:HD12	1.95	0.49
2:B:697:GLU:OE1	3:C:175:PHE:CE2	2.66	0.49
3:C:552:PRO:HB2	3:C:554:LEU:HG	1.93	0.49
3:C:531:ALA:C	3:C:532:THR:HG22	2.33	0.49
2:E:49:TYR:CE1	2:E:81:PRO:HB2	2.48	0.49
2:E:282:ALA:HB2	3:F:148:GLN:HG2	1.94	0.49
1:A:128:LYS:HA	1:A:141:ASN:HD22	1.77	0.49
2:B:53:SER:H	2:B:73:GLU:HG3	1.77	0.49
1:D:287:ILE:CG2	1:D:460:PRO:HB3	2.42	0.49
2:E:294:ARG:HA	3:F:395:TRP:CE2	2.47	0.49
3:F:139:GLU:O	3:F:140:LEU:HD23	2.13	0.49
3:C:195:GLU:O	3:C:198:SER:OG	2.25	0.48
3:F:197:ARG:NH1	3:F:703:ASP:O	2.46	0.48
3:F:741:PHE:HA	3:F:747:VAL:HG22	1.94	0.48
1:A:222:GLU:O	1:A:226:LYS:HB2	2.12	0.48
3:C:28:THR:OG1	3:C:29:VAL:N	2.46	0.48
3:C:634:LEU:HA	3:C:637:LEU:HD12	1.95	0.48
1:D:164:LEU:O	1:D:168:ASN:N	2.46	0.48
1:A:361:THR:HG21	1:D:596:LYS:HE2	1.94	0.48
2:E:22:TYR:HB3	2:E:24:TYR:CD1	2.48	0.48
2:E:467:PHE:O	2:E:470:VAL:HG12	2.13	0.48
2:B:467:PHE:O	2:B:470:VAL:HG12	2.14	0.48
3:C:131:ARG:NH1	3:C:237:GLU:OE1	2.47	0.48
1:D:558:LYS:HE3	3:F:49:LEU:HD11	1.95	0.48
3:F:753:THR:HG22	3:F:754:ALA:O	2.14	0.48
1:A:363:GLU:OE1	1:D:592:ASN:O	2.31	0.48
2:B:123:SER:HB3	3:C:34:THR:HG22	1.96	0.48
1:D:364:GLY:O	2:E:361:ASN:HB3	2.13	0.48
1:D:90:PHE:HB2	1:D:123:LEU:HD21	1.95	0.48
2:E:106:PHE:HB3	2:E:327:ILE:HG23	1.95	0.48
3:F:620:ARG:NH2	3:F:644:THR:O	2.46	0.48
1:A:113:ASP:O	1:A:117:GLN:HG2	2.14	0.48
1:D:434:GLU:HA	1:D:437:LYS:HG2	1.96	0.48
1:D:518:LYS:HG3	1:D:519:HIS:CD2	2.49	0.48
3:F:535:ASP:OD1	3:F:536:LEU:N	2.46	0.48
1:A:635:ASN:ND2	2:B:27:PRO:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:393:LEU:HD21	3:F:467:ARG:CZ	2.44	0.48
3:F:713:SER:HB3	3:F:753:THR:HG21	1.95	0.48
3:C:422:TYR:OH	3:C:445:TYR:O	2.32	0.48
1:D:304:PRO:CG	1:D:310:PRO:HB3	2.41	0.48
1:D:469:LYS:CB	1:D:475:LEU:CD1	2.91	0.48
2:B:409:LEU:HD11	2:B:412:MET:HG2	1.96	0.48
1:D:431:CYS:O	1:D:435:MET:HG3	2.14	0.48
2:E:487:LEU:CD2	2:E:488:PRO:HD2	2.44	0.48
3:F:283:ASN:OD1	3:F:287:LYS:NZ	2.46	0.48
1:A:45:CYS:HB3	1:A:94:ILE:HD11	1.96	0.47
2:B:370:ILE:HD11	2:B:374:LYS:HB2	1.96	0.47
3:C:469:ILE:HG22	3:C:493:LEU:HD13	1.96	0.47
3:F:531:ALA:C	3:F:532:THR:HG22	2.34	0.47
3:F:737:LYS:HA	3:F:750:PHE:O	2.14	0.47
3:C:614:VAL:HG13	3:C:651:GLY:HA3	1.96	0.47
1:D:515:ASN:H	1:D:519:HIS:CD2	2.32	0.47
1:D:586:SER:HB2	1:D:591:GLU:O	2.14	0.47
1:D:695:VAL:HG13	1:D:705:PHE:CD1	2.49	0.47
3:F:397:THR:HA	3:F:497:THR:O	2.15	0.47
3:F:476:LYS:O	3:F:480:SER:OG	2.19	0.47
1:A:219:ASN:HB2	1:A:221:ARG:HH11	1.79	0.47
3:F:551:HIS:O	3:F:551:HIS:ND1	2.47	0.47
1:A:265:MET:HG2	1:A:434:GLU:HG2	1.95	0.47
1:A:151:LEU:O	3:C:713:SER:OG	2.31	0.47
3:C:422:TYR:CZ	3:C:449:MET:HG3	2.49	0.47
2:E:660:HIS:CE1	3:F:106:ASN:HD21	2.33	0.47
1:A:562:ASP:O	1:A:565:SER:OG	2.25	0.47
2:E:18:ILE:HD13	2:E:497:PHE:CD1	2.43	0.47
3:F:349:GLY:HA3	3:F:371:GLU:HG2	1.96	0.47
1:D:128:LYS:HA	1:D:141:ASN:HD22	1.79	0.47
3:F:131:ARG:NH1	3:F:237:GLU:OE1	2.48	0.47
3:F:531:ALA:O	3:F:532:THR:CG2	2.60	0.47
2:B:365:THR:HG22	2:B:366:LYS:HG3	1.97	0.47
2:B:491:PHE:CE1	2:B:493:PHE:HB2	2.50	0.47
2:B:628:PRO:HG3	3:C:205:LEU:HD13	1.97	0.47
3:C:340:MET:HE2	3:C:409:LEU:HD23	1.96	0.47
1:D:391:LYS:O	1:D:430:ASN:ND2	2.43	0.47
1:D:416:GLU:HG2	1:D:420:LYS:HE2	1.97	0.47
3:F:381:SER:HB2	3:F:405:ASP:OD2	2.15	0.47
3:F:422:TYR:OH	3:F:445:TYR:O	2.32	0.47
1:D:113:ASP:O	1:D:117:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:361:ASN:C	2:E:363:ARG:H	2.16	0.47
1:A:316:LEU:HD21	1:A:489:VAL:HG21	1.95	0.47
3:F:139:GLU:O	3:F:140:LEU:HG	2.15	0.47
1:A:518:LYS:HG3	1:A:519:HIS:CD2	2.50	0.47
2:B:147:GLN:NE2	2:B:685:TYR:HD2	2.10	0.47
2:B:497:PHE:O	2:B:503:VAL:HB	2.15	0.47
1:D:222:GLU:O	1:D:226:LYS:HB2	2.15	0.47
2:E:52:THR:HA	2:E:73:GLU:HG2	1.96	0.47
3:F:422:TYR:CZ	3:F:449:MET:HG3	2.50	0.47
1:A:165:ARG:HE	1:A:170:PHE:HZ	1.62	0.46
1:A:115:TYR:CZ	1:A:175:LEU:HD12	2.50	0.46
2:B:22:TYR:HB3	2:B:24:TYR:CD1	2.50	0.46
3:C:393:LEU:HD21	3:C:467:ARG:CZ	2.45	0.46
3:C:272:LYS:HE2	3:C:541:LYS:HA	1.97	0.46
1:D:477:VAL:CG1	1:D:478:PRO:CD	2.91	0.46
2:E:342:ALA:HB3	2:E:343:PRO:HD3	1.97	0.46
2:E:497:PHE:O	2:E:503:VAL:HB	2.15	0.46
3:F:351:LYS:HG2	3:F:369:TRP:NE1	2.30	0.46
3:F:76:GLU:OE2	3:F:80:VAL:HB	2.15	0.46
2:B:532:LYS:O	2:B:535:MET:N	2.48	0.46
1:D:222:GLU:N	1:D:222:GLU:OE1	2.49	0.46
2:E:523:ASP:OD2	2:E:560:TYR:OH	2.24	0.46
1:D:190:THR:O	1:D:194:LEU:HD13	2.16	0.46
1:D:273:LYS:O	1:D:481:MET:HB2	2.16	0.46
3:F:103:ASN:N	3:F:103:ASN:OD1	2.48	0.46
1:A:388:TRP:CH2	1:A:430:ASN:HB3	2.50	0.46
3:C:713:SER:HB3	3:C:753:THR:HG21	1.96	0.46
3:F:157:VAL:O	3:F:160:ARG:HG3	2.15	0.46
3:F:170:GLN:HE21	3:F:211:ALA:HB1	1.80	0.46
3:F:340:MET:HE2	3:F:409:LEU:HD23	1.97	0.46
1:A:199:VAL:HA	1:A:200:PRO:HD3	1.78	0.46
1:A:445:LEU:HD12	1:A:459:VAL:HG11	1.98	0.46
3:C:718:ASP:OD1	3:C:719:PRO:CD	2.63	0.46
1:D:229:GLN:O	1:D:233:ASN:HB2	2.15	0.46
1:D:89:PRO:HG2	1:D:90:PHE:HD1	1.81	0.46
2:E:487:LEU:HD23	2:E:489:GLU:H	1.81	0.46
3:F:533:ILE:HG22	3:F:534:LEU:HG	1.96	0.46
1:A:165:ARG:NH2	2:B:707:ALA:HB2	2.30	0.46
1:A:251:LEU:HD21	1:A:378:PHE:HB2	1.97	0.46
1:A:644:ASN:ND2	2:B:236:GLY:HA3	2.31	0.46
3:C:157:VAL:O	3:C:160:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:562:ASP:OD1	3:F:52:ARG:NH1	2.49	0.46
3:F:692:ARG:HG3	3:F:694:PRO:HD2	1.96	0.46
1:A:382:PHE:HB3	1:A:686:PHE:CD1	2.51	0.46
2:B:436:GLY:HA3	2:B:454:ALA:HA	1.98	0.46
3:C:138:LYS:HG2	3:C:139:GLU:N	2.31	0.46
2:B:303:ASN:ND2	2:B:488:PRO:O	2.49	0.46
3:C:381:SER:HB2	3:C:405:ASP:OD2	2.16	0.46
1:D:280:SER:OG	1:D:464:ARG:NH2	2.49	0.46
2:E:253:PHE:HA	2:E:256:ILE:HD12	1.98	0.46
2:E:350:PHE:HB3	2:E:401:VAL:CG2	2.44	0.46
2:E:303:ASN:ND2	2:E:488:PRO:HA	2.30	0.46
3:C:283:ASN:OD1	3:C:287:LYS:NZ	2.47	0.46
3:C:340:MET:CE	3:C:409:LEU:HD23	2.45	0.46
3:C:600:VAL:HG13	3:C:642:PRO:HA	1.97	0.46
2:E:18:ILE:CD1	2:E:497:PHE:CG	2.97	0.46
1:D:185:MET:CE	2:E:337:ASP:HB3	2.46	0.46
2:B:363:ARG:O	1:D:409:ASN:ND2	2.48	0.46
1:D:316:LEU:HD22	1:D:339:PHE:CE2	2.51	0.46
1:D:658:LYS:HB2	1:D:660:LYS:HE3	1.98	0.46
1:D:183:ILE:HD13	2:E:334:LEU:HD13	1.98	0.46
3:F:453:ILE:HG12	3:F:463:LEU:HD22	1.98	0.46
1:A:646:GLN:HA	1:A:649:ILE:HD12	1.98	0.45
3:C:122:TYR:CD1	3:C:213:MET:HG2	2.51	0.45
1:D:214:GLU:OE1	2:E:336:LYS:NZ	2.48	0.45
2:E:475:GLY:O	2:E:477:ASN:ND2	2.49	0.45
3:F:298:ARG:NH1	3:F:684:ILE:HD11	2.31	0.45
3:F:310:ILE:HD13	3:F:323:CYS:HB3	1.98	0.45
1:A:241:TYR:O	1:A:244:ASN:ND2	2.49	0.45
3:C:265:ASP:O	3:C:269:VAL:HG23	2.16	0.45
1:D:382:PHE:HB3	1:D:686:PHE:CD1	2.51	0.45
1:A:145:PRO:O	1:A:150:LYS:HE3	2.17	0.45
1:A:510:SER:O	1:A:547:LEU:HD12	2.17	0.45
3:C:170:GLN:HE21	3:C:211:ALA:HB1	1.80	0.45
3:C:444:PRO:O	3:C:448:VAL:HG23	2.16	0.45
3:C:76:GLU:OE2	3:C:80:VAL:HB	2.17	0.45
1:D:444:ALA:O	1:D:448:GLU:HG2	2.17	0.45
1:D:566:LYS:HE3	1:D:569:ARG:HH21	1.81	0.45
2:E:705:ILE:H	3:F:744:GLN:HB2	1.80	0.45
3:F:419:ASP:OD2	3:F:467:ARG:NH1	2.49	0.45
3:F:272:LYS:HZ2	3:F:543:THR:HG23	1.81	0.45
1:A:444:ALA:O	1:A:448:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:PHE:HE1	2:B:493:PHE:HB2	1.81	0.45
3:C:236:MET:SD	3:C:239:ILE:HD11	2.56	0.45
3:C:643:PHE:CZ	3:C:658:PHE:HB3	2.52	0.45
1:D:251:LEU:HD21	1:D:378:PHE:HB2	1.99	0.45
3:F:144:LEU:HD21	3:F:228:PHE:HB3	1.97	0.45
1:A:412:GLU:HG2	2:B:601:ASN:ND2	2.32	0.45
1:D:605:ILE:HG13	1:D:623:VAL:HG21	1.99	0.45
3:F:444:PRO:HG2	3:F:533:ILE:HD11	1.99	0.45
3:F:444:PRO:O	3:F:448:VAL:HG23	2.17	0.45
3:F:583:PRO:HD3	3:F:695:LEU:HD11	1.99	0.45
3:C:263:LYS:HA	3:C:266:ILE:HD12	1.98	0.45
2:E:60:VAL:HG23	2:E:61:PHE:CD2	2.52	0.45
1:A:316:LEU:HD22	1:A:339:PHE:CE2	2.52	0.45
3:C:272:LYS:NZ	3:C:543:THR:HG23	2.32	0.45
3:C:59:PHE:N	3:C:60:PRO:HD3	2.32	0.45
2:B:55:GLU:HG3	2:B:66:ARG:HG3	1.98	0.45
3:C:174:LEU:HD23	3:C:175:PHE:HB2	1.99	0.45
3:C:351:LYS:HG2	3:C:369:TRP:NE1	2.30	0.45
1:D:199:VAL:HA	1:D:200:PRO:HD3	1.75	0.45
3:F:469:ILE:HG22	3:F:493:LEU:HD13	1.98	0.45
3:F:384:ALA:HA	3:F:503:ILE:HD12	1.97	0.45
1:A:140:LYS:NZ	1:A:150:LYS:HE2	2.32	0.45
2:B:416:LEU:O	2:B:419:VAL:HB	2.17	0.45
1:D:133:SER:HB2	1:D:137:ARG:HB2	1.97	0.45
2:E:584:ILE:HG21	2:E:590:LEU:HD21	1.99	0.45
3:F:600:VAL:HG13	3:F:642:PRO:HA	1.99	0.45
1:A:419:ASN:ND2	2:B:543:SER:OG	2.50	0.45
3:C:139:GLU:N	3:C:139:GLU:OE1	2.50	0.45
1:A:67:ARG:NH1	3:C:770:ILE:HA	2.32	0.45
2:E:749:ALA:HB1	3:F:16:GLN:HA	1.99	0.45
3:F:330:GLN:HG3	3:F:513:HIS:HB2	1.99	0.45
3:F:197:ARG:HD3	3:F:704:THR:HG22	1.97	0.45
1:A:190:THR:O	1:A:194:LEU:HD13	2.17	0.44
1:A:665:PHE:HB2	2:B:480:LEU:O	2.17	0.44
1:A:405:PRO:HB3	2:B:598:LEU:HG	1.98	0.44
3:C:166:ILE:HD12	3:C:218:PHE:HB2	1.98	0.44
1:A:658:LYS:HB2	1:A:660:LYS:HE3	1.99	0.44
2:E:18:ILE:HD13	2:E:497:PHE:CG	2.52	0.44
2:E:557:ARG:HD3	2:E:563:HIS:HA	1.99	0.44
3:F:174:LEU:HD23	3:F:175:PHE:HB2	1.99	0.44
2:B:52:THR:HA	2:B:73:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:407:LYS:HA	3:C:410:LEU:HD12	2.00	0.44
3:C:517:SER:N	3:C:521:GLU:O	2.41	0.44
2:E:420:LEU:HD11	2:E:474:ILE:HD12	1.98	0.44
3:C:384:ALA:HA	3:C:503:ILE:HD12	1.99	0.44
1:D:140:LYS:NZ	1:D:150:LYS:HE2	2.32	0.44
1:D:282:ALA:C	1:D:284:GLU:H	2.21	0.44
1:D:326:ASP:OD1	1:D:327:ARG:N	2.50	0.44
1:A:275:SER:HB3	1:A:482:ASP:OD2	2.17	0.44
3:F:236:MET:HA	3:F:239:ILE:HG13	1.99	0.44
1:A:431:CYS:SG	1:A:626:VAL:HA	2.58	0.44
2:B:350:PHE:HB3	2:B:401:VAL:CG2	2.45	0.44
3:C:452:TRP:CE3	3:C:453:ILE:HG13	2.53	0.44
3:F:614:VAL:HG13	3:F:651:GLY:HA3	2.00	0.44
3:C:175:PHE:CD1	3:C:177:ASP:HB2	2.52	0.44
1:D:146:MET:N	1:D:149:GLN:OE1	2.49	0.44
3:F:174:LEU:CD2	3:F:175:PHE:HB2	2.48	0.44
3:F:28:THR:OG1	3:F:29:VAL:N	2.51	0.44
3:F:407:LYS:HA	3:F:410:LEU:HD12	1.98	0.44
1:A:586:SER:HB3	1:A:593:LEU:HB2	1.99	0.44
3:C:414:MET:HE2	3:C:463:LEU:HD12	2.00	0.44
3:C:634:LEU:HD23	3:C:696:VAL:HA	1.99	0.44
1:D:194:LEU:HG	2:E:348:ASN:HD22	1.82	0.44
1:A:320:ILE:HG21	1:A:487:ILE:HG21	2.00	0.44
1:A:326:ASP:OD1	1:A:327:ARG:N	2.50	0.44
1:A:681:ASN:HB3	1:A:684:CYS:HB3	2.00	0.44
2:B:221:ILE:O	2:B:225:THR:OG1	2.32	0.44
3:C:393:LEU:HD12	3:C:393:LEU:O	2.18	0.44
3:C:533:ILE:HG22	3:C:534:LEU:HG	2.00	0.44
3:C:704:THR:HB	3:C:707:ALA:HB3	2.00	0.44
1:D:425:VAL:HG12	1:D:426:LEU:HD23	1.99	0.44
2:E:506:LEU:HD12	2:E:540:LEU:HD22	1.99	0.44
3:F:139:GLU:OE1	3:F:139:GLU:N	2.51	0.44
1:A:257:ALA:HA	1:A:376:ARG:HG2	1.99	0.43
2:B:273:LEU:HB2	2:B:418:THR:HG21	1.99	0.43
3:C:124:SER:HB2	3:C:128:ARG:HH21	1.83	0.43
1:D:689:GLN:O	1:D:692:ASN:HB2	2.18	0.43
3:F:161:LEU:HD12	3:F:165:GLU:HG3	1.99	0.43
3:F:463:LEU:HA	3:F:466:SER:HB3	2.00	0.43
1:A:434:GLU:HA	1:A:437:LYS:HG2	2.00	0.43
2:B:475:GLY:O	2:B:477:ASN:ND2	2.51	0.43
2:B:24:TYR:CD1	2:B:507:ALA:HB1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:534:ASN:ND2	2:B:538:ASN:OD1	2.48	0.43
3:C:103:ASN:OD1	3:C:103:ASN:N	2.51	0.43
3:C:174:LEU:CD2	3:C:175:PHE:HB2	2.48	0.43
3:C:197:ARG:HD3	3:C:704:THR:HG22	2.00	0.43
1:D:378:PHE:HA	1:D:379:PRO:HD3	1.83	0.43
3:F:126:PHE:O	3:F:129:LEU:HB3	2.19	0.43
1:A:276:ASP:HB2	1:A:279:ARG:HB2	1.99	0.43
1:A:605:ILE:HG13	1:A:623:VAL:HG21	2.00	0.43
1:D:430:ASN:O	1:D:433:ARG:HB3	2.18	0.43
1:D:410:GLU:HA	3:F:139:GLU:HB3	2.00	0.43
1:A:257:ALA:HB3	1:A:379:PRO:HG3	1.98	0.43
1:A:316:LEU:HD23	1:A:507:PHE:CZ	2.52	0.43
1:A:509:PHE:HB3	1:A:547:LEU:HD11	2.01	0.43
2:B:506:LEU:HD12	2:B:540:LEU:HD22	2.00	0.43
1:D:488:CYS:SG	1:D:504:ILE:HD11	2.57	0.43
1:A:273:LYS:O	1:A:481:MET:HB2	2.18	0.43
2:B:457:TRP:HA	2:B:460:ILE:HD12	2.01	0.43
1:D:450:ARG:HG2	3:F:56:SER:OG	2.19	0.43
1:D:562:ASP:O	1:D:565:SER:OG	2.25	0.43
2:E:436:GLY:HA3	2:E:454:ALA:HA	2.00	0.43
1:A:236:LEU:HD12	1:A:237:PRO:HD2	2.00	0.43
3:C:299:ILE:HG22	3:C:300:GLY:N	2.33	0.43
3:C:335:LEU:HB3	3:C:342:LEU:O	2.19	0.43
1:D:115:TYR:CZ	1:D:175:LEU:HD12	2.53	0.43
1:D:257:ALA:HB3	1:D:379:PRO:HG3	2.00	0.43
1:D:410:GLU:HG3	1:D:410:GLU:H	1.53	0.43
3:F:124:SER:O	3:F:128:ARG:HG3	2.18	0.43
3:F:174:LEU:C	3:F:174:LEU:CD2	2.86	0.43
1:A:317:TRP:NE1	1:A:321:LYS:HD2	2.32	0.43
2:B:493:PHE:O	2:B:496:MET:HB2	2.19	0.43
3:C:236:MET:HA	3:C:239:ILE:HG13	2.01	0.43
3:C:426:ALA:N	3:C:427:PRO:HD3	2.34	0.43
3:C:700:GLU:N	3:C:700:GLU:OE1	2.51	0.43
1:D:402:ALA:O	2:E:550:ARG:HD3	2.18	0.43
1:A:415:ALA:HB1	2:B:546:LEU:HD22	2.00	0.43
1:D:246:PHE:O	1:D:247:ARG:HG2	2.19	0.43
2:E:541:SER:HA	3:F:247:TRP:CZ2	2.54	0.43
1:A:133:SER:HB2	1:A:137:ARG:HB2	2.01	0.43
3:C:154:THR:HG22	3:C:236:MET:HB3	2.01	0.43
3:C:161:LEU:HD12	3:C:165:GLU:HG3	2.00	0.43
3:C:419:ASP:OD2	3:C:467:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:GLN:HG3	1:D:243:GLN:O	2.19	0.43
1:D:316:LEU:HD21	1:D:489:VAL:HG21	2.01	0.43
3:F:393:LEU:O	3:F:393:LEU:HD12	2.19	0.43
3:C:144:LEU:HD23	3:C:244:GLY:O	2.19	0.42
3:C:374:GLU:HG3	3:C:387:SER:HB3	2.01	0.42
3:C:390:GLU:O	3:C:391:ARG:HG2	2.19	0.42
1:D:379:PRO:HB3	1:D:381:TRP:NE1	2.34	0.42
3:F:131:ARG:NH1	3:F:234:GLU:OE1	2.46	0.42
3:F:426:ALA:N	3:F:427:PRO:HD3	2.34	0.42
1:A:307:GLY:HA2	1:A:523:THR:HG23	2.01	0.42
3:C:197:ARG:NH1	3:C:703:ASP:O	2.52	0.42
1:D:529:HIS:HA	1:D:546:PRO:HA	2.00	0.42
2:E:340:SER:O	2:E:343:PRO:HD2	2.18	0.42
2:E:680:ALA:HA	2:E:683:LYS:HE3	2.02	0.42
1:A:285:ILE:HG22	1:A:289:PHE:CD2	2.54	0.42
2:B:342:ALA:HB3	2:B:343:PRO:HD3	2.01	0.42
3:C:443:ILE:HD11	3:C:533:ILE:HG21	2.00	0.42
1:D:236:LEU:HD23	1:D:665:PHE:O	2.18	0.42
2:E:97:MET:HA	2:E:426:CYS:SG	2.58	0.42
3:F:472:THR:HG23	3:F:492:SER:HB3	2.00	0.42
1:A:164:LEU:O	1:A:168:ASN:N	2.52	0.42
1:A:338:GLU:HG2	3:F:254:ALA:CB	2.49	0.42
1:D:452:PHE:CD1	1:D:457:LYS:HD2	2.54	0.42
2:E:457:TRP:HA	2:E:460:ILE:HD12	2.01	0.42
3:F:414:MET:HE2	3:F:463:LEU:HD12	2.01	0.42
3:F:59:PHE:N	3:F:60:PRO:HD3	2.33	0.42
1:A:410:GLU:HG3	1:A:410:GLU:H	1.58	0.42
2:E:273:LEU:HB2	2:E:418:THR:HG21	2.01	0.42
2:E:427:TYR:CD2	2:E:431:GLU:HB2	2.54	0.42
3:F:122:TYR:CD1	3:F:213:MET:HG2	2.55	0.42
3:F:269:VAL:O	3:F:273:VAL:HG23	2.19	0.42
1:A:350:ILE:HB	2:B:368:VAL:HG22	2.01	0.42
2:B:584:ILE:HG21	2:B:590:LEU:HD21	2.01	0.42
3:C:150:ARG:CB	3:C:152:VAL:HG23	2.48	0.42
2:B:720:GLU:HG2	3:C:725:THR:HG22	2.02	0.42
2:E:251:ARG:N	2:E:252:PRO:HD2	2.35	0.42
1:A:244:ASN:O	1:A:705:PHE:HA	2.20	0.42
1:A:327:ARG:NE	1:A:329:MET:SD	2.93	0.42
2:B:4:ASN:HB3	2:B:7:LEU:HG	2.01	0.42
1:D:477:VAL:CG1	1:D:478:PRO:N	2.83	0.42
3:F:138:LYS:HE2	3:F:250:GLU:HG2	1.10	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:340:MET:CE	3:F:409:LEU:HD23	2.49	0.42
1:A:357:GLN:O	1:A:361:THR:N	2.46	0.42
3:C:147:ARG:N	3:C:227:VAL:O	2.39	0.42
1:D:112:ASP:OD1	1:D:112:ASP:N	2.53	0.42
1:D:145:PRO:O	1:D:150:LYS:HE3	2.20	0.42
1:D:236:LEU:HD12	1:D:237:PRO:HD2	2.02	0.42
2:E:487:LEU:CG	2:E:488:PRO:CD	2.87	0.42
2:E:576:ILE:O	2:E:579:GLU:HG2	2.19	0.42
3:F:714:VAL:HG22	3:F:750:PHE:CE2	2.55	0.42
3:F:412:MET:HE3	3:F:412:MET:HB3	1.92	0.42
1:A:246:PHE:O	1:A:247:ARG:HG2	2.20	0.42
2:B:363:ARG:HA	1:D:409:ASN:CB	2.50	0.42
2:B:359:LEU:HD11	2:B:378:TYR:CE2	2.55	0.42
3:C:195:GLU:O	3:C:199:LYS:HG2	2.20	0.42
3:C:695:LEU:HD11	3:C:734:PHE:CZ	2.51	0.42
1:D:681:ASN:HB3	1:D:684:CYS:HB3	2.02	0.42
2:E:150:VAL:HG12	2:E:154:LYS:HE3	2.02	0.42
2:E:304:ILE:HG22	2:E:485:GLY:HA3	2.02	0.42
3:F:81:ALA:O	3:F:82:LEU:HD23	2.20	0.42
1:A:170:PHE:O	1:A:173:ILE:HG22	2.20	0.41
1:A:430:ASN:O	1:A:433:ARG:HB3	2.20	0.41
1:A:569:ARG:NH2	2:B:514:THR:HG21	2.35	0.41
3:C:626:GLN:O	3:C:632:TYR:HB3	2.19	0.41
2:E:302:VAL:HG22	2:E:486:SER:O	2.20	0.41
2:E:660:HIS:HE1	3:F:106:ASN:HD21	1.66	0.41
3:F:138:LYS:HZ1	3:F:250:GLU:CG	2.25	0.41
3:F:299:ILE:HG22	3:F:300:GLY:N	2.35	0.41
3:F:693:VAL:HG23	3:F:694:PRO:HD3	2.01	0.41
1:D:598:LEU:HD23	1:D:617:LEU:HD23	2.02	0.41
3:F:138:LYS:HE2	3:F:250:GLU:OE2	2.04	0.41
3:F:739:ARG:HA	3:F:749:THR:HG22	2.01	0.41
1:A:521:LYS:HD2	1:A:552:ARG:NH1	2.35	0.41
1:A:671:LEU:HA	1:A:674:ILE:HD12	2.02	0.41
2:B:491:PHE:CE2	2:B:498:PHE:CD2	3.08	0.41
3:C:734:PHE:HA	3:C:752:ARG:HG3	2.02	0.41
3:C:739:ARG:HA	3:C:749:THR:HG22	2.01	0.41
3:C:737:LYS:HA	3:C:750:PHE:O	2.20	0.41
3:F:117:VAL:O	3:F:121:VAL:HG23	2.20	0.41
2:B:364:LYS:HD3	2:B:364:LYS:HA	1.95	0.41
1:D:646:GLN:HA	1:D:649:ILE:HD12	2.03	0.41
2:E:493:PHE:O	2:E:496:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:138:LYS:HZ3	3:F:250:GLU:CG	2.04	0.41
1:A:452:PHE:CD1	1:A:457:LYS:HD2	2.55	0.41
1:A:280:SER:OG	1:A:464:ARG:NH2	2.53	0.41
1:D:302:ASP:O	1:D:304:PRO:HD3	2.21	0.41
1:D:510:SER:O	1:D:547:LEU:HD12	2.20	0.41
1:D:504:ILE:HG22	1:D:554:THR:O	2.20	0.41
1:D:5:PHE:HA	1:D:8:ILE:HD12	2.02	0.41
3:F:467:ARG:HD3	3:F:467:ARG:HA	1.93	0.41
1:A:364:GLY:O	2:B:361:ASN:HB3	2.21	0.41
3:C:398:ILE:O	3:C:499:GLN:N	2.45	0.41
1:D:316:LEU:HD23	1:D:507:PHE:CZ	2.55	0.41
1:D:469:LYS:CD	1:D:475:LEU:CD1	2.95	0.41
3:F:139:GLU:O	3:F:139:GLU:HG2	2.20	0.41
3:F:322:LEU:O	3:F:325:SER:OG	2.29	0.41
3:F:324:LYS:NZ	3:F:331:LEU:HD22	2.35	0.41
3:F:452:TRP:CE3	3:F:453:ILE:HG13	2.55	0.41
3:F:758:ALA:O	3:F:762:ASP:HB2	2.20	0.41
3:F:76:GLU:HG2	3:F:77:HIS:H	1.86	0.41
1:A:201:LEU:HD21	2:B:87:ILE:HD11	2.03	0.41
3:F:195:GLU:O	3:F:199:LYS:HG2	2.20	0.41
1:A:89:PRO:HG2	1:A:90:PHE:HD1	1.86	0.41
1:A:99:GLU:OE2	1:A:128:LYS:NZ	2.50	0.41
2:B:150:VAL:HG12	2:B:154:LYS:HE3	2.03	0.41
2:B:663:ARG:O	3:C:62:ILE:HD12	2.20	0.41
3:C:76:GLU:HG3	3:C:82:LEU:HD11	2.01	0.41
1:D:134:TYR:HB3	1:D:161:ALA:HB2	2.02	0.41
3:F:272:LYS:NZ	3:F:543:THR:HG23	2.36	0.41
2:B:304:ILE:HG13	2:B:450:LEU:HB3	2.02	0.41
2:E:491:PHE:CD1	2:E:492:GLU:N	2.89	0.41
2:E:55:GLU:HG3	2:E:66:ARG:HG3	2.02	0.41
3:F:753:THR:HG22	3:F:754:ALA:N	2.36	0.41
1:A:431:CYS:SG	1:A:626:VAL:HG22	2.60	0.41
3:C:124:SER:O	3:C:128:ARG:HG3	2.21	0.41
3:F:595:TYR:CZ	3:F:620:ARG:HG3	2.56	0.41
1:A:229:GLN:O	1:A:233:ASN:HB2	2.21	0.41
1:A:245:LYS:HA	1:A:706:PHE:CB	2.51	0.41
1:A:441:THR:HG21	1:A:461:ILE:HA	2.03	0.41
1:A:287:ILE:HG21	1:A:460:PRO:HB3	2.03	0.41
2:E:632:PHE:CE1	3:F:102:ILE:HG23	2.56	0.41
3:F:202:ASN:O	3:F:204:PRO:HD3	2.21	0.41
3:F:236:MET:SD	3:F:239:ILE:HD11	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:332:GLY:HA3	3:F:512:ILE:HG22	2.02	0.41
1:A:391:LYS:O	1:A:430:ASN:ND2	2.49	0.40
3:C:479:SER:HB2	3:C:497:THR:HB	2.02	0.40
1:D:355:LEU:HG	2:E:368:VAL:HG11	2.03	0.40
3:C:582:ILE:N	3:C:583:PRO:HD2	2.36	0.40
1:D:101:GLN:NE2	1:D:128:LYS:HE3	2.36	0.40
1:D:320:ILE:HG21	1:D:487:ILE:HG21	2.03	0.40
3:F:288:LEU:O	3:F:292:ILE:HG12	2.21	0.40
1:A:302:ASP:O	1:A:304:PRO:HD3	2.20	0.40
1:A:586:SER:HB2	1:A:591:GLU:O	2.21	0.40
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.94	0.40
3:C:299:ILE:N	3:C:302:THR:O	2.52	0.40
1:A:154:PHE:HB3	3:C:714:VAL:HB	2.03	0.40
1:D:396:THR:HG21	1:D:468:ARG:HG3	2.01	0.40
2:E:404:LEU:HA	2:E:405:PRO:HD3	1.79	0.40
3:F:390:GLU:O	3:F:391:ARG:HG2	2.21	0.40
3:F:398:ILE:O	3:F:499:GLN:N	2.45	0.40
3:F:578:GLY:HA2	3:F:734:PHE:CD2	2.57	0.40
2:B:346:PHE:HA	2:B:349:LYS:HB3	2.04	0.40
2:B:580:PHE:HD1	3:C:107:PHE:HB2	1.86	0.40
3:C:639:LYS:HD3	3:C:674:PHE:CD1	2.56	0.40
1:D:235:LYS:NZ	2:E:464:ILE:HG22	2.36	0.40
2:E:4:ASN:HB3	2:E:7:LEU:HG	2.03	0.40
3:F:175:PHE:HE1	3:F:177:ASP:HB2	1.86	0.40
3:F:263:LYS:HA	3:F:266:ILE:HD12	2.04	0.40
2:B:420:LEU:HD11	2:B:474:ILE:HD12	2.04	0.40
3:C:243:GLY:HA2	3:C:247:TRP:HB2	2.02	0.40
3:C:267:ARG:CZ	3:C:317:SER:HB2	2.52	0.40
3:C:697:VAL:C	3:C:698:GLY:O	2.59	0.40
1:A:17:ALA:HB2	3:C:763:VAL:HG11	2.02	0.40
1:D:140:LYS:HZ1	1:D:150:LYS:HE2	1.86	0.40
2:E:105:PHE:HE2	2:E:264:ILE:HG23	1.85	0.40
3:F:479:SER:HB2	3:F:497:THR:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	685/709 (97%)	643 (94%)	42 (6%)	0	100	100
1	D	685/709 (97%)	645 (94%)	40 (6%)	0	100	100
2	B	703/754 (93%)	666 (95%)	35 (5%)	2 (0%)	41	75
2	E	703/754 (93%)	673 (96%)	27 (4%)	3 (0%)	34	71
3	C	756/782 (97%)	688 (91%)	63 (8%)	5 (1%)	22	60
3	F	756/782 (97%)	686 (91%)	67 (9%)	3 (0%)	34	71
All	All	4288/4490 (96%)	4001 (93%)	274 (6%)	13 (0%)	41	75

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	405	PRO
3	C	698	GLY
2	E	405	PRO
2	B	503	VAL
2	E	503	VAL
3	F	550	GLN
3	C	428	ALA
3	C	533	ILE
3	C	550	GLN
3	F	428	ALA
3	F	533	ILE
2	E	23	PRO
3	C	47	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	618/631 (98%)	603 (98%)	15 (2%)	49	69
1	D	618/631 (98%)	608 (98%)	10 (2%)	62	79
2	B	629/669 (94%)	620 (99%)	9 (1%)	67	81
2	E	629/669 (94%)	618 (98%)	11 (2%)	60	78
3	C	669/686 (98%)	660 (99%)	9 (1%)	69	82
3	F	669/686 (98%)	655 (98%)	14 (2%)	53	73
All	All	3832/3972 (96%)	3764 (98%)	68 (2%)	59	77

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	163	PHE
1	A	170	PHE
1	A	220	PRO
1	A	276	ASP
1	A	366	LYS
1	A	410	GLU
1	A	468	ARG
1	A	471	MET
1	A	475	LEU
1	A	477	VAL
1	A	482	ASP
1	A	490	LYS
1	A	506	THR
1	A	554	THR
2	B	68	PHE
2	B	166	LEU
2	B	273	LEU
2	B	279	GLU
2	B	302	VAL
2	B	362	LYS
2	B	491	PHE
2	B	502	PHE
2	B	540	LEU
3	C	4	LEU
3	C	103	ASN
3	C	135	ILE

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Mol	Chain	Res	Type
3	C	160	ARG
3	C	175	PHE
3	C	445	TYR
3	C	450	MET
3	C	594	LEU
3	C	611	ARG
1	D	38	ILE
1	D	48	PHE
1	D	163	PHE
1	D	170	PHE
1	D	276	ASP
1	D	366	LYS
1	D	410	GLU
1	D	490	LYS
1	D	506	THR
1	D	554	THR
2	E	68	PHE
2	E	89	SER
2	E	166	LEU
2	E	273	LEU
2	E	279	GLU
2	E	302	VAL
2	E	362	LYS
2	E	491	PHE
2	E	502	PHE
2	E	540	LEU
2	E	657	VAL
3	F	4	LEU
3	F	103	ASN
3	F	135	ILE
3	F	152	VAL
3	F	160	ARG
3	F	175	PHE
3	F	270	CYS
3	F	323	CYS
3	F	445	TYR
3	F	450	MET
3	F	594	LEU
3	F	611	ARG
3	F	695	LEU
3	F	725	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	101	GLN
1	A	141	ASN
1	A	494	HIS
1	A	519	HIS
1	A	561	ASN
1	A	635	ASN
1	A	644	ASN
1	A	680	ASN
2	B	147	GLN
2	B	303	ASN
2	B	461	HIS
2	B	537	ASN
2	B	627	ASN
2	B	660	HIS
2	B	686	GLN
3	C	148	GLN
3	C	550	GLN
3	C	717	ASN
1	D	31	HIS
1	D	101	GLN
1	D	141	ASN
1	D	494	HIS
1	D	519	HIS
1	D	561	ASN
1	D	680	ASN
2	E	303	ASN
2	E	315	GLN
2	E	316	GLN
2	E	477	ASN
2	E	537	ASN
2	E	627	ASN
2	E	660	HIS
2	E	686	GLN
3	F	148	GLN
3	F	550	GLN
3	F	717	ASN
3	F	744	GLN
3	F	756	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	693/709 (97%)	-0.05	17 (2%)	57	47	132, 195, 269, 299	0
1	D	693/709 (97%)	-0.11	5 (0%)	87	82	129, 191, 258, 295	0
2	B	711/754 (94%)	-0.03	13 (1%)	68	59	131, 192, 256, 317	0
2	E	711/754 (94%)	0.06	26 (3%)	41	32	130, 184, 266, 315	0
3	C	762/782 (97%)	0.01	23 (3%)	50	38	149, 222, 285, 358	0
3	F	762/782 (97%)	0.13	24 (3%)	49	38	134, 224, 287, 343	0
All	All	4332/4490 (96%)	0.00	108 (2%)	57	47	129, 202, 275, 358	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	242	ALA	6.2
2	E	237	LYS	5.3
3	F	631	HIS	4.8
3	C	1	MET	4.8
3	C	696	VAL	4.6
1	A	499	ASP	4.5
3	C	703	ASP	4.4
2	B	441	GLY	4.4
2	E	497	PHE	4.3
1	D	499	ASP	4.3
2	E	241	ARG	4.1
3	F	630	GLY	4.1
2	E	25	THR	3.8
2	B	237	LYS	3.8
3	F	695	LEU	3.8
3	C	282	MET	3.7
2	E	441	GLY	3.6
3	F	687	HIS	3.6
2	B	25	THR	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	365	GLN	3.6
1	A	95	PHE	3.5
3	F	696	VAL	3.5
2	E	502	PHE	3.4
2	B	504	SER	3.4
3	F	703	ASP	3.4
2	B	443	GLN	3.3
2	E	498	PHE	3.3
2	B	502	PHE	3.1
2	E	231	LYS	3.1
2	B	236	GLY	3.0
3	F	149	ARG	3.0
3	C	149	ARG	3.0
3	F	594	LEU	3.0
1	A	63	LEU	3.0
1	A	102	PHE	2.9
3	F	629	THR	2.9
2	E	449	VAL	2.9
1	A	386	TRP	2.9
2	E	230	ALA	2.9
3	F	586	ILE	2.9
3	C	439	LEU	2.9
3	C	574	ARG	2.8
3	C	200	PHE	2.8
3	F	431	THR	2.8
2	B	490	LEU	2.8
3	C	767	VAL	2.8
2	E	32	HIS	2.7
2	E	492	GLU	2.7
2	E	491	PHE	2.7
3	F	571	LEU	2.6
1	A	132	PHE	2.6
3	C	284	ALA	2.6
3	C	594	LEU	2.6
3	C	95	VAL	2.6
3	C	443	ILE	2.6
2	E	504	SER	2.6
3	C	687	HIS	2.6
2	E	29	PRO	2.6
2	E	442	LEU	2.6
2	E	232	ASP	2.6
2	E	490	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	35	ILE	2.5
3	F	357	TYR	2.5
2	B	442	LEU	2.4
3	C	702	MET	2.4
3	F	91	LYS	2.4
2	E	239	GLN	2.4
2	B	497	PHE	2.3
2	E	236	GLY	2.3
3	C	328	GLY	2.3
3	F	652	MET	2.3
1	A	62	VAL	2.3
1	A	64	ILE	2.3
2	E	451	PHE	2.3
2	B	23	PRO	2.3
1	A	123	LEU	2.3
3	F	204	PRO	2.3
3	C	523	PHE	2.2
1	A	100	LYS	2.2
3	C	367	GLU	2.2
3	F	700	GLU	2.2
2	E	238	LEU	2.2
3	C	355	THR	2.2
1	A	522	TYR	2.2
2	B	22	TYR	2.2
3	F	689	ILE	2.2
2	B	231	LYS	2.2
1	D	468	ARG	2.2
3	C	642	PRO	2.2
1	A	101	GLN	2.1
1	A	91	LEU	2.1
3	C	41	SER	2.1
2	E	190	VAL	2.1
1	D	525	PHE	2.1
3	F	432	MET	2.1
1	A	134	TYR	2.1
3	F	685	TYR	2.1
3	F	702	MET	2.1
1	A	651	MET	2.1
3	F	148	GLN	2.1
3	C	431	THR	2.1
3	F	665	VAL	2.1
1	A	665	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	625	THR	2.0
1	D	651	MET	2.0
2	E	506	LEU	2.0
1	A	67	ARG	2.0
2	E	452	ALA	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 carbohydrates 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
4	MG	A	800	1/1	0.89	0.07	204,204,204,204	0
4	MG	D	801	1/1	0.89	0.16	182,182,182,182	0
4	MG	D	800	1/1	0.94	0.10	200,200,200,200	0
4	MG	A	801	1/1	0.94	0.10	185,185,185,185	0

6.5 Other polymers (i)

There are no such residues in this entry.