



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 11:54 am GMT

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 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:

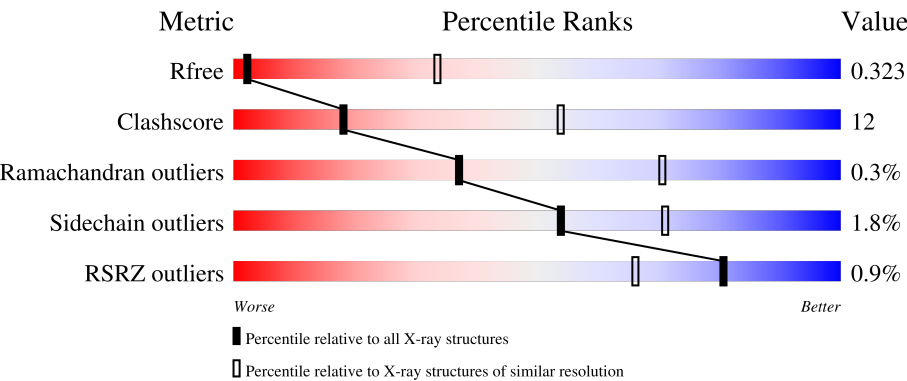
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 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}	164625	1157 (4.10-3.70)
Clashscore	180529	1219 (4.10-3.70)
Ramachandran outliers	177936	1177 (4.10-3.70)
Sidechain outliers	177891	1169 (4.10-3.70)
RSRZ outliers	164620	1157 (4.10-3.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	709	<div><div></div><div>67%30%..</div></div>
1	D	709	<div><div>%</div><div>68%29%..</div></div>
2	B	754	<div><div>%</div><div>74%19%6%</div></div>
2	E	754	<div><div>%</div><div>73%20%6%</div></div>
3	C	782	<div><div>%</div><div>70%26%..</div></div>

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Mol	Chain	Length	Quality of chain
3	F	782	<div><div><div>%</div><div><div></div></div><div>67%</div><div>29%</div><div>..</div></div></div>

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

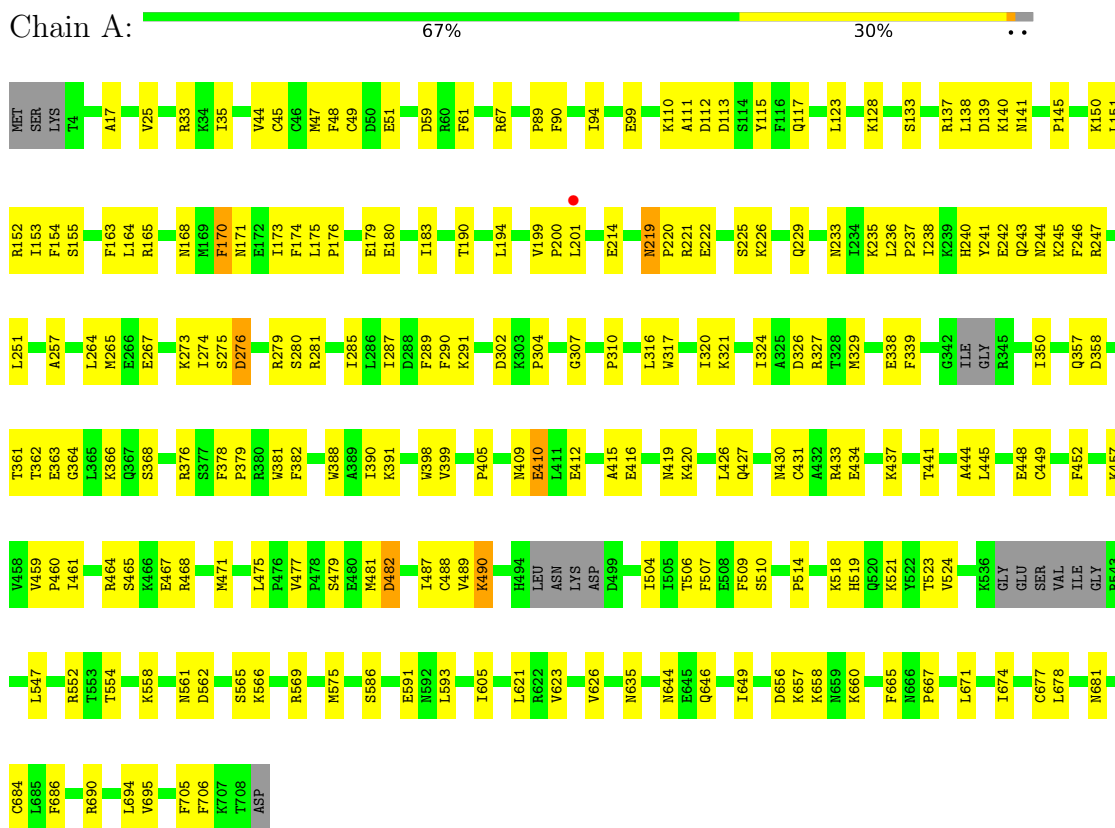
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

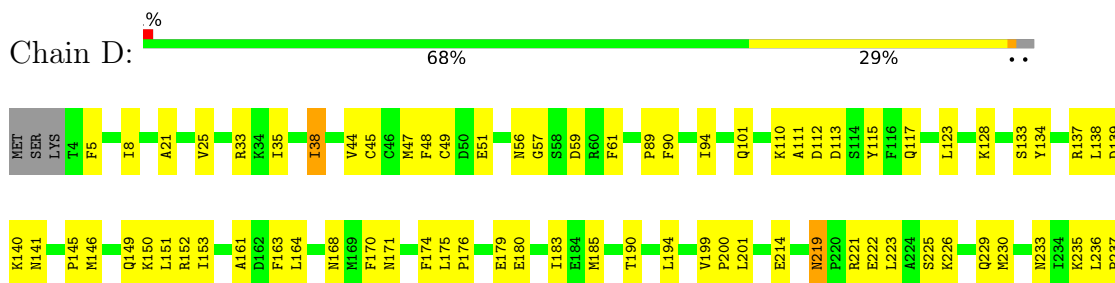
3 Residue-property plots

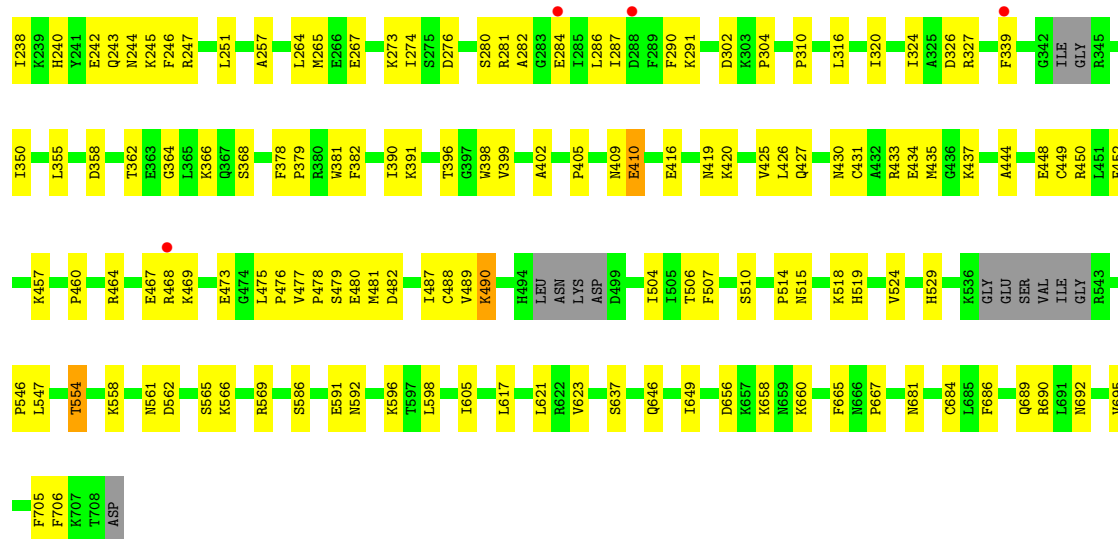
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Polymerase acidic protein

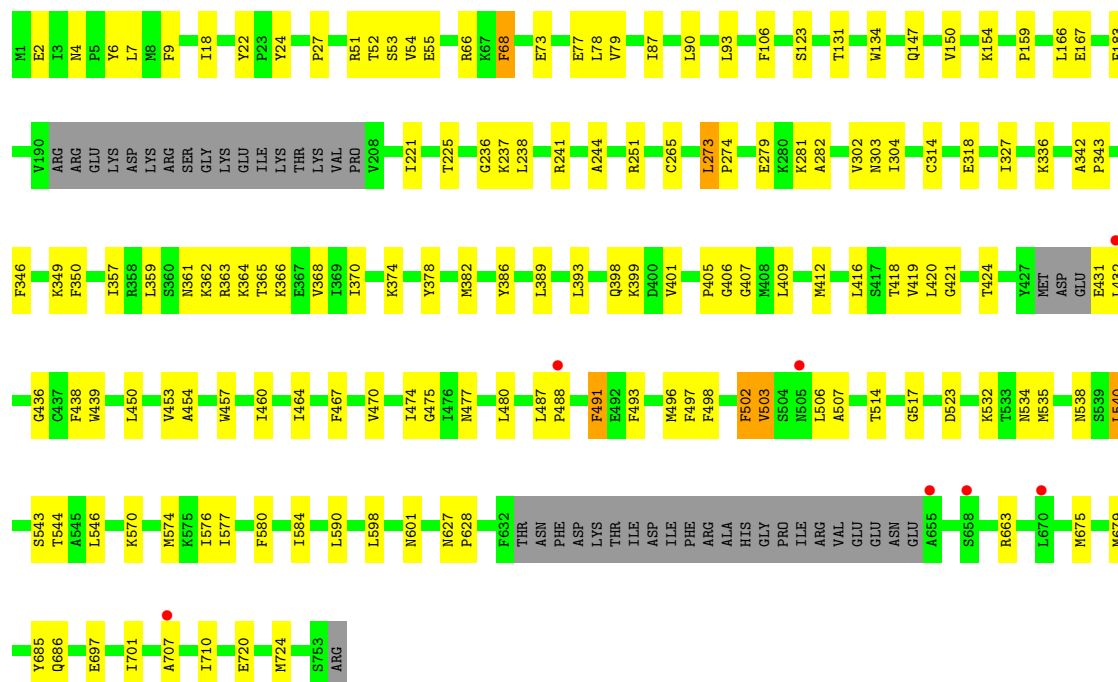
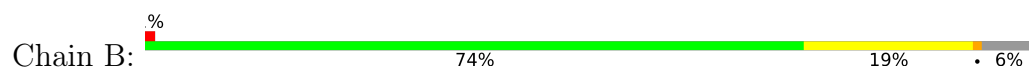


• Molecule 1: Polymerase acidic protein

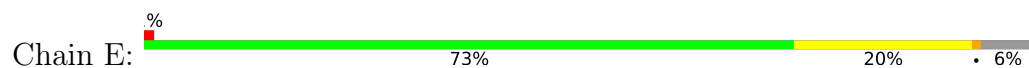


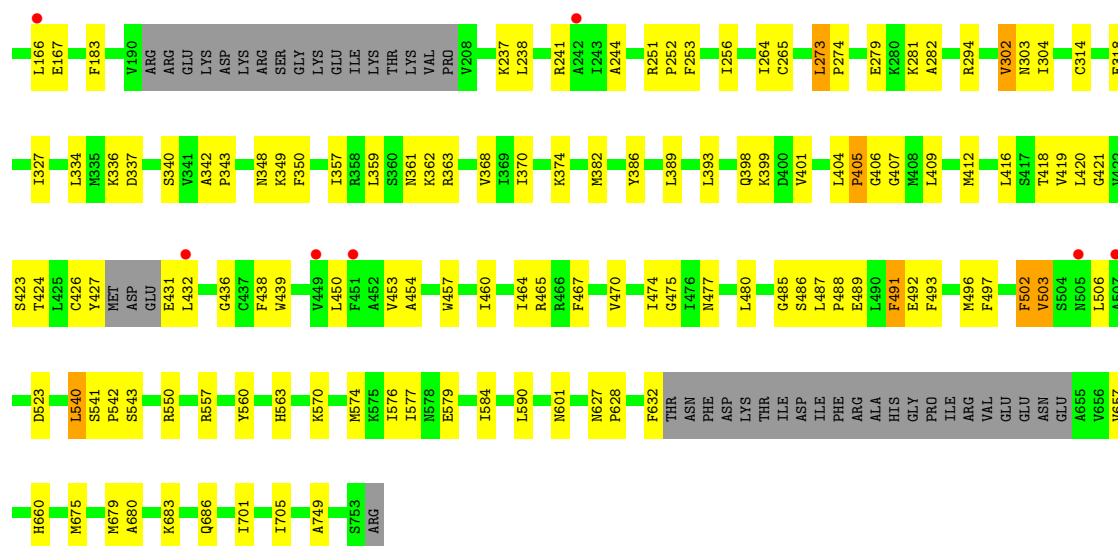


• Molecule 2: RNA-directed RNA polymerase catalytic subunit



• Molecule 2: RNA-directed RNA polymerase catalytic subunit





• Molecule 3: Polymerase basic protein 2



• Molecule 3: Polymerase basic protein 2



GLN	G688	Q550	P427	K343	I239	H1
	I691	H551	A428	S346	W247	L4
	R692	P552	T429	G349	I248	Q16
	V693	D553	K438	V350	E250	T28
	P694	L554	R441	K351	T253	V29
	L695	T665	P444	T355	A254	K37
	Y696	L575	Y445	I358	K263	W38
	D703	G578	V448	GLN	W264	T39
	T704	M449	M449	GLY	D265	L49
	S713	M450	M450	VAL	I266	R52
	V714	P583	M451	ARG	R267	W53
	C715	I586	W452	ALA	A268	S56
	E716	I586	I453	VAL	V269	S57
	H717	Y591	L463	Q365	C270	A58
	D718	L594	S466	W369	R271	F59
	P719	Y595	R467	S370	K272	P60
	K720	V600	G468	E371	V273	E76
	A721	V600	I469	E374	L275	H77
	T725	I607	T472	S381	A277	V80
	F734	R611	K476	A384	S280	A81
	K737	K612	S479	S387	N283	L82
	V738	G613	S480	E390	K287	E87
	R739	V614	S492	R391	L288	ASP
	F741	R620	L493	S392	T292	VAL
	Q744	Q626	T497	L393	R298	SER
	V747	V627	I498	E394	T299	K91
	R748	Y632	Q499	W395	G300	I102
	T749	S633	I503	L396	E308	M103
	F750	L634	D504	I397	L309	N106
	K751	L637	I512	I398	I310	C111
	R752	P642	H513	D405	S317	V117
	T753	F643	S517	K406	F316	V121
	A754	T644	E521	L409	E319	Y122
	A758	G651	E521	L410	V320	K123
	D762	F658	A531	M412	T321	S124
	K769	N670	T532	C413	L322	R125
	I770	W676	I533	M414	C323	F126
	K771	L534	L534	I415	K324	G127
HET	SER	ALA	L536	F416	S325	R128
SER	ASN	ALA	L536	C417	Q330	L129
ASN	ALA	ARG	L536	R418	L331	F130
ARG	ALA	L536	L536	C419	G332	R131
GLU	GLU	S681	P537	D419	K333	I135
ASN	ASN	I684	T543	Y422	M340	M136
LEU	LEU	Y685	V547	A426		
TYR	TYR					
PHE	PHE					

4 Data and refinement statistics

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 50.01 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.01-3.90) 98.8 (50.01-3.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	4770 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)	0.29 , 156.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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(°)	Ideal(°)
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:HD23	3:C:174:LEU:C	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:583:PRO:CB	3:C:695:LEU:HD13	2.27	0.63
3:C:693:VAL:N	3:C:694:PRO:CD	2.62	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:OE1	1:A:242:GLU:N	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:51:ARG:NH2	2:B:77:GLU:O	2.39	0.56
3:F:174:LEU:HD23	3:F:174:LEU:O	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:338:GLU:HG2	3:F:254:ALA:HB1	1.88	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
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:HD23	3:C:174:LEU:O	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:274:ILE:HA	1:A:481:MET:HB3	1.90	0.53
1:A:409:ASN:OD1	1:A:409:ASN:N	2.41	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
2:E:294:ARG:HG3	3:F:395:TRP:CH2	2.43	0.53
3:F:271:ARG:O	3:F:275:LEU:HG	2.09	0.53
3:C:565:THR:HG22	3:C:685:TYR:HB3	1.90	0.53
3:C:575:LEU:HD13	3:C:582:ILE:HG13	1.91	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:O	3:C:551:HIS:ND1	2.43	0.51
3:F:393:LEU:HD22	3:F:396:ILE:HD11	1.92	0.51
2:B:359:LEU:HB2	2:B:368:VAL:HB	1.92	0.51
2:B:361:ASN:C	2:B:363:ARG:H	2.14	0.51
2:E:79:VAL:HB	2:E:480:LEU:HD11	1.92	0.51
2:E:244:ALA:HB3	2:E:409:LEU:HD13	1.91	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:155:SER:HB3	3:C:713:SER:OG	2.11	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: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
2:B:363:ARG:HD3	3:F:139:GLU:CD	2.32	0.49
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
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:287:ILE:CG2	1:A:460:PRO:HB3	2.43	0.49
1:A:416:GLU:HG2	1:A:420:LYS:HE2	1.94	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
1:A:361:THR:HG21	1:D:596:LYS:HE2	1.94	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
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:151:LEU:O	3:C:713:SER:OG	2.31	0.47
1:A:265:MET:HG2	1:A:434:GLU:HG2	1.95	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
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:128:LYS:HA	1:D:141:ASN:HD22	1.79	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:131:ARG:NH1	3:F:237:GLU:OE1	2.48	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
3:F:531:ALA:O	3:F:532:THR:CG2	2.60	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:115:TYR:CZ	1:A:175:LEU:HD12	2.50	0.46
1:A:165:ARG:HE	1:A:170:PHE:HZ	1.62	0.46
2:B:22:TYR:HB3	2:B:24:TYR:CD1	2.50	0.46
3:C:272:LYS:HE2	3:C:541:LYS:HA	1.97	0.46
3:C:393:LEU:HD21	3:C:467:ARG:CZ	2.45	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:76:GLU:OE2	3:F:80:VAL:HB	2.15	0.46
3:F:351:LYS:HG2	3:F:369:TRP:NE1	2.30	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:OD1	3:F:103:ASN:N	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:89:PRO:HG2	1:D:90:PHE:HD1	1.81	0.46
1:D:229:GLN:O	1:D:233:ASN:HB2	2.15	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:303:ASN:ND2	2:E:488:PRO:HA	2.30	0.46
2:E:350:PHE:HB3	2:E:401:VAL:CG2	2.44	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
1:D:185:MET:CE	2:E:337:ASP:HB3	2.46	0.46
2:E:18:ILE:CD1	2:E:497:PHE:CG	2.97	0.46
2:B:363:ARG:O	1:D:409:ASN:ND2	2.48	0.46
1:D:183:ILE:HD13	2:E:334:LEU:HD13	1.98	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
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:76:GLU:OE2	3:C:80:VAL:HB	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
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:272:LYS:HZ2	3:F:543:THR:HG23	1.81	0.45
3:F:419:ASP:OD2	3:F:467:ARG:NH1	2.49	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:59:PHE:N	3:C:60:PRO:HD3	2.32	0.45
3:C:272:LYS:NZ	3:C:543:THR:HG23	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:384:ALA:HA	3:F:503:ILE:HD12	1.97	0.45
3:F:469:ILE:HG22	3:F:493:LEU:HD13	1.98	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:67:ARG:NH1	3:C:770:ILE:HA	2.32	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
2:E:749:ALA:HB1	3:F:16:GLN:HA	1.99	0.45
3:F:197:ARG:HD3	3:F:704:THR:HG22	1.97	0.45
3:F:330:GLN:HG3	3:F:513:HIS:HB2	1.99	0.45
1:A:190:THR:O	1:A:194:LEU:HD13	2.17	0.44
1:A:405:PRO:HB3	2:B:598:LEU:HG	1.98	0.44
1:A:665:PHE:HB2	2:B:480:LEU:O	2.17	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:28:THR:OG1	3:F:29:VAL:N	2.51	0.44
3:F:174:LEU:CD2	3:F:175:PHE:HB2	2.48	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:N	3:F:139:GLU:OE1	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:24:TYR:CD1	2:B:507:ALA:HB1	2.54	0.43
2:B:475:GLY:O	2:B:477:ASN:ND2	2.51	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:N	3:C:103:ASN:OD1	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:410:GLU:HA	3:F:139:GLU:HB3	2.00	0.43
1:D:430:ASN:O	1:D:433:ARG:HB3	2.18	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:H	1:D:410:GLU:HG3	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:OE1	3:C:700:GLU:N	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:HD12	3:F:393:LEU:O	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:59:PHE:N	3:F:60:PRO:HD3	2.33	0.42
3:F:414:MET:HE2	3:F:463:LEU:HD12	2.01	0.42
1:A:410:GLU:H	1:A:410:GLU:HG3	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
2:B:720:GLU:HG2	3:C:725:THR:HG22	2.02	0.42
3:C:150:ARG:CB	3:C:152:VAL:HG23	2.48	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:N	1:D:112:ASP:OD1	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:359:LEU:HD11	2:B:378:TYR:CE2	2.55	0.42
2:B:363:ARG:HA	1:D:409:ASN:CB	2.50	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:737:LYS:HA	3:C:750:PHE:O	2.20	0.41
3:C:739:ARG:HA	3:C:749:THR:HG22	2.01	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:280:SER:OG	1:A:464:ARG:NH2	2.53	0.41
1:A:452:PHE:CD1	1:A:457:LYS:HD2	2.55	0.41
1:D:5:PHE:HA	1:D:8:ILE:HD12	2.02	0.41
1:D:302:ASP:O	1:D:304:PRO:HD3	2.21	0.41
1:D:504:ILE:HG22	1:D:554:THR:O	2.20	0.41
1:D:510:SER:O	1:D:547:LEU:HD12	2.20	0.41
3:F:467:ARG:HA	3:F:467:ARG:HD3	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:76:GLU:HG2	3:F:77:HIS:H	1.86	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
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
1:A:431:CYS:SG	1:A:626:VAL:HG22	2.60	0.41
2:B:304:ILE:HG13	2:B:450:LEU:HB3	2.02	0.41
3:C:124:SER:O	3:C:128:ARG:HG3	2.21	0.41
2:E:55:GLU:HG3	2:E:66:ARG:HG3	2.02	0.41
2:E:491:PHE:CD1	2:E:492:GLU:N	2.89	0.41
3:F:595:TYR:CZ	3:F:620:ARG:HG3	2.56	0.41
3:F:753:THR:HG22	3:F:754:ALA:N	2.36	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:287:ILE:HG21	1:A:460:PRO:HB3	2.03	0.41
1:A:441:THR:HG21	1:A:461:ILE:HA	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:154:PHE:HB3	3:C:714:VAL:HB	2.03	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: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
1:A:17:ALA:HB2	3:C:763:VAL:HG11	2.02	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: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%)	37	70
2	E	703/754 (93%)	673 (96%)	27 (4%)	3 (0%)	30	65
3	C	756/782 (97%)	688 (91%)	63 (8%)	5 (1%)	19	54
3	F	756/782 (97%)	686 (91%)	67 (9%)	3 (0%)	30	65
All	All	4288/4490 (96%)	4001 (93%)	274 (6%)	13 (0%)	37	70

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%)	44	63
1	D	618/631 (98%)	608 (98%)	10 (2%)	58	73
2	B	629/669 (94%)	620 (99%)	9 (1%)	62	75
2	E	629/669 (94%)	618 (98%)	11 (2%)	56	72
3	C	669/686 (98%)	660 (99%)	9 (1%)	65	76
3	F	669/686 (98%)	655 (98%)	14 (2%)	48	67
All	All	3832/3972 (96%)	3764 (98%)	68 (2%)	54	71

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

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	693/709 (97%)	-0.46	1 (0%)	92 89	132, 195, 269, 299	0
1	D	693/709 (97%)	-0.36	4 (0%)	85 73	129, 191, 258, 295	0
2	B	711/754 (94%)	-0.45	7 (0%)	79 64	131, 192, 256, 317	0
2	E	711/754 (94%)	-0.37	8 (1%)	77 62	130, 184, 266, 315	0
3	C	762/782 (97%)	-0.23	10 (1%)	74 58	149, 222, 285, 358	0
3	F	762/782 (97%)	-0.14	10 (1%)	74 58	134, 224, 287, 343	0
All	All	4332/4490 (96%)	-0.33	40 (0%)	81 66	129, 202, 275, 358	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	695	LEU	5.0
3	C	696	VAL	4.0
2	E	242	ALA	3.7
2	E	166	LEU	3.4
3	F	586	ILE	3.1
3	F	358	ILE	3.0
2	E	505	ASN	3.0
2	E	451	PHE	2.9
3	F	141	ARG	2.9
3	C	170	GLN	2.9
3	C	695	LEU	2.8
3	C	200	PHE	2.8
3	F	429	THR	2.8
3	C	767	VAL	2.8
1	A	201	LEU	2.6
1	D	284	GLU	2.5
2	E	432	LEU	2.5
3	F	200	PHE	2.4
3	C	252	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	339	PHE	2.4
2	B	505	ASN	2.4
2	B	670	LEU	2.4
2	B	658	SER	2.4
3	F	750	PHE	2.3
1	D	288	ASP	2.3
2	B	432	LEU	2.3
3	F	696	VAL	2.3
3	F	202	ASN	2.2
2	E	507	ALA	2.2
3	F	37	LYS	2.2
2	B	655	ALA	2.2
2	E	89	SER	2.2
1	D	468	ARG	2.1
3	C	390	GLU	2.1
3	C	215	GLU	2.1
3	C	358	ILE	2.1
2	E	449	VAL	2.1
2	B	707	ALA	2.0
3	C	183	SER	2.0
2	B	488	PRO	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, 95th 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(\AA^2)	Q<0.9
4	MG	D	800	1/1	0.72	0.15	200,200,200,200	0
4	MG	A	800	1/1	0.74	0.10	204,204,204,204	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	D	801	1/1	0.74	0.14	182,182,182,182	0
4	MG	A	801	1/1	0.93	0.06	185,185,185,185	0

6.5 Other polymers [i](#)

There are no such residues in this entry.