



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:33 PM UTC

PDB ID : 5D98 / pdb_00005d98
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

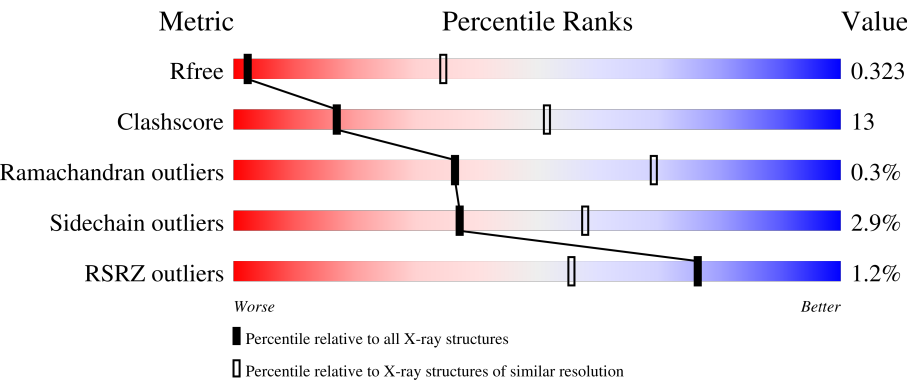
1 Overall quality at a glance i

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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (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	66%31%..
1	D	709	% 66%30%..
2	B	754	% 71%22%6%
2	E	754	% 70%22%6%
3	C	782	% 69%27%. .

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Mol	Chain	Length	Quality of chain
3	F	782	% 67% 29%

2 Entry composition [i](#)

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

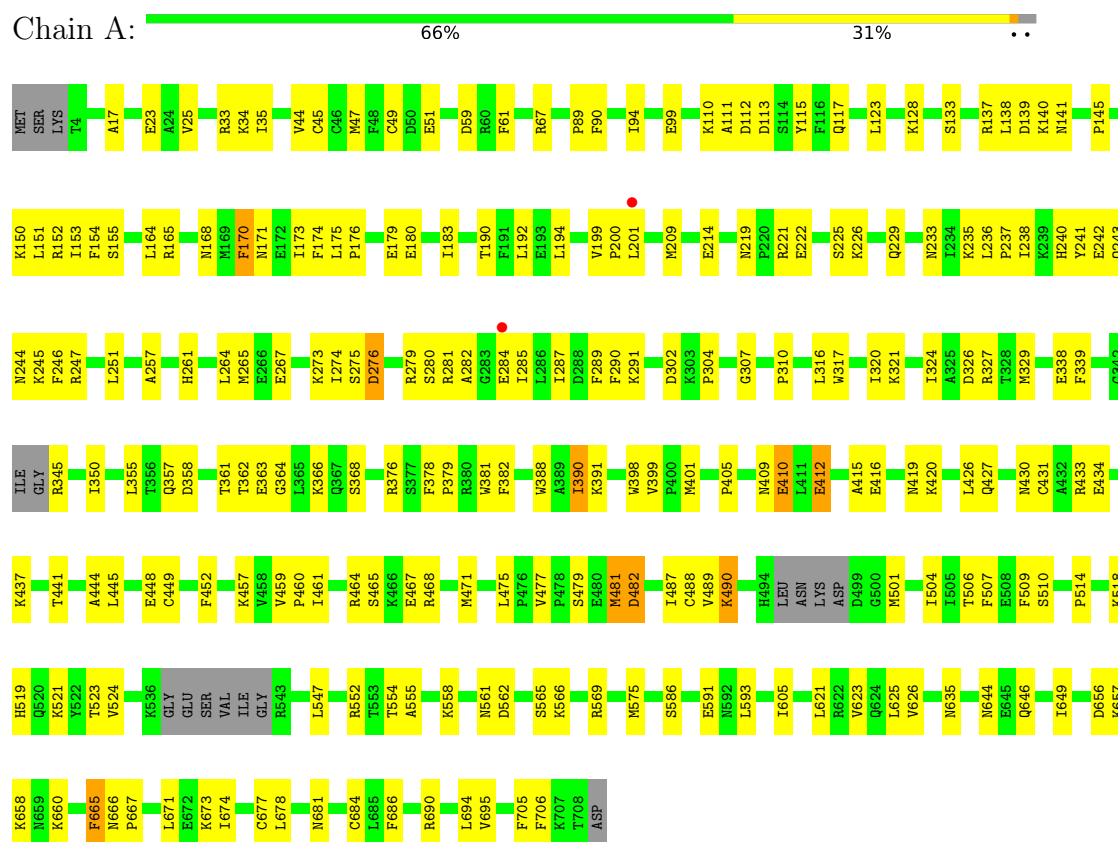
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

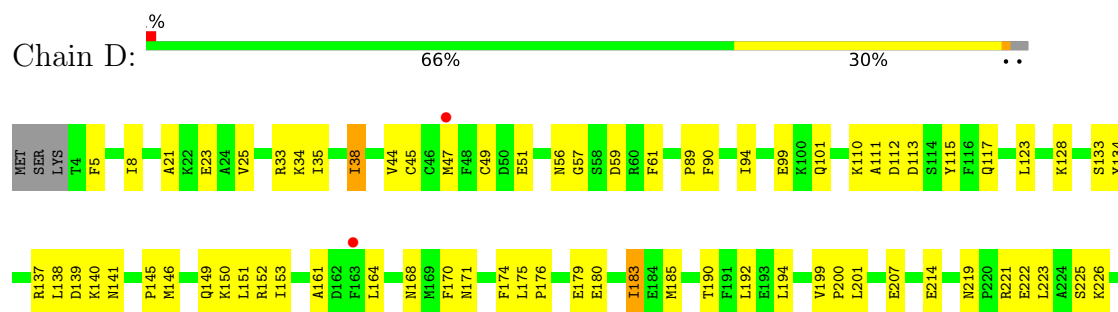
3 Residue-property plots

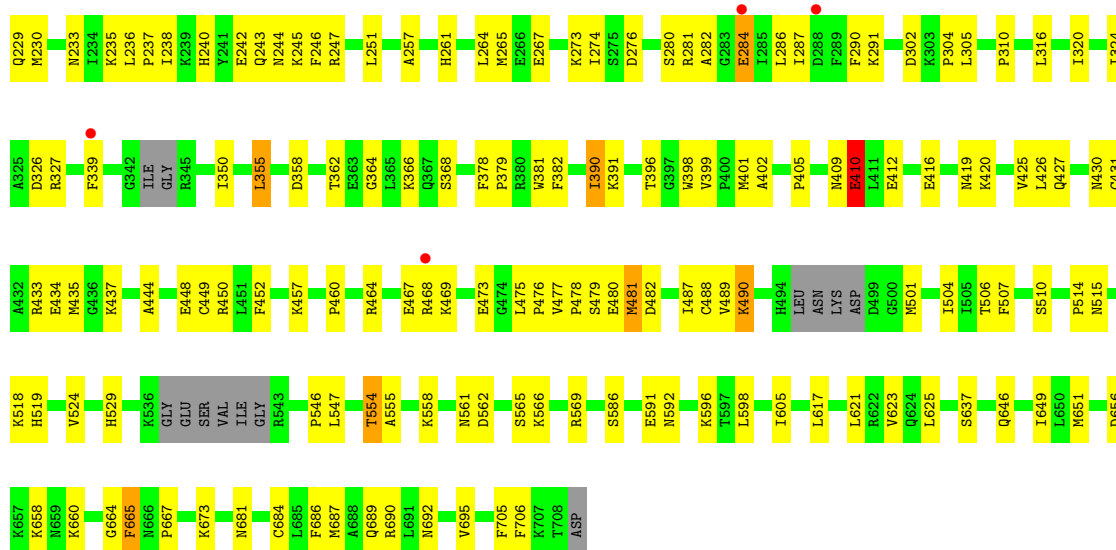
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

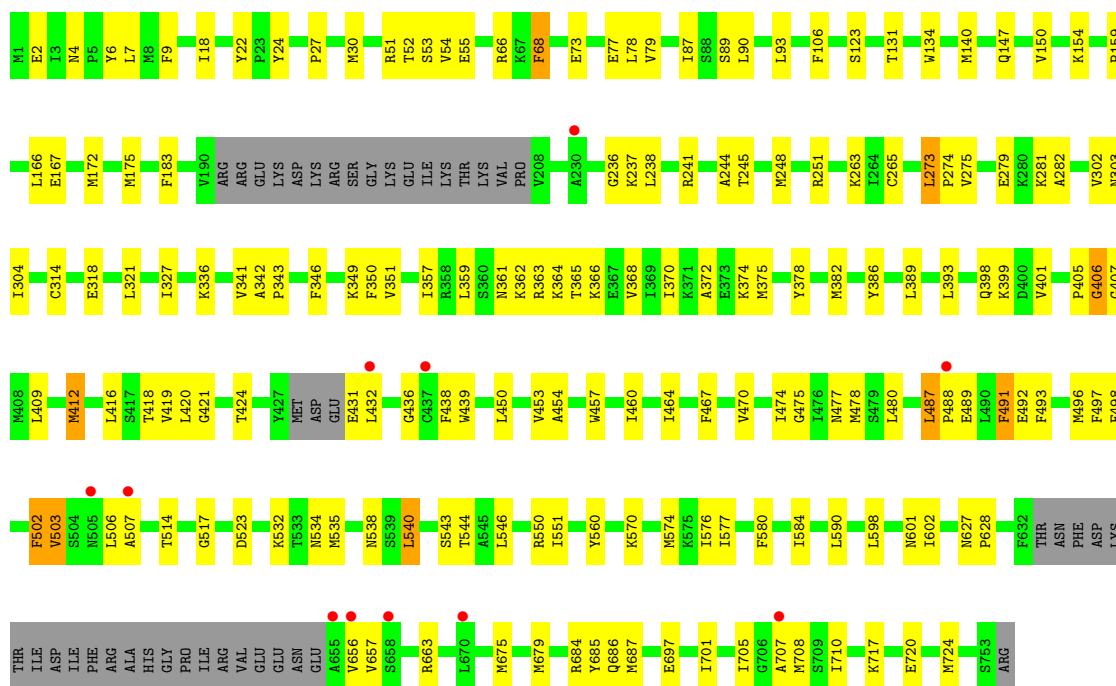


• Molecule 1: Polymerase acidic protein

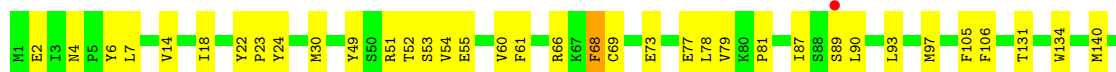


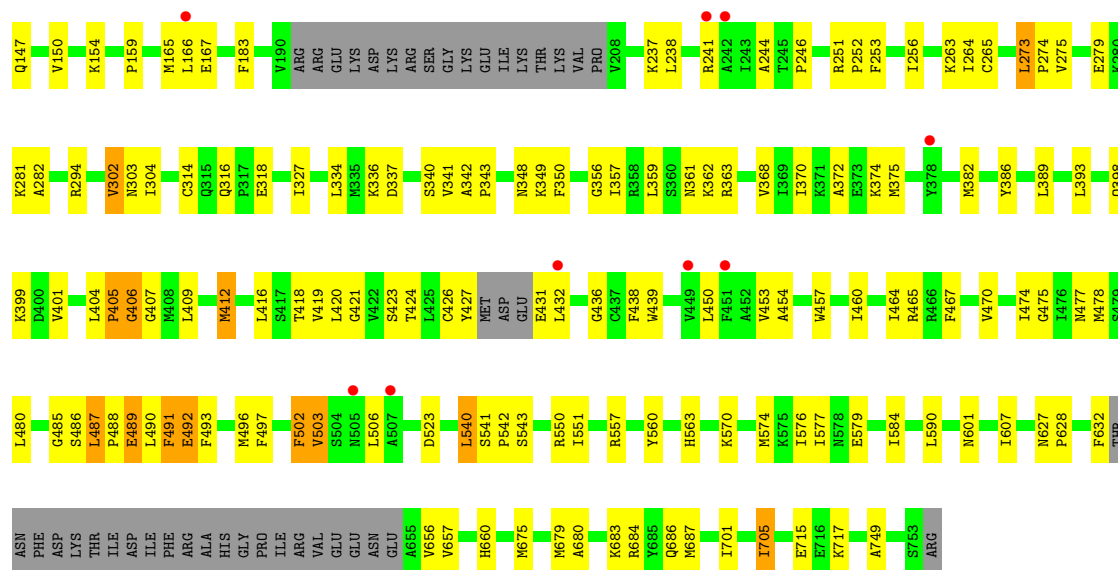


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

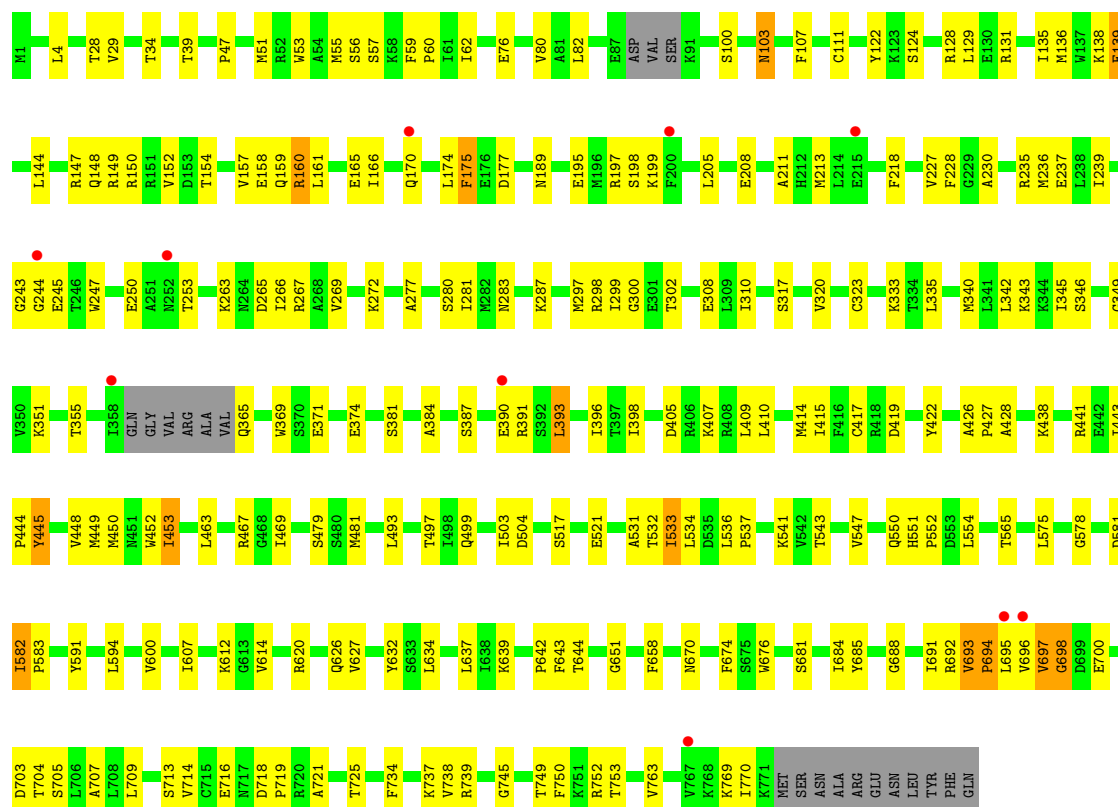


• Molecule 2: RNA-directed RNA polymerase catalytic subunit





• Molecule 3: Polymerase basic protein 2



• Molecule 3: Polymerase basic protein 2





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	4772 reflections (5.01%)	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	0.54	0/5746	0.88	4/7717 (0.1%)
1	D	0.56	0/5746	0.88	4/7717 (0.1%)
2	B	0.56	0/5749	0.91	5/7723 (0.1%)
2	E	0.57	0/5749	0.89	6/7723 (0.1%)
3	C	0.56	0/6185	0.89	6/8322 (0.1%)
3	F	0.57	0/6185	0.88	4/8322 (0.0%)
All	All	0.56	0/35360	0.89	29/47524 (0.1%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	406	GLY	N-CA-C	7.22	121.40	112.73
1	A	481	MET	N-CA-C	6.39	117.01	108.38
3	F	245	GLU	N-CA-C	6.37	119.04	111.71
1	D	284	GLU	N-CA-C	-6.17	105.79	113.38
2	E	489	GLU	N-CA-C	6.16	117.99	111.28
3	C	139	GLU	N-CA-C	6.15	119.15	108.76
3	C	245	GLU	N-CA-C	5.88	118.64	111.82
3	C	693	VAL	CA-C-N	5.87	125.56	119.05
3	C	693	VAL	C-N-CA	5.87	125.56	119.05
3	C	694	PRO	N-CA-C	5.70	121.45	113.53
2	E	487	LEU	N-CA-C	-5.62	101.86	110.01
2	B	489	GLU	N-CA-C	5.60	117.38	111.28
2	B	487	LEU	N-CA-C	-5.54	101.98	110.01
1	A	666	ASN	CA-C-N	5.49	125.14	119.05
1	A	666	ASN	C-N-CA	5.49	125.14	119.05
3	C	705	SER	N-CA-C	-5.45	106.64	113.28
2	B	406	GLY	N-CA-C	5.38	119.66	112.77
2	E	607	ILE	N-CA-C	5.36	113.18	107.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	481	MET	N-CA-C	5.36	115.61	108.38
1	D	665	PHE	N-CA-C	5.33	116.78	111.07
2	E	316	GLN	CA-C-N	5.28	124.94	119.56
2	E	316	GLN	C-N-CA	5.28	124.94	119.56
2	B	245	THR	CA-C-N	5.21	126.35	119.84
2	B	245	THR	C-N-CA	5.21	126.35	119.84
1	A	665	PHE	N-CA-C	5.15	116.90	111.28
3	F	202	ASN	N-CA-C	5.15	116.98	111.36
3	F	250	GLU	N-CA-C	5.13	116.98	109.24
3	F	135	ILE	CB-CA-C	-5.03	107.01	111.74
1	D	410	GLU	N-CA-C	5.02	116.44	110.97

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	155	0
1	D	5630	0	5632	175	0
2	B	5652	0	5749	141	0
2	E	5652	0	5749	140	0
3	C	6076	0	6183	190	0
3	F	6076	0	6183	205	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
All	All	34720	0	35128	888	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 13.

All (888) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:138:LYS:CE	3:F:250:GLU:HG2	1.34	1.48
3:F:138:LYS:CE	3:F:250:GLU:CD	1.86	1.46
3:F:138:LYS:HE3	3:F:250:GLU:CD	1.42	1.38
3:F:138:LYS:CE	3:F:250:GLU:CG	1.83	1.36
3:F:138:LYS:NZ	3:F:250:GLU:HG2	1.33	1.36
3:C:718:ASP:CG	3:C:719:PRO:HD3	1.59	1.28
3:F:718:ASP:CG	3:F:719:PRO:HD3	1.60	1.26
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
3:F:138:LYS:HE2	3:F:250:GLU:CD	1.67	1.02
2:E:487:LEU:HG	2:E:488:PRO:HD2	1.43	0.98
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
3:F:138:LYS:HZ3	3:F:250:GLU:HG2	1.28	0.93
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:C:694:PRO:C	3:C:695:LEU:HD23	1.94	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:718:ASP:CG	3:F:719:PRO:CD	2.52	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
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
3:C:718:ASP:CG	3:C:719:PRO:CD	2.51	0.72
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:174:LEU:HD23	3:C:174:LEU:C	2.15	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:174:LEU:C	3:F:174:LEU:HD23	2.15	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:401:MET:HE1	2:B:551:ILE:HD11	1.73	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
2:E:131:THR:HG21	2:E:251:ARG:HD2	1.74	0.69
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:697:VAL:O	3:C:698:GLY:C	2.37	0.65
3:F:415:ILE:HD11	3:F:453:ILE:HD13	1.77	0.65
1:A:345:ARG:HD3	3:F:136:MET:HE3	1.78	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
3:F:340:MET:HE2	3:F:409:LEU:HD23	1.79	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
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:F:138:LYS:HZ1	3:F:250:GLU:CG	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:340:MET:HE2	3:C:409:LEU:HD23	1.80	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
3:C:51:MET:HE3	3:C:55:MET:HG2	1.81	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
2:B:357:ILE:O	2:B:370:ILE:HG22	2.01	0.60
1:D:185:MET:HE2	2:E:337:ASP:HB3	1.83	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
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
3:C:272:LYS:HZ2	3:C:543:THR:HG23	1.68	0.59
1:D:469:LYS:HD3	1:D:475:LEU:CD1	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:421:GLY:O	2:B:424:THR:OG1	2.15	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:656:VAL:HG13	3:C:213:MET:HE1	1.85	0.56
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:372:ALA:HA	2:E:375:MET:HE2	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ARG:NH2	2:B:77:GLU:O	2.39	0.56
2:B:361:ASN:C	2:B:363:ARG:H	2.14	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
2:E:656:VAL:HG13	3:F:213:MET:HE1	1.88	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
3:F:174:LEU:HD23	3:F:174:LEU:O	2.06	0.56
1:D:59:ASP:OD2	3:F:769:LYS:NZ	2.38	0.56
1:A:261:HIS:CD2	1:A:265:MET:HE3	2.40	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
2:B:363:ARG:HD3	3:F:139:GLU:CD	2.32	0.54
2:B:244:ALA:HB3	2:B:409:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:531:ALA:C	3:C:532:THR:HG22	2.33	0.53
2:E:438:PHE:HB2	2:E:453:VAL:HB	1.89	0.53
1:A:34:LYS:HZ3	1:A:180:GLU:HG3	1.74	0.53
3:C:333:LYS:HE3	3:C:343:LYS:HD3	1.90	0.53
3:F:272:LYS:HZ2	3:F:543:THR:HG23	1.73	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:444:PRO:HG2	3:C:533:ILE:HD11	1.91	0.53
1:D:401:MET:HE1	2:E:551:ILE:HD11	1.90	0.53
3:F:51:MET:HE3	3:F:55:MET:HG2	1.89	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
1:D:687:MET:HE3	2:E:6:TYR:CE2	2.42	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:266:ILE:HG12	3:C:297:MET:HE3	1.91	0.53
3:C:693:VAL:N	3:C:694:PRO:HD2	2.23	0.53
2:E:246:PRO:HG2	2:E:412:MET:HE2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TRP:CE3	1:A:465:SER:HB2	2.44	0.52
2:E:684:ARG:HA	2:E:687:MET:HE2	1.91	0.52
3:F:531:ALA:C	3:F:532:THR:HG22	2.34	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
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
2:B:140:MET:HE2	2:B:675:MET:HE1	1.92	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
2:E:361:ASN:C	2:E:363:ARG:H	2.16	0.51
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: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:C:414:MET:HE3	3:C:467:ARG:HE	1.76	0.51
3:F:266:ILE:HG12	3:F:297:MET:HE3	1.92	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
1:A:562:ASP:O	1:A:565:SER:OG	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:235:LYS:HZ3	2:B:464:ILE:HG22	1.74	0.51
2:B:684:ARG:HA	2:B:687:MET:HE2	1.92	0.51
2:B:701:ILE:HD11	3:C:208:GLU:HA	1.92	0.51
3:C:53:TRP:O	3:C:56:SER:OG	2.24	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
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: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
3:C:195:GLU:O	3:C:198:SER:OG	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:E:356:GLY:HA2	2:E:375:MET:HE1	1.94	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
1:D:282:ALA:C	1:D:284:GLU:H	2.21	0.49
1:D:34:LYS:HZ3	1:D:180:GLU:HG3	1.78	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:372:ALA:HA	2:B:375:MET:HE2	1.95	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:414:MET:HE3	3:F:467:ARG:HE	1.77	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
3:C:174:LEU:C	3:C:174:LEU:CD2	2.86	0.48
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
2:E:715:GLU:OE2	3:F:11:TYR:OH	2.30	0.47
3:F:174:LEU:C	3:F:174:LEU:CD2	2.86	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
1:A:219:ASN:HB2	1:A:221:ARG:HH11	1.79	0.47
2:E:523:ASP:OD2	2:E:560:TYR:OH	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:HIS:CD2	1:D:265:MET:HE3	2.50	0.47
2:E:660:HIS:CE1	3:F:106:ASN:HD21	2.33	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
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
1:D:501:MET:HE2	1:D:555:ALA:HB1	1.96	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
3:F:718:ASP:OD1	3:F:719:PRO:HD3	2.07	0.47
1:D:113:ASP:O	1:D:117:GLN:HG2	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:MET:HE1	2:B:251:ARG:HD3	1.97	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:185:MET:CE	2:E:337:ASP:HB3	2.46	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
2:B:172:MET:HA	2:B:175:MET:HE2	1.99	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
3:C:697:VAL:C	3:C:698:GLY:O	2.59	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:195:GLU:O	3:F:198:SER:OG	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:269:VAL:HG21	3:F:297:MET:HE1	1.99	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:282:ALA:C	1:A:284:GLU:H	2.24	0.44
1:A:658:LYS:HB2	1:A:660:LYS:HE3	1.99	0.44
3:C:581:ASP:C	3:C:583:PRO:HD2	2.42	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
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: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
1:D:651:MET:HE1	2:E:490:LEU:HD22	2.00	0.44
2:E:491:PHE:CD1	2:E:491:PHE:C	2.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:476:PRO:C	1:D:477:VAL:HG23	2.42	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
3:F:152:VAL:HG13	3:F:236:MET:HE2	2.01	0.43
1:A:434:GLU:HA	1:A:437:LYS:HG2	2.00	0.43
1:A:501:MET:HE2	1:A:555:ALA:HB1	1.99	0.43
2:B:24:TYR:CD1	2:B:507:ALA:HB1	2.54	0.43
2:B:361:ASN:C	2:B:363:ARG:N	2.77	0.43
2:B:475:GLY:O	2:B:477:ASN:ND2	2.51	0.43
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
3:F:58:LYS:C	3:F:60:PRO:HD3	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:552:PRO:C	3:F:554:LEU:H	2.26	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
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
2:B:523:ASP:OD2	2:B:560:TYR:OH	2.24	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:238:ILE:HG21	1:D:664:GLY:C	2.44	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:410:LEU:HD11	3:C:481:MET:HE3	2.00	0.43
3:C:419:ASP:OD2	3:C:467:ARG:NH1	2.52	0.43
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:F:414:MET:HE1	3:F:463:LEU:O	2.19	0.43
2:B:351:VAL:C	2:B:401:VAL:HG23	2.43	0.42
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:410:LEU:HD11	3:F:481:MET:HE3	2.00	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
2:B:535:MET:HE1	2:B:602:ILE:HG23	2.00	0.42
3:C:197:ARG:NH1	3:C:703:ASP:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:419:ASN:CG	2:B:550:ARG:HH22	2.27	0.42
2:B:273:LEU:C	2:B:275:VAL:H	2.26	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
1:A:410:GLU:H	1:A:410:GLU:HG3	1.58	0.42
3:C:694:PRO:O	3:C:709:LEU:C	2.63	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
2:E:140:MET:HE2	2:E:675:MET:HE1	2.00	0.42
3:F:138:LYS:HE2	3:F:250:GLU:HG2	1.10	0.42
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
3:C:718:ASP:OD1	3:C:719:PRO:CD	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:714:VAL:HG22	3:F:750:PHE:CE2	2.55	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: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
2:B:708:MET:HG3	3:C:745:GLY:C	2.46	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:477:VAL:CG1	1:D:478:PRO:N	2.83	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:361:ASN:C	2:E:363:ARG:N	2.79	0.41
3:F:76:GLU:HG2	3:F:77:HIS:H	1.86	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
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:209:MET:HE1	2:B:321:LEU:HG	2.03	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:139:GLU:O	3:F:139:GLU:HG2	2.20	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
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
2:E:273:LEU:C	2:E:275:VAL:H	2.28	0.40
3:F:288:LEU:O	3:F:292:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:GLU:OE2	1:D:128:LYS:NZ	2.53	0.40
1:D:396:THR:HG21	1:D:468:ARG:HG3	2.01	0.40
2:E:165:MET:HE1	2:E:252:PRO:HB3	2.03	0.40
2:E:404:LEU:HA	2:E:405:PRO:HD3	1.79	0.40
3:F:339:PRO:HD2	3:F:412:MET:HE1	2.03	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
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	36	69
2	E	703/754 (93%)	673 (96%)	27 (4%)	3 (0%)	30	64
3	C	756/782 (97%)	688 (91%)	63 (8%)	5 (1%)	18	53
3	F	756/782 (97%)	686 (91%)	67 (9%)	3 (0%)	30	64
All	All	4288/4490 (96%)	4001 (93%)	274 (6%)	13 (0%)	36	69

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%)	599 (97%)	19 (3%)	35	57
1	D	618/631 (98%)	600 (97%)	18 (3%)	37	58
2	B	629/669 (94%)	610 (97%)	19 (3%)	36	57
2	E	629/669 (94%)	609 (97%)	20 (3%)	34	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	669/686 (98%)	653 (98%)	16 (2%)	43	63
3	F	669/686 (98%)	650 (97%)	19 (3%)	38	59
All	All	3832/3972 (96%)	3721 (97%)	111 (3%)	37	58

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	170	PHE
1	A	192	LEU
1	A	276	ASP
1	A	355	LEU
1	A	366	LYS
1	A	390	ILE
1	A	410	GLU
1	A	412	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
1	A	625	LEU
1	A	673	LYS
2	B	30	MET
2	B	68	PHE
2	B	89	SER
2	B	166	LEU
2	B	263	LYS
2	B	273	LEU
2	B	279	GLU
2	B	302	VAL
2	B	341	VAL
2	B	362	LYS
2	B	412	MET
2	B	478	MET
2	B	491	PHE
2	B	492	GLU
2	B	502	PHE

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Mol	Chain	Res	Type
2	B	540	LEU
2	B	657	VAL
2	B	705	ILE
2	B	717	LYS
3	C	4	LEU
3	C	103	ASN
3	C	129	LEU
3	C	135	ILE
3	C	136	MET
3	C	160	ARG
3	C	175	PHE
3	C	281	ILE
3	C	345	ILE
3	C	393	LEU
3	C	445	TYR
3	C	450	MET
3	C	453	ILE
3	C	582	ILE
3	C	594	LEU
3	C	697	VAL
1	D	23	GLU
1	D	38	ILE
1	D	170	PHE
1	D	183	ILE
1	D	192	LEU
1	D	207	GLU
1	D	276	ASP
1	D	305	LEU
1	D	355	LEU
1	D	366	LYS
1	D	390	ILE
1	D	410	GLU
1	D	412	GLU
1	D	490	LYS
1	D	506	THR
1	D	554	THR
1	D	625	LEU
1	D	673	LYS
2	E	30	MET
2	E	68	PHE
2	E	89	SER
2	E	147	GLN

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Mol	Chain	Res	Type
2	E	166	LEU
2	E	263	LYS
2	E	273	LEU
2	E	279	GLU
2	E	302	VAL
2	E	341	VAL
2	E	362	LYS
2	E	412	MET
2	E	478	MET
2	E	491	PHE
2	E	492	GLU
2	E	502	PHE
2	E	540	LEU
2	E	657	VAL
2	E	705	ILE
2	E	717	LYS
3	F	4	LEU
3	F	103	ASN
3	F	129	LEU
3	F	135	ILE
3	F	152	VAL
3	F	160	ARG
3	F	175	PHE
3	F	270	CYS
3	F	281	ILE
3	F	323	CYS
3	F	393	LEU
3	F	445	TYR
3	F	450	MET
3	F	453	ILE
3	F	582	ILE
3	F	594	LEU
3	F	695	LEU
3	F	725	THR
3	F	738	VAL

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

Mol	Chain	Res	Type
1	A	31	HIS
1	A	43	GLN
1	A	101	GLN

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Mol	Chain	Res	Type
1	A	141	ASN
1	A	243	GLN
1	A	248	GLN
1	A	494	HIS
1	A	519	HIS
1	A	561	ASN
1	A	627	GLN
1	A	644	ASN
2	B	108	HIS
2	B	147	GLN
2	B	303	ASN
2	B	461	HIS
2	B	537	ASN
2	B	623	ASN
2	B	627	ASN
2	B	660	HIS
3	C	155	GLN
3	C	212	HIS
3	C	249	GLN
3	C	454	GLN
3	C	550	GLN
3	C	631	HIS
3	C	766	ASN
1	D	31	HIS
1	D	101	GLN
1	D	141	ASN
1	D	248	GLN
1	D	261	HIS
1	D	315	ASN
1	D	332	ASN
1	D	336	HIS
1	D	494	HIS
1	D	519	HIS
1	D	529	HIS
1	D	561	ASN
1	D	615	GLN
1	D	628	GLN
1	D	644	ASN
2	E	108	HIS
2	E	303	ASN
2	E	316	GLN
2	E	456	ASN

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Mol	Chain	Res	Type
2	E	477	ASN
2	E	537	ASN
2	E	554	GLN
2	E	627	ASN
2	E	660	HIS
2	E	667	ASN
2	E	686	GLN
3	F	148	GLN
3	F	155	GLN
3	F	212	HIS
3	F	403	ASN
3	F	454	GLN
3	F	550	GLN
3	F	631	HIS

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%)	-0.28	2 (0%)	90 78	132, 195, 269, 299	0
1	D	693/709 (97%)	-0.19	6 (0%)	81 62	129, 191, 258, 295	0
2	B	711/754 (94%)	-0.28	11 (1%)	72 50	131, 192, 256, 317	0
2	E	711/754 (94%)	-0.20	10 (1%)	73 52	130, 184, 266, 315	0
3	C	762/782 (97%)	-0.06	10 (1%)	75 54	149, 222, 285, 358	0
3	F	762/782 (97%)	0.03	11 (1%)	73 52	134, 224, 287, 343	0
All	All	4332/4490 (96%)	-0.16	50 (1%)	76 55	129, 202, 275, 358	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	695	LEU	4.9
3	C	696	VAL	4.2
2	E	242	ALA	3.9
2	E	166	LEU	3.4
3	F	586	ILE	3.2
3	F	141	ARG	3.2
2	E	451	PHE	3.1
3	F	358	ILE	3.1
3	C	767	VAL	3.0
2	E	505	ASN	3.0
3	C	200	PHE	3.0
3	C	170	GLN	2.9
3	C	695	LEU	2.9
3	F	429	THR	2.8
1	D	284	GLU	2.8
1	A	201	LEU	2.6
3	F	200	PHE	2.6
2	E	432	LEU	2.6
1	D	339	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	288	ASP	2.5
3	F	696	VAL	2.5
3	C	252	ASN	2.5
3	F	750	PHE	2.5
2	B	505	ASN	2.5
2	B	670	LEU	2.4
2	E	507	ALA	2.4
1	D	468	ARG	2.4
2	B	655	ALA	2.4
2	B	432	LEU	2.3
3	F	37	LYS	2.3
3	C	390	GLU	2.3
3	C	215	GLU	2.3
3	F	202	ASN	2.3
2	E	449	VAL	2.3
2	B	707	ALA	2.2
2	B	658	SER	2.2
2	E	378	TYR	2.2
3	C	358	ILE	2.2
2	B	488	PRO	2.2
2	B	230	ALA	2.1
1	A	284	GLU	2.1
2	B	507	ALA	2.1
2	E	241	ARG	2.1
3	C	244	GLY	2.1
1	D	47	MET	2.1
2	B	437	CYS	2.1
2	E	89	SER	2.1
1	D	163	PHE	2.0
2	B	656	VAL	2.0
3	F	205	LEU	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 oligosaccharides 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(Å ²)	Q<0.9
4	MG	D	800	1/1	0.69	0.15	200,200,200,200	0
4	MG	A	800	1/1	0.71	0.11	204,204,204,204	0
4	MG	D	801	1/1	0.72	0.14	182,182,182,182	0
4	MG	A	801	1/1	0.92	0.06	185,185,185,185	0

6.5 Other polymers [i](#)

There are no such residues in this entry.