



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 PM UTC

PDB ID : 1DE4 / pdb_00001de4
Title : HEMOCHROMATOSIS PROTEIN HFE COMPLEXED WITH TRANSFERRIN RECEPTOR
Authors : Bennett, M.J.; Lebron, J.A.; Bjorkman, P.J.
Deposited on : 1999-11-12
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

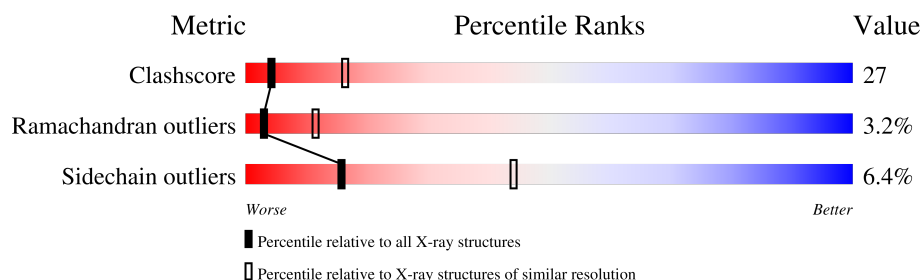
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	48% 41% 8% ..
1	D	275	49% 41% 7% ..
1	G	275	48% 43% 7% ..
2	B	99	52% 44% .
2	E	99	49% 45% 5%
2	H	99	52% 43% 5%
3	C	640	53% 39% 7% .
3	F	640	52% 41% 6% .

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Mol	Chain	Length	Quality of chain
3	I	640	55% 38% 6% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24315 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 HEMOCHROMATOSIS PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2242	1424	390	416	12			
1	D	272	Total	C	N	O	S	0	0	0
			2242	1424	390	416	12			
1	G	272	Total	C	N	O	S	0	0	0
			2242	1424	390	416	12			

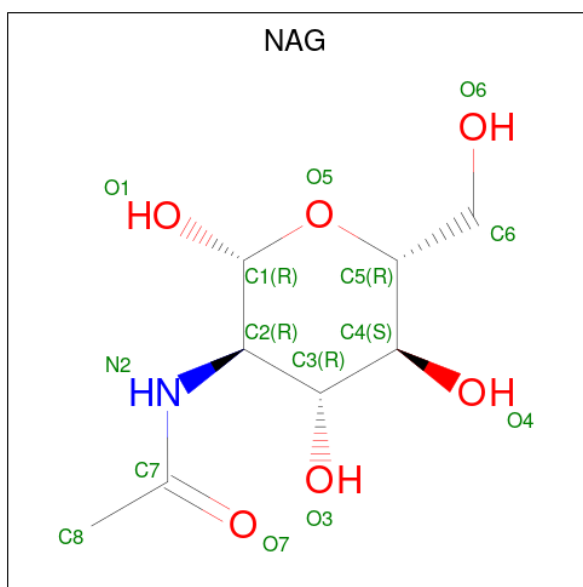
- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	522	138	158	3			
2	E	99	Total	C	N	O	S	0	0	0
			821	522	138	158	3			
2	H	99	Total	C	N	O	S	0	0	0
			821	522	138	158	3			

- Molecule 3 is a protein called TRANSFERRIN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	635	Total	C	N	O	S	0	0	0
			5022	3223	845	940	14			
3	F	635	Total	C	N	O	S	0	0	0
			5022	3223	845	940	14			
3	I	635	Total	C	N	O	S	0	0	0
			5022	3223	845	940	14			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

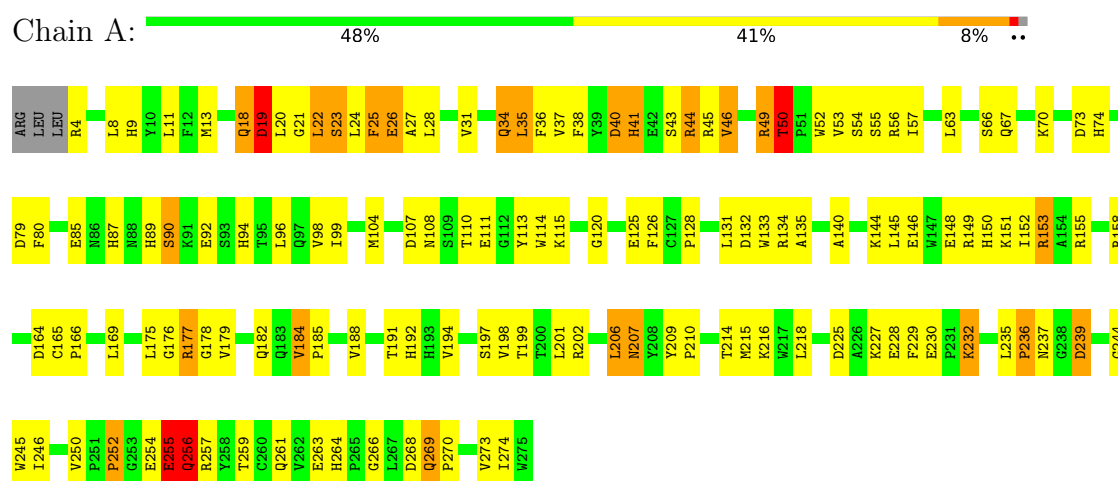
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	4	Total	O	0	0
			4	4		
7	F	2	Total	O	0	0
			2	2		
7	I	3	Total	O	0	0
			3	3		

3 Residue-property plots

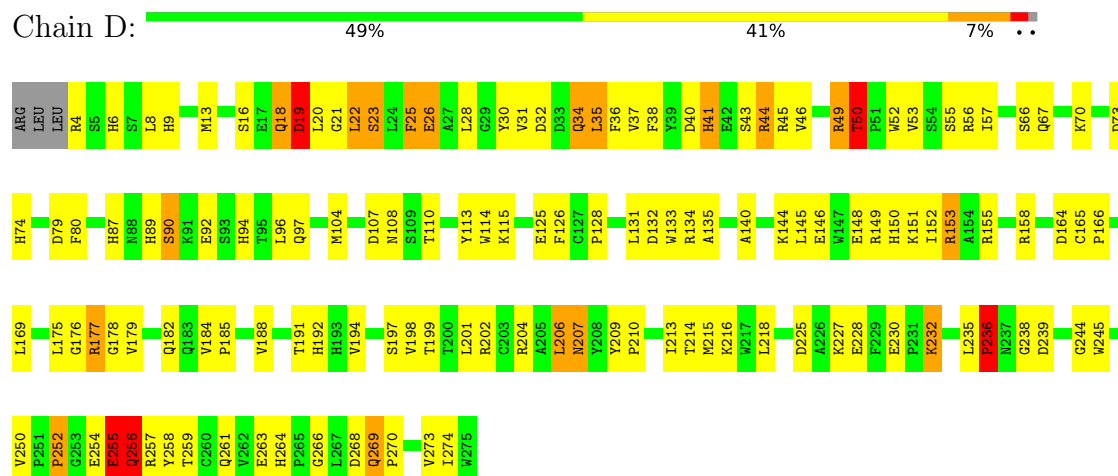
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: HEMOCHROMATOSIS PROTEIN

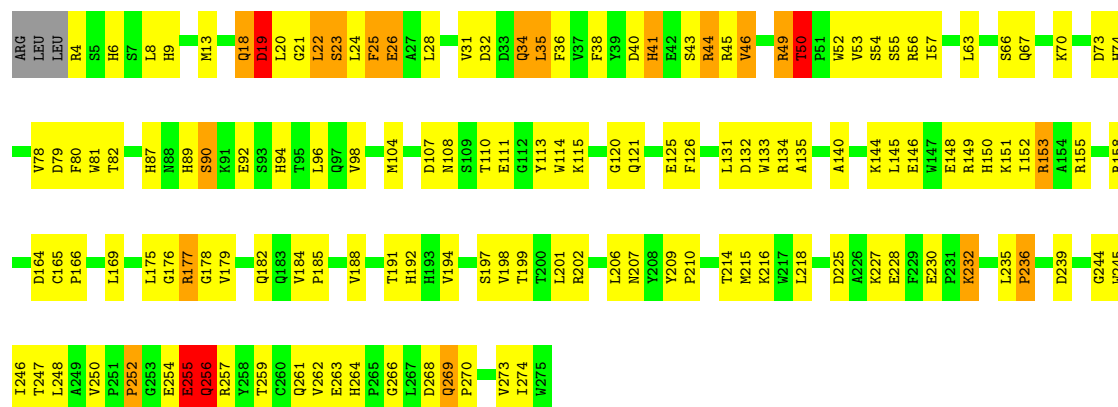


• Molecule 1: HEMOCHROMATOSIS PROTEIN

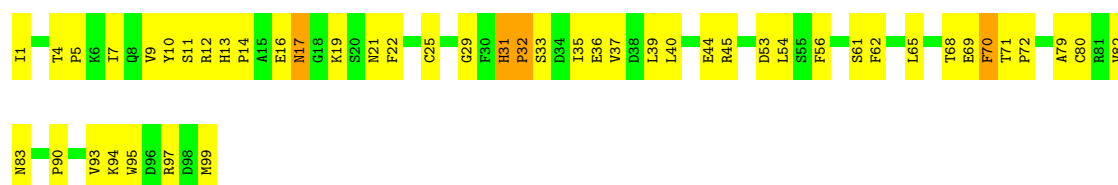


• Molecule 1: HEMOCHROMATOSIS PROTEIN

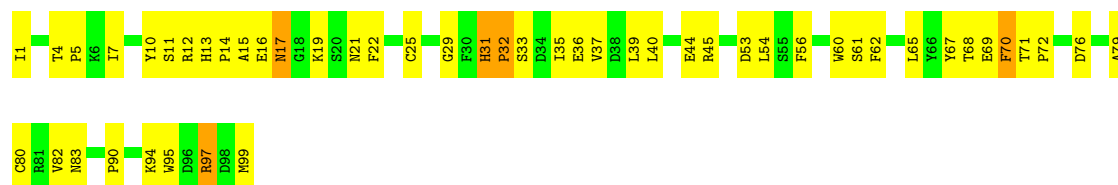




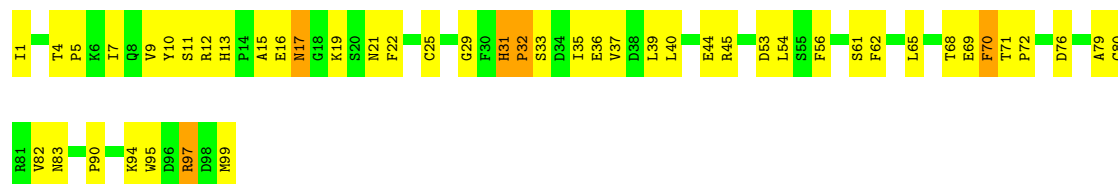
• Molecule 2: BETA-2-MICROGLOBULIN



• Molecule 2: BETA-2-MICROGLOBULIN



• Molecule 2: BETA-2-MICROGLOBULIN



• Molecule 3: TRANSFERRIN RECEPTOR

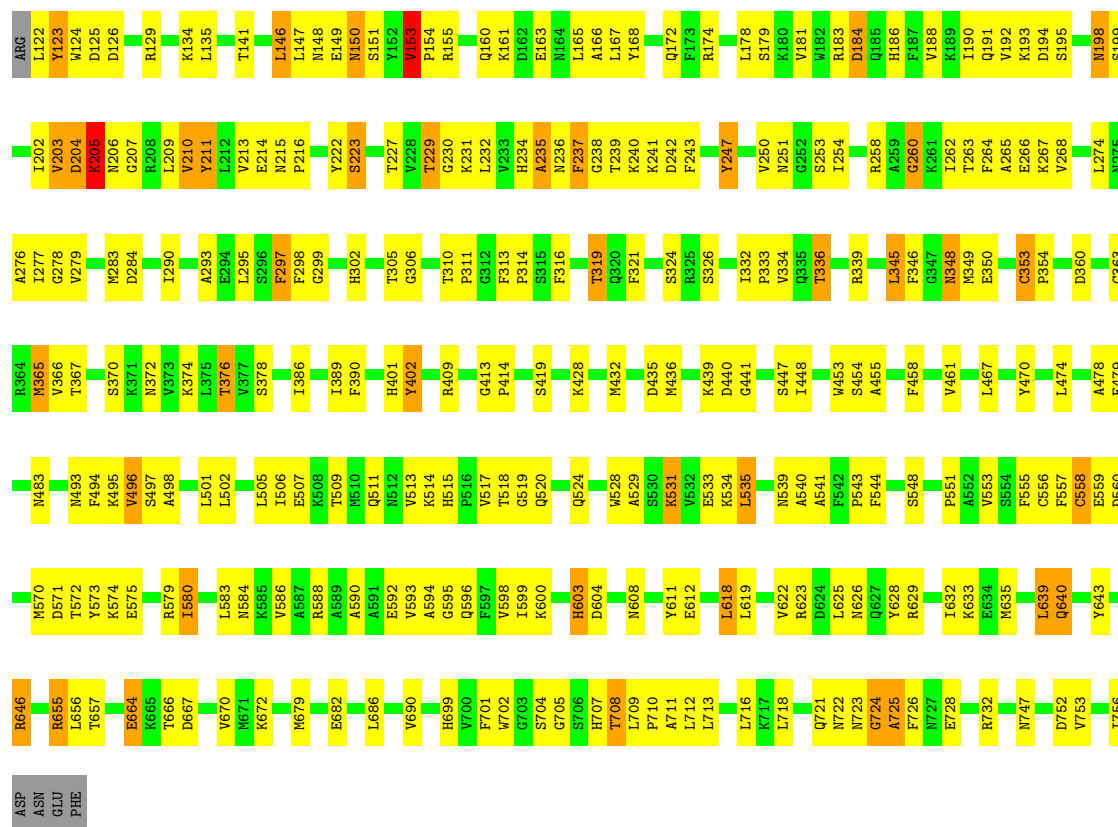




G724	A725	F726	N727	E728	T729	R732	W740	N747	D752	V753	L756	ASP	ASN	GLU	PHE	Y628	R629	I632	K633	E634	M635	L639	Q640	V641	L642	Y643	R646	R655	L656	T657	E664	K665	T666	D667	V670	M679	R680	V681	E682	L686	V690	H699	F701	W702	G703	S704	G705	S706	H707	T708	L709	P710	A711	L712	L713	L716	K717	L718	R719	T720	Q721	W722	Y628	K205	N206	G207	R208	L209	V210	Y211	L212	V213	E214	N215	P216	G217	Y222	S223	T227	V228	T229	G230	K231	L232	V233	H234	A235	D236	E237	L238	G238	L239	K241	D242	F243	E244	Y247	V250	N251	G252	S253	L254	V255	G256	V257	R258	A259	I260	K261	L262	T263	F264	A265	E266	K267	N268	S269	V268	Y272	K273	L274	N275	A276	T277	G278	V279	M283	L284	I290	A293	L295	E294	S296	F297	G298	H302	T305	G306	T310	P311	N312	G313	P314	F316	T319	G320	P322	P323	S324	K325	S326	N331	I332	P333	V334	Q335	T336	R339	L344	L345	F346	G347	N348	K349	C353	Y470	P354	S473	L474	K365	V366	T367	S370	K371	N372	V373	K374	L375	V377	S378	I386	N387	G388	I389	F390	H401	Y402	R409	G413	F414	S419	K428	L429	F432	M433	S434	D435	M436	N528	A529	S530	K531	V532	E533	K534	L535	T536	L537	D538	N539	A540	A541	F542	P543	L625	Q721	W626	Y470	P354	S473	L474	K365	V366	T367	S370	K371	N372	V373	K374	L375	V377	S378	I386	N387	G388	I389	F390	H401	Y402	R409	G413	F414	S419	K428	L429	F432	M433	S434	D435	M436	N528	A529	S530	K531	V532	E533	K534	L535	T536	L537	D538	N539	A540	A541	F542	P543	L625	Q721	W626	Y470	P354	S473	L474	K365	V366	T367	S370	K371	N372	V373	K374	L375	V377	S378	I386	N387	G388	I389	F390	H401	Y402	R409	G413	F414	S419	K428	L429	F432	M433	S434	D435	M436	N528	A529	S530	K531	V532	E533	K534	L535	T536	L537	D538	N539	A
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- Molecule 3: TRANSFERRIN RECEPTOR

Chain I: 55% 38% 6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.40Å 144.40Å 327.10Å 90.00° 93.60° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	94.3 (30.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.231 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24315	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/2310	0.92	11/3143 (0.3%)
1	D	0.40	0/2310	0.92	6/3143 (0.2%)
1	G	0.43	0/2310	0.91	9/3143 (0.3%)
2	B	0.36	0/844	0.83	1/1144 (0.1%)
2	E	0.34	0/844	0.82	1/1144 (0.1%)
2	H	0.35	0/844	0.82	1/1144 (0.1%)
3	C	0.47	0/5142	0.98	24/6973 (0.3%)
3	F	0.46	0/5142	0.98	21/6973 (0.3%)
3	I	0.52	0/5142	1.00	23/6973 (0.3%)
All	All	0.45	0/24888	0.95	97/33780 (0.3%)

There are no bond length outliers.

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	I	215	ASN	CA-C-N	7.65	127.71	119.90
3	I	215	ASN	C-N-CA	7.65	127.71	119.90
3	I	153	VAL	CA-C-N	-7.42	110.56	119.84
3	I	153	VAL	C-N-CA	-7.42	110.56	119.84
3	C	557	PHE	N-CA-C	-7.42	93.01	107.62
3	I	211	TYR	N-CA-C	7.34	122.12	112.72
3	F	557	PHE	N-CA-C	-7.30	93.23	107.62
3	F	153	VAL	CA-C-N	-7.18	110.86	119.84
3	F	153	VAL	C-N-CA	-7.18	110.86	119.84
1	A	25	PHE	N-CA-C	7.14	121.30	109.95
3	I	557	PHE	N-CA-C	-7.11	93.61	107.62
1	G	25	PHE	N-CA-C	7.06	121.18	109.95
1	D	25	PHE	N-CA-C	6.96	121.02	109.95
3	I	198	ASN	N-CA-C	-6.85	100.38	110.52
3	C	153	VAL	CA-C-N	-6.82	111.32	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	153	VAL	C-N-CA	-6.82	111.32	119.84
3	I	235	ALA	N-CA-C	-6.80	99.90	110.17
3	C	314	PRO	N-CA-C	6.74	121.77	111.19
3	F	235	ALA	N-CA-C	-6.66	100.11	110.17
3	I	603	HIS	N-CA-C	6.53	118.98	111.02
3	C	580	ILE	CA-C-N	6.51	126.44	119.28
3	C	580	ILE	C-N-CA	6.51	126.44	119.28
3	I	580	ILE	CA-C-N	6.51	126.44	119.28
3	I	580	ILE	C-N-CA	6.51	126.44	119.28
3	C	603	HIS	N-CA-C	6.49	118.94	111.02
3	C	198	ASN	N-CA-C	-6.43	101.01	110.52
3	F	198	ASN	N-CA-C	-6.42	101.02	110.52
3	C	235	ALA	N-CA-C	-6.38	100.53	110.17
1	D	164	ASP	N-CA-C	6.37	117.92	110.97
3	F	580	ILE	CA-C-N	6.37	126.28	119.28
3	F	580	ILE	C-N-CA	6.37	126.28	119.28
1	A	164	ASP	N-CA-C	6.35	117.89	110.97
1	G	206	LEU	N-CA-C	6.33	119.89	110.52
1	A	206	LEU	N-CA-C	6.31	119.86	110.52
1	D	206	LEU	N-CA-C	6.28	119.81	110.52
1	G	50	THR	CA-C-N	6.27	126.17	119.28
1	G	50	THR	C-N-CA	6.27	126.17	119.28
1	G	164	ASP	N-CA-C	6.21	117.74	110.97
3	I	260	GLY	N-CA-C	6.13	118.27	112.08
1	D	50	THR	CA-C-N	6.11	126.00	119.28
1	D	50	THR	C-N-CA	6.11	126.00	119.28
1	A	50	THR	CA-C-N	6.10	126.00	119.28
1	A	50	THR	C-N-CA	6.10	126.00	119.28
3	I	402	TYR	N-CA-C	5.90	117.22	108.60
3	F	215	ASN	CA-C-N	5.87	127.18	119.84
3	F	215	ASN	C-N-CA	5.87	127.18	119.84
3	F	402	TYR	N-CA-C	5.85	117.14	108.60
3	F	223	SER	N-CA-C	-5.84	102.66	110.55
3	F	314	PRO	N-CA-C	5.75	121.15	111.32
3	C	215	ASN	CA-C-N	5.75	127.02	119.84
3	C	215	ASN	C-N-CA	5.75	127.02	119.84
3	I	314	PRO	N-CA-C	5.72	121.10	111.32
3	C	478	ALA	N-CA-C	-5.70	100.52	109.25
3	C	260	GLY	N-CA-C	5.65	117.79	112.08
1	D	26	GLU	N-CA-C	-5.65	100.68	109.72
3	C	223	SER	N-CA-C	-5.63	102.95	110.55
3	F	604	ASP	N-CA-C	5.62	117.16	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	686	LEU	N-CA-C	-5.62	100.83	109.76
3	F	478	ALA	N-CA-C	-5.60	100.68	109.25
3	I	534	LYS	N-CA-C	5.57	117.88	110.53
3	C	402	TYR	N-CA-C	5.57	116.72	108.60
3	C	604	ASP	N-CA-C	5.50	117.00	109.18
3	C	686	LEU	N-CA-C	-5.50	101.01	109.76
3	F	207	GLY	N-CA-C	-5.47	107.55	115.27
3	I	604	ASP	N-CA-C	5.47	116.95	109.18
1	A	184	VAL	CA-C-N	5.46	123.59	119.66
1	A	184	VAL	C-N-CA	5.46	123.59	119.66
3	I	223	SER	N-CA-C	-5.44	103.21	110.55
3	F	560	ASP	N-CA-C	-5.40	106.65	113.18
3	I	686	LEU	N-CA-C	-5.36	101.23	109.76
3	I	560	ASP	N-CA-C	-5.36	106.70	113.18
3	I	205	LYS	N-CA-C	5.35	122.20	110.80
1	G	46	VAL	N-CA-C	5.29	114.92	106.88
3	C	560	ASP	N-CA-C	-5.26	106.81	113.18
1	A	46	VAL	N-CA-C	5.26	114.88	106.88
2	B	25	CYS	N-CA-C	-5.24	99.57	108.26
3	F	264	PHE	N-CA-C	-5.23	105.47	111.07
2	H	25	CYS	N-CA-C	-5.23	99.58	108.26
2	E	25	CYS	N-CA-C	-5.21	99.61	108.26
3	I	264	PHE	N-CA-C	-5.21	105.50	111.07
3	I	478	ALA	N-CA-C	-5.20	101.29	109.25
1	A	26	GLU	N-CA-C	-5.15	101.76	109.95
3	F	534	LYS	N-CA-C	5.15	117.32	110.53
1	G	24	LEU	N-CA-C	5.11	119.47	112.88
3	F	260	GLY	N-CA-C	5.11	117.24	112.08
3	C	406	GLY	N-CA-C	5.06	118.49	111.10
1	G	262	VAL	N-CA-C	5.06	115.33	107.28
1	A	40	ASP	N-CA-C	5.05	117.92	110.59
3	F	565	TYR	N-CA-C	5.04	119.28	113.18
3	C	210	VAL	N-CA-C	5.04	115.83	108.53
3	C	493	ASN	N-CA-C	5.03	117.51	109.81
1	A	24	LEU	N-CA-C	5.02	119.36	112.88
1	G	26	GLU	N-CA-C	-5.02	101.97	109.95
3	C	264	PHE	N-CA-C	-5.01	105.70	111.07
3	C	363	CYS	N-CA-C	5.01	117.14	110.53
3	C	548	SER	N-CA-C	5.00	117.62	111.82
3	I	672	LYS	N-CA-C	-5.00	105.74	111.14

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	2242	0	2126	146	0
1	D	2242	0	2126	148	0
1	G	2242	0	2126	142	0
2	B	821	0	772	52	0
2	E	821	0	772	56	0
2	H	821	0	772	51	0
3	C	5022	0	4965	266	0
3	F	5022	0	4965	264	0
3	I	5022	0	4965	251	0
4	C	14	0	13	0	0
4	F	14	0	13	0	0
4	I	14	0	13	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
6	G	6	0	8	3	0
7	C	4	0	0	0	0
7	F	2	0	0	0	0
7	I	3	0	0	0	0
All	All	24315	0	23636	1300	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 27.

All (1300) 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:C:708:THR:HG22	3:C:711:ALA:H	1.18	1.09
3:C:708:THR:HG23	3:C:710:PRO:HD2	1.29	1.08
3:I:708:THR:HG23	3:I:710:PRO:HD2	1.29	1.07
3:F:708:THR:HG23	3:F:710:PRO:HD2	1.31	1.04
3:I:708:THR:HG22	3:I:711:ALA:H	1.18	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:708:THR:HG22	3:F:711:ALA:H	1.19	1.02
3:I:539:ASN:HD22	3:I:541:ALA:H	1.11	0.99
3:C:539:ASN:HD22	3:C:541:ALA:H	1.10	0.96
1:A:146:GLU:HG2	3:C:640:GLN:HE21	1.31	0.96
3:F:239:THR:HG22	3:F:241:LYS:H	1.32	0.95
3:F:515:HIS:HD2	3:F:517:VAL:H	1.14	0.95
3:F:539:ASN:HD22	3:F:541:ALA:H	1.14	0.95
3:C:515:HIS:HD2	3:C:517:VAL:H	1.12	0.94
1:D:22:LEU:HD12	3:F:619:LEU:HD23	1.48	0.94
3:I:202:ILE:HB	3:I:211:TYR:HB2	1.50	0.93
1:D:202:ARG:HE	2:E:99:MET:HG2	1.33	0.92
3:I:239:THR:HG22	3:I:241:LYS:H	1.35	0.91
3:I:515:HIS:HD2	3:I:517:VAL:H	1.14	0.91
3:C:239:THR:HG22	3:C:241:LYS:H	1.35	0.91
3:C:664:GLU:CD	3:C:664:GLU:H	1.80	0.90
3:I:204:ASP:O	3:I:206:ASN:N	2.05	0.90
1:G:146:GLU:HG2	3:I:640:GLN:HE21	1.37	0.88
3:F:664:GLU:H	3:F:664:GLU:CD	1.80	0.88
2:E:31:HIS:HB3	2:E:32:PRO:HD3	1.58	0.85
3:I:664:GLU:CD	3:I:664:GLU:H	1.83	0.85
2:B:31:HIS:HB3	2:B:32:PRO:HD3	1.57	0.84
2:H:31:HIS:HB3	2:H:32:PRO:HD3	1.59	0.84
3:I:708:THR:HG23	3:I:710:PRO:CD	2.09	0.83
3:C:386:ILE:HG23	3:C:454:SER:HB3	1.61	0.83
1:A:146:GLU:HG2	3:C:640:GLN:NE2	1.95	0.82
3:I:493:ASN:HB2	3:I:495:LYS:HZ2	1.46	0.81
3:C:493:ASN:HB2	3:C:495:LYS:HZ2	1.45	0.81
3:F:386:ILE:HG23	3:F:454:SER:HB3	1.60	0.81
3:C:239:THR:HB	3:C:242:ASP:OD1	1.81	0.80
3:C:655:ARG:HB2	3:C:655:ARG:HH11	1.45	0.80
3:C:153:VAL:HG23	3:C:154:PRO:HD2	1.64	0.80
3:F:655:ARG:HH11	3:F:655:ARG:HB2	1.44	0.80
3:C:515:HIS:CD2	3:C:517:VAL:H	1.99	0.80
3:C:708:THR:HG23	3:C:710:PRO:CD	2.10	0.80
2:E:79:ALA:HB2	2:E:94:LYS:HA	1.63	0.80
1:G:57:ILE:HA	1:G:175:LEU:HD21	1.64	0.80
1:D:206:LEU:HD11	2:E:14:PRO:HD3	1.62	0.79
2:B:79:ALA:HB2	2:B:94:LYS:HA	1.63	0.79
2:H:79:ALA:HB2	2:H:94:LYS:HA	1.64	0.79
3:I:386:ILE:HG23	3:I:454:SER:HB3	1.62	0.79
3:I:153:VAL:HG23	3:I:154:PRO:HD2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:295:LEU:HD22	3:I:570:MET:HE2	1.63	0.79
3:I:539:ASN:ND2	3:I:541:ALA:H	1.81	0.79
3:C:295:LEU:HD22	3:C:570:MET:HE2	1.64	0.79
3:F:708:THR:HG23	3:F:710:PRO:CD	2.11	0.79
1:D:21:GLY:C	1:D:22:LEU:HD23	2.08	0.79
1:G:26:GLU:HG3	1:G:41:HIS:ND1	1.98	0.79
1:G:36:PHE:HB2	1:G:53:VAL:HG11	1.65	0.78
3:I:239:THR:HB	3:I:242:ASP:OD1	1.83	0.78
1:G:21:GLY:C	1:G:22:LEU:HD23	2.08	0.78
1:D:26:GLU:HG3	1:D:41:HIS:ND1	1.97	0.78
3:F:153:VAL:HG23	3:F:154:PRO:HD2	1.64	0.78
1:A:57:ILE:HA	1:A:175:LEU:HD21	1.65	0.77
3:C:539:ASN:ND2	3:C:541:ALA:H	1.82	0.77
3:F:239:THR:HB	3:F:242:ASP:OD1	1.84	0.77
3:F:295:LEU:HD22	3:F:570:MET:HE2	1.66	0.77
1:D:22:LEU:HD12	3:F:619:LEU:CD2	2.14	0.77
1:A:36:PHE:HB2	1:A:53:VAL:HG11	1.66	0.77
1:D:36:PHE:HB2	1:D:53:VAL:HG11	1.65	0.77
1:A:26:GLU:HG3	1:A:41:HIS:ND1	2.00	0.77
3:F:493:ASN:HB2	3:F:495:LYS:HZ2	1.50	0.76
3:I:655:ARG:HB2	3:I:655:ARG:HH11	1.47	0.76
1:A:21:GLY:C	1:A:22:LEU:HD23	2.08	0.76
1:D:202:ARG:NE	2:E:99:MET:HG2	2.01	0.76
3:I:209:LEU:HD12	3:I:210:VAL:H	1.49	0.76
1:G:146:GLU:HG2	3:I:640:GLN:NE2	2.01	0.76
1:D:198:VAL:HA	1:D:252:PRO:HG3	1.67	0.76
3:F:515:HIS:CD2	3:F:517:VAL:H	2.02	0.76
1:G:56:ARG:O	1:G:175:LEU:HD11	1.85	0.76
1:D:145:LEU:HD22	1:D:149:ARG:NH2	2.01	0.76
6:G:309:GOL:H32	3:I:646:ARG:HH21	1.51	0.76
1:D:259:THR:HG22	1:D:274:ILE:HG22	1.67	0.75
1:D:268:ASP:HB2	1:D:269:GLN:HE21	1.51	0.75
1:D:57:ILE:HA	1:D:175:LEU:HD21	1.66	0.75
1:A:268:ASP:HB2	1:A:269:GLN:HE21	1.52	0.75
3:F:495:LYS:HD3	3:F:558:CYS:SG	2.27	0.75
1:G:259:THR:HG22	1:G:274:ILE:HG22	1.68	0.75
3:F:539:ASN:ND2	3:F:541:ALA:H	1.84	0.75
1:A:259:THR:HG22	1:A:274:ILE:HG22	1.69	0.75
3:F:493:ASN:HD22	3:F:495:LYS:HZ2	1.33	0.75
1:G:268:ASP:HB2	1:G:269:GLN:HE21	1.51	0.75
1:A:202:ARG:HE	2:B:99:MET:HG2	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:655:ARG:HH11	3:F:655:ARG:CB	1.99	0.74
1:G:165:CYS:HB3	1:G:166:PRO:HD3	1.69	0.74
1:D:56:ARG:O	1:D:175:LEU:HD11	1.86	0.74
1:D:146:GLU:HG2	3:F:640:GLN:HE21	1.52	0.74
1:D:207:ASN:HD21	2:E:13:HIS:CD2	2.04	0.74
3:C:202:ILE:HB	3:C:211:TYR:HB2	1.68	0.74
2:E:19:LYS:HD2	2:E:19:LYS:N	2.03	0.74
3:I:515:HIS:CD2	3:I:517:VAL:H	2.02	0.74
2:B:19:LYS:HD2	2:B:19:LYS:N	2.03	0.73
3:I:210:VAL:HG12	3:I:211:TYR:HD1	1.54	0.73
1:A:20:LEU:HD13	1:A:20:LEU:O	1.89	0.73
3:C:206:ASN:HD22	3:C:206:ASN:C	1.94	0.73
1:D:165:CYS:HB3	1:D:166:PRO:HD3	1.69	0.73
3:I:655:ARG:HH11	3:I:655:ARG:CB	2.01	0.73
1:A:198:VAL:HA	1:A:252:PRO:HG3	1.70	0.73
3:C:655:ARG:HH11	3:C:655:ARG:CB	2.01	0.73
1:G:145:LEU:HD22	1:G:149:ARG:NH2	2.03	0.73
3:F:263:THR:HG22	3:F:265:ALA:N	2.04	0.72
3:C:495:LYS:HD3	3:C:558:CYS:SG	2.29	0.72
1:G:18:GLN:O	1:G:19:ASP:HB2	1.89	0.72
2:H:19:LYS:N	2:H:19:LYS:HD2	2.05	0.72
3:I:428:LYS:HE2	3:I:428:LYS:HA	1.71	0.72
1:D:25:PHE:O	1:D:44:ARG:NH1	2.23	0.72
1:D:206:LEU:CD1	2:E:14:PRO:HD3	2.19	0.72
3:F:428:LYS:HA	3:F:428:LYS:HE2	1.71	0.72
3:I:263:THR:HG22	3:I:265:ALA:N	2.05	0.72
3:C:153:VAL:HG23	3:C:161:LYS:HE3	1.72	0.72
1:D:18:GLN:O	1:D:19:ASP:HB2	1.90	0.72
3:C:122:LEU:O	3:C:123:TYR:HB2	1.90	0.71
3:F:635:MET:CE	3:F:728:GLU:HG3	2.20	0.71
3:I:495:LYS:HD3	3:I:558:CYS:SG	2.29	0.71
1:A:56:ARG:O	1:A:175:LEU:HD11	1.90	0.71
3:C:497:SER:HB3	3:C:535:LEU:HD13	1.71	0.71
1:D:194:VAL:HG22	1:D:199:THR:HG23	1.73	0.71
2:H:31:HIS:O	2:H:32:PRO:C	2.34	0.71
3:I:705:GLY:O	3:I:708:THR:HB	1.90	0.71
1:G:20:LEU:O	1:G:20:LEU:HD13	1.91	0.71
1:G:198:VAL:HA	1:G:252:PRO:HG3	1.73	0.71
3:C:263:THR:HG22	3:C:265:ALA:N	2.05	0.71
1:G:202:ARG:HE	2:H:99:MET:HG2	1.54	0.71
3:C:211:TYR:O	3:C:212:LEU:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:O	1:A:19:ASP:HB2	1.89	0.71
3:C:236:ASN:C	3:C:238:GLY:H	1.99	0.71
3:C:428:LYS:HA	3:C:428:LYS:HE2	1.73	0.71
3:F:153:VAL:HG23	3:F:161:LYS:HE3	1.72	0.71
1:A:202:ARG:NE	2:B:99:MET:HG2	2.05	0.70
3:F:236:ASN:C	3:F:238:GLY:H	1.99	0.70
1:D:20:LEU:HD13	1:D:20:LEU:O	1.91	0.70
3:C:705:GLY:O	3:C:708:THR:HB	1.90	0.70
3:F:239:THR:HG22	3:F:241:LYS:N	2.04	0.70
1:G:150:HIS:HD2	1:G:153:ARG:H	1.40	0.70
1:A:165:CYS:HB3	1:A:166:PRO:HD3	1.71	0.70
1:G:150:HIS:CD2	1:G:152:ILE:HB	2.26	0.70
1:A:194:VAL:HG22	1:A:199:THR:HG23	1.73	0.70
3:I:497:SER:HB3	3:I:535:LEU:HD13	1.72	0.70
3:I:122:LEU:O	3:I:123:TYR:HB2	1.91	0.70
3:C:635:MET:CE	3:C:728:GLU:HG3	2.22	0.70
1:D:28:LEU:HD23	1:D:38:PHE:HD1	1.56	0.70
1:D:150:HIS:HD2	1:D:153:ARG:H	1.38	0.70
1:G:50:THR:O	1:G:53:VAL:HG22	1.91	0.69
3:F:306:GLY:HA2	3:F:461:VAL:HA	1.75	0.69
3:C:239:THR:HG22	3:C:241:LYS:N	2.08	0.69
3:I:306:GLY:HA2	3:I:461:VAL:HA	1.73	0.69
2:E:39:LEU:HD23	2:E:80:CYS:HB3	1.75	0.69
2:B:31:HIS:O	2:B:32:PRO:C	2.35	0.69
1:D:50:THR:O	1:D:53:VAL:HG22	1.92	0.69
1:A:145:LEU:HD22	1:A:149:ARG:NH2	2.08	0.69
3:C:626:ASN:HA	3:C:629:ARG:HG3	1.75	0.69
1:A:50:THR:O	1:A:53:VAL:HG22	1.93	0.68
1:D:185:PRO:HB3	1:D:266:GLY:O	1.93	0.68
3:I:153:VAL:HG23	3:I:161:LYS:HE3	1.74	0.68
3:I:236:ASN:C	3:I:238:GLY:H	1.99	0.68
3:F:497:SER:HB3	3:F:535:LEU:HD13	1.76	0.68
1:D:52:TRP:O	1:D:56:ARG:HB2	1.93	0.68
3:F:626:ASN:HA	3:F:629:ARG:HG3	1.74	0.68
1:G:194:VAL:HG22	1:G:199:THR:HG23	1.74	0.68
2:H:31:HIS:O	2:H:33:SER:N	2.26	0.68
3:I:239:THR:HG22	3:I:241:LYS:N	2.06	0.68
1:A:22:LEU:HD12	3:C:619:LEU:HD23	1.75	0.68
3:C:153:VAL:HB	3:C:154:PRO:HD3	1.76	0.68
3:C:753:VAL:HG13	3:F:473:SER:HB3	1.74	0.68
1:A:198:VAL:HG22	1:A:199:THR:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:LEU:HD23	2:H:80:CYS:HB3	1.75	0.68
2:E:31:HIS:O	2:E:32:PRO:C	2.35	0.68
3:I:493:ASN:HD22	3:I:495:LYS:NZ	1.91	0.68
2:B:39:LEU:HD23	2:B:80:CYS:HB3	1.75	0.68
3:C:306:GLY:HA2	3:C:461:VAL:HA	1.74	0.68
3:C:493:ASN:HD22	3:C:495:LYS:HZ2	1.41	0.68
3:C:600:LYS:HD2	3:C:608:ASN:ND2	2.09	0.68
1:D:215:MET:HE1	1:D:244:GLY:C	2.19	0.68
2:E:31:HIS:O	2:E:33:SER:N	2.26	0.68
3:F:122:LEU:O	3:F:123:TYR:HB2	1.92	0.68
1:G:185:PRO:HB3	1:G:266:GLY:O	1.93	0.68
1:G:202:ARG:NE	2:H:99:MET:HG2	2.09	0.68
3:I:626:ASN:HA	3:I:629:ARG:HG3	1.76	0.68
3:C:708:THR:CG2	3:C:711:ALA:H	2.02	0.67
3:F:153:VAL:HB	3:F:154:PRO:HD3	1.75	0.67
3:F:213:VAL:HG11	3:F:345:LEU:HD22	1.74	0.67
3:F:600:LYS:HD2	3:F:608:ASN:ND2	2.09	0.67
3:C:718:LEU:HD13	3:C:725:ALA:HB1	1.75	0.67
1:D:198:VAL:HG22	1:D:199:THR:N	2.09	0.67
3:F:705:GLY:O	3:F:708:THR:HB	1.93	0.67
3:I:402:TYR:HB3	3:I:447:SER:HB2	1.76	0.67
3:F:236:ASN:HB3	3:F:242:ASP:OD2	1.93	0.67
3:F:718:LEU:HD13	3:F:725:ALA:HB1	1.77	0.67
1:G:52:TRP:O	1:G:56:ARG:HB2	1.93	0.67
3:C:539:ASN:HD22	3:C:541:ALA:N	1.91	0.67
1:D:150:HIS:CD2	1:D:152:ILE:HB	2.29	0.67
3:F:188:VAL:HG21	3:F:386:ILE:HD11	1.76	0.67
3:F:493:ASN:HD22	3:F:495:LYS:NZ	1.92	0.67
3:I:470:TYR:O	3:I:474:LEU:HD13	1.94	0.67
1:A:133:TRP:O	1:A:144:LYS:HE2	1.95	0.67
3:F:198:ASN:HD21	3:F:378:SER:H	1.42	0.67
3:I:345:LEU:HB3	3:I:349:MET:HE2	1.77	0.67
3:I:497:SER:HB3	3:I:535:LEU:CD1	2.23	0.67
3:F:498:ALA:HB2	3:F:553:VAL:HG23	1.76	0.67
3:F:708:THR:CG2	3:F:711:ALA:H	2.02	0.67
1:G:215:MET:HE1	1:G:244:GLY:C	2.19	0.67
3:I:213:VAL:HG11	3:I:345:LEU:HD22	1.75	0.67
1:A:28:LEU:HD23	1:A:38:PHE:HD1	1.59	0.67
1:D:133:TRP:O	1:D:144:LYS:HE2	1.95	0.67
3:I:493:ASN:HD22	3:I:495:LYS:HZ2	1.43	0.67
1:A:150:HIS:CD2	1:A:152:ILE:HB	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:263:THR:HG22	3:C:265:ALA:H	1.59	0.67
2:B:31:HIS:O	2:B:33:SER:N	2.28	0.67
3:C:188:VAL:HG21	3:C:386:ILE:HD11	1.77	0.67
3:I:236:ASN:HB3	3:I:242:ASP:OD2	1.95	0.67
1:A:4:ARG:HD3	1:A:4:ARG:N	2.10	0.67
3:C:402:TYR:HB3	3:C:447:SER:HB2	1.77	0.67
3:C:198:ASN:ND2	3:C:378:SER:H	1.93	0.66
1:D:4:ARG:HD3	1:D:4:ARG:N	2.10	0.66
1:G:25:PHE:O	1:G:44:ARG:NH1	2.27	0.66
1:A:215:MET:HE1	1:A:244:GLY:C	2.20	0.66
3:C:236:ASN:HB3	3:C:242:ASP:OD2	1.95	0.66
3:C:470:TYR:O	3:C:474:LEU:HD13	1.96	0.66
3:F:402:TYR:HB3	3:F:447:SER:HB2	1.76	0.66
3:I:153:VAL:HB	3:I:154:PRO:HD3	1.76	0.66
3:F:198:ASN:ND2	3:F:378:SER:H	1.92	0.66
3:F:263:THR:HG22	3:F:265:ALA:H	1.60	0.66
3:I:718:LEU:HD13	3:I:725:ALA:HB1	1.78	0.66
3:F:540:ALA:O	3:F:543:PRO:HD2	1.94	0.66
1:G:198:VAL:HG22	1:G:199:THR:N	2.10	0.66
1:A:52:TRP:O	1:A:56:ARG:HB2	1.96	0.66
1:A:150:HIS:HD2	1:A:153:ARG:H	1.41	0.66
1:G:4:ARG:HD3	1:G:4:ARG:N	2.11	0.66
3:I:699:HIS:HD2	3:I:702:TRP:H	1.43	0.66
3:C:297:PHE:O	3:C:336:THR:HG21	1.96	0.66
1:A:214:THR:HB	1:A:263:GLU:HB2	1.78	0.66
1:D:214:THR:HB	1:D:263:GLU:HB2	1.77	0.66
3:F:297:PHE:O	3:F:336:THR:HG21	1.96	0.66
1:G:225:ASP:OD2	1:G:227:LYS:HB3	1.96	0.66
1:D:28:LEU:CD2	1:D:38:PHE:HD1	2.09	0.65
3:C:323:PRO:HG3	3:F:729:THR:HG22	1.76	0.65
3:I:708:THR:CG2	3:I:711:ALA:H	2.02	0.65
1:A:185:PRO:HB3	1:A:266:GLY:O	1.96	0.65
1:D:225:ASP:OD2	1:D:227:LYS:HB3	1.95	0.65
3:C:198:ASN:HD21	3:C:378:SER:H	1.42	0.65
3:C:497:SER:HB3	3:C:535:LEU:CD1	2.27	0.65
3:F:699:HIS:HD2	3:F:702:TRP:H	1.45	0.65
3:I:198:ASN:ND2	3:I:378:SER:H	1.93	0.65
3:I:635:MET:CE	3:I:728:GLU:HG3	2.26	0.65
1:A:28:LEU:CD2	1:A:38:PHE:HD1	2.10	0.65
1:A:67:GLN:HE22	3:C:657:THR:HB	1.62	0.65
3:C:635:MET:HE2	3:C:728:GLU:HG3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:498:ALA:HB2	3:I:553:VAL:HG23	1.79	0.65
3:C:699:HIS:HD2	3:C:702:TRP:H	1.45	0.65
3:I:297:PHE:O	3:I:336:THR:HG21	1.96	0.65
3:I:600:LYS:HD2	3:I:608:ASN:ND2	2.11	0.65
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.79	0.65
3:C:493:ASN:HD22	3:C:495:LYS:NZ	1.93	0.65
3:I:205:LYS:HE3	3:I:370:SER:HA	1.79	0.65
3:C:278:GLY:HA2	3:C:333:PRO:O	1.97	0.65
1:A:225:ASP:OD2	1:A:227:LYS:HB3	1.97	0.64
2:H:33:SER:HB2	2:H:54:LEU:HD21	1.78	0.64
2:B:31:HIS:HB3	2:B:32:PRO:CD	2.28	0.64
3:F:470:TYR:O	3:F:474:LEU:HD13	1.98	0.64
1:G:214:THR:HB	1:G:263:GLU:HB2	1.78	0.64
3:I:278:GLY:HA2	3:I:333:PRO:O	1.97	0.64
3:F:345:LEU:HB3	3:F:349:MET:HE2	1.77	0.64
3:F:497:SER:HB3	3:F:535:LEU:CD1	2.27	0.64
1:G:28:LEU:HD23	1:G:38:PHE:HD1	1.62	0.64
3:C:345:LEU:HB3	3:C:349:MET:HE2	1.78	0.64
6:G:309:GOL:H32	3:I:646:ARG:NH2	2.12	0.64
3:C:213:VAL:HG11	3:C:345:LEU:HD22	1.78	0.64
3:F:575:GLU:O	3:F:579:ARG:HG3	1.98	0.64
3:F:635:MET:HE2	3:F:728:GLU:HG3	1.79	0.64
3:C:498:ALA:HB2	3:C:553:VAL:HG23	1.78	0.63
3:F:278:GLY:HA2	3:F:333:PRO:O	1.97	0.63
3:I:198:ASN:HD21	3:I:378:SER:H	1.45	0.63
1:D:145:LEU:HD22	1:D:149:ARG:HH22	1.64	0.63
1:G:28:LEU:CD2	1:G:38:PHE:HD1	2.10	0.63
3:I:155:ARG:HD2	3:I:409:ARG:O	1.98	0.62
3:I:635:MET:HE2	3:I:728:GLU:HG3	1.81	0.62
1:A:132:ASP:HB2	1:A:148:GLU:OE2	1.98	0.62
3:F:204:ASP:O	3:F:206:ASN:N	2.32	0.62
1:G:133:TRP:O	1:G:144:LYS:HE2	1.98	0.62
2:E:31:HIS:HB3	2:E:32:PRO:CD	2.28	0.62
2:E:7:ILE:HD12	2:E:7:ILE:H	1.64	0.62
1:A:25:PHE:O	1:A:44:ARG:NH1	2.29	0.62
3:F:319:THR:HG22	3:F:321:PHE:H	1.64	0.62
3:I:188:VAL:HG21	3:I:386:ILE:HD11	1.81	0.62
3:I:667:ASP:HB3	3:I:670:VAL:HG12	1.81	0.62
1:G:218:LEU:HB2	1:G:259:THR:OG1	2.00	0.62
3:I:192:VAL:HG12	3:I:193:LYS:N	2.15	0.62
3:F:192:VAL:HG12	3:F:193:LYS:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:153:VAL:HB	3:I:154:PRO:CD	2.30	0.62
3:I:263:THR:HG22	3:I:265:ALA:H	1.63	0.62
1:D:74:HIS:HB3	3:F:646:ARG:NH1	2.14	0.61
1:D:236:PRO:HG2	2:E:65:LEU:HD22	1.82	0.61
3:F:258:ARG:HD2	3:F:284:ASP:OD1	2.00	0.61
3:F:302:HIS:HE1	3:F:326:SER:OG	1.83	0.61
1:G:132:ASP:HB2	1:G:148:GLU:OE2	2.00	0.61
3:I:618:LEU:HD13	3:I:701:PHE:HZ	1.65	0.61
2:H:31:HIS:HB3	2:H:32:PRO:CD	2.30	0.61
3:C:263:THR:HB	3:C:266:GLU:HG3	1.82	0.61
1:D:132:ASP:HB2	1:D:148:GLU:OE2	2.00	0.61
2:B:7:ILE:HD12	2:B:7:ILE:H	1.66	0.61
2:H:16:GLU:HG2	2:H:19:LYS:HD3	1.82	0.61
3:C:575:GLU:O	3:C:579:ARG:HG3	1.99	0.61
3:C:590:ALA:O	3:C:593:VAL:HG22	2.01	0.61
3:F:618:LEU:HD13	3:F:701:PHE:HZ	1.66	0.61
3:C:153:VAL:HB	3:C:154:PRO:CD	2.30	0.61
3:C:192:VAL:HG12	3:C:193:LYS:N	2.15	0.61
3:C:155:ARG:HD2	3:C:409:ARG:O	2.00	0.61
2:E:33:SER:HB2	2:E:54:LEU:HD21	1.81	0.60
3:F:539:ASN:HD22	3:F:541:ALA:N	1.93	0.60
3:I:203:VAL:HG11	3:I:207:GLY:HA2	1.81	0.60
3:F:209:LEU:HD12	3:F:210:VAL:H	1.65	0.60
2:E:79:ALA:CB	2:E:94:LYS:HA	2.31	0.60
2:H:79:ALA:CB	2:H:94:LYS:HA	2.31	0.60
3:C:319:THR:HG22	3:C:321:PHE:H	1.66	0.60
3:F:153:VAL:HB	3:F:154:PRO:CD	2.30	0.60
3:F:618:LEU:CD1	3:F:701:PHE:HZ	2.14	0.60
3:I:319:THR:HG22	3:I:321:PHE:H	1.66	0.60
3:C:155:ARG:HH12	3:C:419:SER:HB3	1.66	0.60
3:C:611:TYR:CZ	3:C:656:LEU:HD23	2.37	0.60
1:D:218:LEU:HB2	1:D:259:THR:OG1	2.02	0.60
1:G:43:SER:O	1:G:45:ARG:N	2.35	0.60
3:I:501:LEU:HD23	3:I:611:TYR:HA	1.83	0.60
2:E:7:ILE:HD12	2:E:7:ILE:N	2.16	0.60
1:A:43:SER:O	1:A:45:ARG:N	2.35	0.60
3:F:611:TYR:CZ	3:F:656:LEU:HD23	2.36	0.60
3:I:590:ALA:O	3:I:593:VAL:HG22	2.02	0.60
3:F:667:ASP:HB3	3:F:670:VAL:HG12	1.83	0.60
3:I:540:ALA:O	3:I:543:PRO:HD2	2.02	0.60
3:C:174:ARG:HG2	3:C:174:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:386:ILE:CG2	3:C:454:SER:HB3	2.32	0.59
3:C:540:ALA:O	3:C:543:PRO:HD2	2.02	0.59
3:I:258:ARG:HD2	3:I:284:ASP:OD1	2.02	0.59
2:B:16:GLU:HG2	2:B:19:LYS:HD3	1.83	0.59
3:F:580:ILE:HD11	3:F:586:VAL:HG21	1.84	0.59
3:I:580:ILE:HD11	3:I:586:VAL:HG21	1.83	0.59
3:F:155:ARG:HD2	3:F:409:ARG:O	2.02	0.59
3:F:664:GLU:CD	3:F:664:GLU:N	2.57	0.59
2:H:7:ILE:H	2:H:7:ILE:HD12	1.67	0.59
2:B:12:ARG:NH2	2:B:22:PHE:CE2	2.70	0.59
1:D:74:HIS:HB3	3:F:646:ARG:HH12	1.68	0.59
1:D:146:GLU:HG2	3:F:640:GLN:NE2	2.18	0.59
3:F:263:THR:HB	3:F:266:GLU:HG3	1.84	0.59
3:I:263:THR:HB	3:I:266:GLU:HG3	1.84	0.59
3:C:600:LYS:HB3	3:C:608:ASN:HD22	1.67	0.59
3:I:174:ARG:HH11	3:I:174:ARG:HG2	1.66	0.59
2:B:79:ALA:CB	2:B:94:LYS:HA	2.30	0.59
1:D:21:GLY:O	1:D:22:LEU:O	2.20	0.59
1:A:184:VAL:HG12	1:A:209:TYR:HB3	1.84	0.59
3:C:258:ARG:HD2	3:C:284:ASP:OD1	2.03	0.59
3:C:664:GLU:CD	3:C:664:GLU:N	2.57	0.59
2:E:31:HIS:O	2:E:62:PHE:HD2	1.85	0.59
1:G:145:LEU:HD22	1:G:149:ARG:HH22	1.66	0.59
3:I:539:ASN:HD22	3:I:541:ALA:N	1.91	0.59
1:A:63:LEU:HD21	3:C:657:THR:HG22	1.85	0.58
3:C:618:LEU:HD13	3:C:701:PHE:HZ	1.68	0.58
1:D:43:SER:O	1:D:45:ARG:N	2.35	0.58
2:B:7:ILE:HD12	2:B:7:ILE:N	2.19	0.58
3:F:141:THR:OG1	3:F:584:ASN:HB2	2.03	0.58
3:F:590:ALA:O	3:F:593:VAL:HG22	2.03	0.58
3:I:575:GLU:O	3:I:579:ARG:HG3	2.03	0.58
3:I:600:LYS:HB3	3:I:608:ASN:HD22	1.68	0.58
3:C:146:LEU:HD22	3:C:146:LEU:O	2.03	0.58
1:A:87:HIS:HB3	1:A:89:HIS:CE1	2.38	0.58
3:F:155:ARG:HH12	3:F:419:SER:HB3	1.67	0.58
3:I:203:VAL:CG1	3:I:204:ASP:N	2.67	0.58
1:D:150:HIS:HE1	3:F:641:TRP:HA	1.69	0.58
3:C:401:HIS:CE1	3:C:679:MET:HE1	2.38	0.58
3:C:580:ILE:HD11	3:C:586:VAL:HG21	1.86	0.58
3:C:667:ASP:HB3	3:C:670:VAL:HG12	1.85	0.58
3:I:721:GLN:O	3:I:723:ASN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:HIS:O	2:B:62:PHE:HD2	1.86	0.58
3:C:501:LEU:HD23	3:C:611:TYR:HA	1.86	0.58
3:F:134:LYS:HZ1	3:F:435:ASP:HB3	1.67	0.58
3:F:600:LYS:HB3	3:F:608:ASN:HD22	1.69	0.58
1:D:53:VAL:HB	1:D:57:ILE:CD1	2.33	0.58
2:E:12:ARG:NH2	2:E:22:PHE:CE2	2.72	0.58
3:I:699:HIS:CD2	3:I:702:TRP:CD1	2.91	0.58
3:F:174:ARG:HG2	3:F:174:ARG:HH11	1.68	0.58
3:I:501:LEU:CD2	3:I:611:TYR:HA	2.33	0.58
3:C:699:HIS:CD2	3:C:702:TRP:CD1	2.92	0.58
3:C:618:LEU:CD1	3:C:701:PHE:HZ	2.17	0.57
1:D:268:ASP:HB2	1:D:269:GLN:NE2	2.18	0.57
3:F:721:GLN:O	3:F:723:ASN:N	2.37	0.57
3:I:134:LYS:HZ1	3:I:435:ASP:HB3	1.68	0.57
3:C:473:SER:HB3	3:F:753:VAL:HG13	1.86	0.57
3:F:496:VAL:HG11	3:F:506:ILE:HD13	1.87	0.57
1:G:184:VAL:HG12	1:G:209:TYR:HB3	1.85	0.57
2:H:12:ARG:NH2	2:H:22:PHE:CE2	2.71	0.57
2:H:31:HIS:O	2:H:62:PHE:HD2	1.87	0.57
3:I:611:TYR:CZ	3:I:656:LEU:HD23	2.39	0.57
3:I:155:ARG:HH12	3:I:419:SER:HB3	1.68	0.57
1:D:87:HIS:HB3	1:D:89:HIS:CE1	2.39	0.57
1:D:184:VAL:HG12	1:D:209:TYR:HB3	1.86	0.57
1:A:43:SER:O	1:A:45:ARG:HG2	2.04	0.57
1:D:43:SER:O	1:D:45:ARG:HG2	2.04	0.57
3:C:721:GLN:O	3:C:723:ASN:N	2.37	0.57
3:F:153:VAL:HG23	3:F:154:PRO:CD	2.34	0.57
3:I:496:VAL:HG11	3:I:506:ILE:HD13	1.87	0.57
3:C:141:THR:HG23	3:C:573:TYR:OH	2.05	0.57
3:F:467:LEU:HD21	3:F:544:PHE:CE2	2.40	0.57
1:A:218:LEU:HB2	1:A:259:THR:OG1	2.03	0.56
3:C:141:THR:OG1	3:C:584:ASN:HB2	2.05	0.56
3:C:230:GLY:O	3:C:372:ASN:HB2	2.05	0.56
2:H:7:ILE:HD12	2:H:7:ILE:N	2.20	0.56
3:C:728:GLU:O	3:C:732:ARG:HG3	2.06	0.56
1:D:80:PHE:HA	1:D:96:LEU:HD22	1.86	0.56
2:E:16:GLU:HG2	2:E:19:LYS:HD3	1.86	0.56
1:A:149:ARG:O	1:A:151:LYS:HG2	2.04	0.56
3:C:150:ASN:O	3:C:153:VAL:HG22	2.05	0.56
3:F:635:MET:HE1	3:F:726:PHE:HZ	1.70	0.56
3:F:728:GLU:O	3:F:732:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:SER:O	1:G:45:ARG:HG2	2.06	0.56
2:H:19:LYS:O	2:H:72:PRO:HD2	2.06	0.56
3:I:141:THR:OG1	3:I:584:ASN:HB2	2.05	0.56
3:I:401:HIS:CE1	3:I:679:MET:HE1	2.40	0.56
3:I:551:PRO:HD3	3:I:682:GLU:HG2	1.87	0.56
1:A:21:GLY:O	1:A:22:LEU:O	2.23	0.56
3:F:386:ILE:CG2	3:F:454:SER:HB3	2.32	0.56
3:I:150:ASN:O	3:I:153:VAL:HG22	2.04	0.56
3:F:501:LEU:CD2	3:F:611:TYR:HA	2.35	0.56
1:D:79:ASP:OD1	1:D:153:ARG:NH2	2.39	0.56
3:F:146:LEU:O	3:F:146:LEU:HD22	2.04	0.56
1:G:225:ASP:OD1	1:G:228:GLU:HG2	2.06	0.56
1:D:192:HIS:HB2	1:D:201:LEU:HD23	1.88	0.56
3:I:153:VAL:HG23	3:I:154:PRO:CD	2.34	0.56
1:A:216:LYS:HE3	1:A:261:GLN:NE2	2.20	0.56
1:D:225:ASP:OD1	1:D:228:GLU:HG2	2.06	0.56
1:G:268:ASP:HB2	1:G:269:GLN:NE2	2.17	0.56
3:I:295:LEU:HD22	3:I:570:MET:CE	2.36	0.56
1:A:80:PHE:HA	1:A:96:LEU:HD22	1.87	0.56
3:C:346:PHE:HA	3:C:349:MET:HE3	1.87	0.56
3:F:346:PHE:HA	3:F:349:MET:HE3	1.87	0.56
3:F:501:LEU:HD23	3:F:611:TYR:HA	1.86	0.56
1:G:192:HIS:HB2	1:G:201:LEU:HD23	1.87	0.56
1:A:268:ASP:HB2	1:A:269:GLN:NE2	2.18	0.56
2:E:19:LYS:O	2:E:72:PRO:HD2	2.06	0.56
3:I:302:HIS:HE1	3:I:326:SER:OG	1.89	0.56
3:I:635:MET:HE1	3:I:726:PHE:HZ	1.71	0.56
3:C:134:LYS:HZ1	3:C:435:ASP:HB3	1.71	0.55
3:C:153:VAL:HG23	3:C:154:PRO:CD	2.35	0.55
2:B:19:LYS:O	2:B:72:PRO:HD2	2.06	0.55
1:D:191:THR:HG23	1:D:202:ARG:HB3	1.88	0.55
3:F:401:HIS:CE1	3:F:679:MET:HE1	2.40	0.55
1:A:151:LYS:O	1:A:155:ARG:HG3	2.06	0.55
3:F:213:VAL:HG11	3:F:345:LEU:CD2	2.36	0.55
3:C:699:HIS:CD2	3:C:702:TRP:H	2.24	0.55
1:D:235:LEU:HD13	2:E:10:TYR:CE1	2.41	0.55
3:C:134:LYS:NZ	3:C:435:ASP:HB3	2.22	0.55
3:F:518:THR:C	3:F:520:GLN:H	2.15	0.55
1:G:21:GLY:O	1:G:22:LEU:O	2.23	0.55
1:G:87:HIS:HB3	1:G:89:HIS:CE1	2.42	0.55
3:I:134:LYS:NZ	3:I:435:ASP:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:635:MET:HE1	3:C:726:PHE:HZ	1.72	0.55
3:F:428:LYS:HE2	3:F:428:LYS:CA	2.37	0.55
3:F:699:HIS:CD2	3:F:702:TRP:H	2.24	0.55
3:C:206:ASN:C	3:C:206:ASN:ND2	2.63	0.55
3:C:632:ILE:HG21	3:C:639:LEU:HD13	1.88	0.55
3:F:231:LYS:O	3:F:253:SER:HB2	2.07	0.55
1:A:35:LEU:HD22	1:A:49:ARG:HG3	1.88	0.55
3:F:514:LYS:HD2	3:F:519:GLY:O	2.06	0.55
3:F:632:ILE:HG21	3:F:639:LEU:HD13	1.89	0.55
3:I:618:LEU:CD1	3:I:701:PHE:HZ	2.19	0.55
1:A:192:HIS:HB2	1:A:201:LEU:HD23	1.88	0.55
1:A:225:ASP:OD1	1:A:228:GLU:HG2	2.07	0.55
3:F:134:LYS:NZ	3:F:435:ASP:HB3	2.21	0.55
3:F:283:MET:HE2	3:F:297:PHE:CG	2.42	0.55
1:G:149:ARG:O	1:G:151:LYS:HG2	2.07	0.55
1:G:151:LYS:O	1:G:155:ARG:HG3	2.07	0.55
1:G:50:THR:HG22	1:G:52:TRP:HD1	1.71	0.55
1:A:53:VAL:HB	1:A:57:ILE:CD1	2.36	0.54
3:F:493:ASN:HB2	3:F:495:LYS:NZ	2.21	0.54
1:G:191:THR:HG23	1:G:202:ARG:HB3	1.88	0.54
3:I:147:LEU:C	3:I:148:ASN:HD22	2.14	0.54
3:I:632:ILE:HG21	3:I:639:LEU:HD13	1.89	0.54
1:D:97:GLN:HB2	2:E:60:TRP:CE3	2.42	0.54
3:F:295:LEU:HD22	3:F:570:MET:CE	2.37	0.54
3:F:297:PHE:N	3:F:297:PHE:CD2	2.75	0.54
3:I:297:PHE:CD2	3:I:297:PHE:N	2.75	0.54
3:C:518:THR:C	3:C:520:GLN:H	2.15	0.54
3:F:150:ASN:O	3:F:153:VAL:HG22	2.07	0.54
3:I:141:THR:HG23	3:I:573:TYR:OH	2.06	0.54
3:C:501:LEU:CD2	3:C:611:TYR:HA	2.37	0.54
3:C:514:LYS:HD2	3:C:519:GLY:O	2.07	0.54
3:F:231:LYS:HG3	3:F:253:SER:HB3	1.89	0.54
1:D:206:LEU:HD22	2:E:12:ARG:O	2.08	0.54
3:I:213:VAL:HG11	3:I:345:LEU:CD2	2.37	0.54
1:A:145:LEU:HD22	1:A:149:ARG:HH22	1.71	0.54
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.42	0.54
3:C:153:VAL:CB	3:C:154:PRO:CD	2.86	0.54
1:D:216:LYS:HE3	1:D:261:GLN:NE2	2.23	0.54
3:F:153:VAL:CB	3:F:154:PRO:CD	2.85	0.54
3:I:231:LYS:O	3:I:253:SER:HB2	2.07	0.54
1:A:198:VAL:HG22	1:A:199:THR:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LEU:C	3:C:148:ASN:HD22	2.15	0.54
3:C:254:ILE:HA	3:C:277:ILE:O	2.08	0.54
3:F:655:ARG:HH11	3:F:655:ARG:CG	2.21	0.54
3:C:231:LYS:HG3	3:C:253:SER:HB3	1.89	0.54
1:D:151:LYS:O	1:D:155:ARG:HG3	2.08	0.54
1:G:79:ASP:OD1	1:G:153:ARG:NH2	2.41	0.54
3:C:213:VAL:HG11	3:C:345:LEU:CD2	2.38	0.54
1:D:50:THR:HG22	1:D:52:TRP:HD1	1.72	0.53
3:I:153:VAL:CB	3:I:154:PRO:CD	2.86	0.53
1:D:232:LYS:HD2	1:D:232:LYS:O	2.08	0.53
1:G:198:VAL:HG22	1:G:199:THR:H	1.73	0.53
3:I:728:GLU:O	3:I:732:ARG:HG3	2.08	0.53
3:C:231:LYS:O	3:C:253:SER:HB2	2.08	0.53
1:D:198:VAL:HG22	1:D:199:THR:H	1.71	0.53
3:F:214:GLU:O	3:F:216:PRO:HD3	2.09	0.53
1:A:79:ASP:OD1	1:A:153:ARG:NH2	2.42	0.53
3:C:278:GLY:H	3:C:332:ILE:HB	1.74	0.53
3:C:493:ASN:HB2	3:C:495:LYS:NZ	2.20	0.53
3:C:496:VAL:HG11	3:C:506:ILE:HD13	1.90	0.53
3:C:214:GLU:O	3:C:216:PRO:HD3	2.09	0.53
3:C:234:HIS:ND1	3:C:235:ALA:O	2.41	0.53
3:C:250:VAL:CG1	3:C:276:ALA:HB2	2.38	0.53
3:F:154:PRO:HD2	3:F:161:LYS:HE3	1.91	0.53
3:I:655:ARG:HH11	3:I:655:ARG:CG	2.21	0.53
3:C:297:PHE:N	3:C:297:PHE:CD2	2.76	0.53
3:C:664:GLU:C	3:C:666:THR:H	2.16	0.53
3:I:346:PHE:HA	3:I:349:MET:HE3	1.91	0.53
3:I:278:GLY:H	3:I:332:ILE:HB	1.74	0.53
1:A:125:GLU:HB3	1:A:134:ARG:HG2	1.90	0.53
1:D:235:LEU:HD13	2:E:10:TYR:CZ	2.44	0.53
3:F:699:HIS:CD2	3:F:702:TRP:CD1	2.96	0.53
1:A:50:THR:HG22	1:A:52:TRP:HD1	1.73	0.53
3:C:154:PRO:HD2	3:C:161:LYS:HE3	1.90	0.53
1:D:125:GLU:HB3	1:D:134:ARG:HG2	1.89	0.53
1:G:216:LYS:HE3	1:G:261:GLN:NE2	2.23	0.53
1:A:191:THR:HG23	1:A:202:ARG:HB3	1.91	0.53
3:F:310:THR:HG22	3:F:313:PHE:CE1	2.44	0.53
1:G:80:PHE:HA	1:G:96:LEU:HD22	1.91	0.53
3:C:302:HIS:HE1	3:C:326:SER:OG	1.91	0.52
3:C:199:SER:OG	3:C:376:THR:HG23	2.08	0.52
2:E:71:THR:HG23	2:E:71:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:71:THR:HG23	2:H:71:THR:O	2.10	0.52
3:I:230:GLY:O	3:I:372:ASN:HB2	2.09	0.52
3:I:283:MET:HE2	3:I:297:PHE:CG	2.44	0.52
3:I:467:LEU:HD21	3:I:544:PHE:CE2	2.43	0.52
1:D:35:LEU:HD22	1:D:49:ARG:HG3	1.91	0.52
3:F:135:LEU:HD23	3:F:432:MET:SD	2.50	0.52
3:I:146:LEU:O	3:I:146:LEU:HD22	2.09	0.52
3:I:250:VAL:CG1	3:I:276:ALA:HB2	2.40	0.52
3:C:231:LYS:HG3	3:C:253:SER:CB	2.38	0.52
3:C:551:PRO:HD3	3:C:682:GLU:HG2	1.91	0.52
1:G:150:HIS:NE2	1:G:152:ILE:HB	2.24	0.52
3:I:386:ILE:CG2	3:I:454:SER:HB3	2.36	0.52
3:F:147:LEU:C	3:F:148:ASN:HD22	2.16	0.52
2:H:21:ASN:CG	2:H:22:PHE:H	2.17	0.52
3:I:514:LYS:HD2	3:I:519:GLY:O	2.08	0.52
3:F:230:GLY:O	3:F:372:ASN:HB2	2.09	0.52
3:I:518:THR:C	3:I:520:GLN:H	2.17	0.52
3:C:729:THR:HG22	3:F:323:PRO:HG3	1.92	0.52
1:D:206:LEU:HD11	2:E:14:PRO:CD	2.36	0.52
3:F:254:ILE:HA	3:F:277:ILE:O	2.10	0.52
3:F:278:GLY:H	3:F:332:ILE:HB	1.75	0.52
1:G:50:THR:CG2	1:G:52:TRP:HD1	2.22	0.52
3:I:664:GLU:C	3:I:666:THR:H	2.18	0.52
3:F:141:THR:HG23	3:F:573:TYR:OH	2.08	0.52
1:G:125:GLU:HB3	1:G:134:ARG:HG2	1.91	0.52
1:G:188:VAL:HB	1:G:273:VAL:HG21	1.91	0.52
3:I:493:ASN:HB2	3:I:495:LYS:NZ	2.22	0.52
3:C:354:PRO:HD3	3:C:365:MET:SD	2.50	0.52
2:H:33:SER:HB3	2:H:62:PHE:CE2	2.45	0.52
3:C:150:ASN:HA	3:C:153:VAL:HG22	1.92	0.51
3:F:184:ASP:HB2	3:F:390:PHE:HE1	1.75	0.51
3:F:237:PHE:O	3:F:267:LYS:HG2	2.10	0.51
1:G:35:LEU:HD22	1:G:49:ARG:HG3	1.91	0.51
1:G:49:ARG:O	1:G:50:THR:HB	2.10	0.51
1:G:81:TRP:CH2	3:I:623:ARG:HB2	2.44	0.51
3:I:231:LYS:HG3	3:I:253:SER:HB3	1.92	0.51
3:I:699:HIS:CD2	3:I:702:TRP:H	2.24	0.51
3:C:295:LEU:HD22	3:C:570:MET:CE	2.37	0.51
1:D:50:THR:CG2	1:D:52:TRP:HD1	2.23	0.51
1:D:53:VAL:HB	1:D:57:ILE:HD12	1.92	0.51
3:F:250:VAL:CG1	3:F:276:ALA:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:297:PHE:N	3:F:297:PHE:HD2	2.07	0.51
3:I:297:PHE:N	3:I:297:PHE:HD2	2.08	0.51
3:I:310:THR:HG22	3:I:313:PHE:CE1	2.45	0.51
3:I:354:PRO:HD3	3:I:365:MET:SD	2.51	0.51
3:C:414:PRO:HB2	3:C:571:ASP:O	2.10	0.51
3:I:401:HIS:ND1	3:I:679:MET:HE1	2.25	0.51
1:A:107:ASP:O	1:A:108:ASN:HB2	2.09	0.51
3:C:122:LEU:O	3:C:123:TYR:CB	2.59	0.51
3:C:237:PHE:O	3:C:267:LYS:HG2	2.10	0.51
1:D:150:HIS:NE2	1:D:152:ILE:HB	2.25	0.51
3:F:205:LYS:HE3	3:F:370:SER:HA	1.93	0.51
3:F:231:LYS:HG3	3:F:253:SER:CB	2.40	0.51
1:G:8:LEU:HB2	1:G:169:LEU:HD13	1.92	0.51
1:A:50:THR:CG2	1:A:52:TRP:HD1	2.23	0.51
3:C:283:MET:HE2	3:C:297:PHE:CG	2.46	0.51
3:F:203:VAL:CG1	3:F:204:ASP:N	2.71	0.51
1:G:53:VAL:HB	1:G:57:ILE:CD1	2.40	0.51
3:I:254:ILE:HA	3:I:277:ILE:O	2.11	0.51
3:I:625:LEU:HD13	3:I:713:LEU:HD21	1.91	0.51
1:A:49:ARG:O	1:A:50:THR:HB	2.11	0.51
3:C:236:ASN:C	3:C:238:GLY:N	2.65	0.51
1:D:67:GLN:HE22	3:F:657:THR:HB	1.75	0.51
3:F:551:PRO:HD3	3:F:682:GLU:HG2	1.92	0.51
3:I:305:THR:HG21	3:I:543:PRO:HG3	1.93	0.51
3:I:414:PRO:HB2	3:I:571:ASP:O	2.10	0.51
3:F:229:THR:HG22	3:F:374:LYS:HG3	1.93	0.51
3:I:154:PRO:HD2	3:I:161:LYS:HE3	1.92	0.51
3:I:231:LYS:HG3	3:I:253:SER:CB	2.41	0.51
3:I:150:ASN:HA	3:I:153:VAL:HG22	1.92	0.51
3:I:199:SER:OG	3:I:376:THR:HG23	2.10	0.51
1:D:49:ARG:O	1:D:50:THR:HB	2.11	0.51
3:F:414:PRO:HB2	3:F:571:ASP:O	2.10	0.51
1:G:215:MET:HE1	1:G:245:TRP:N	2.25	0.51
3:I:724:GLY:O	3:I:725:ALA:C	2.53	0.51
3:C:625:LEU:HD13	3:C:713:LEU:HD21	1.92	0.51
1:D:264:HIS:ND1	1:D:266:GLY:N	2.48	0.51
3:F:708:THR:HG22	3:F:711:ALA:N	2.04	0.51
1:G:232:LYS:HD2	1:G:232:LYS:O	2.11	0.51
1:A:188:VAL:HB	1:A:273:VAL:HG21	1.93	0.50
2:B:71:THR:O	2:B:71:THR:HG23	2.10	0.50
3:C:135:LEU:HD23	3:C:432:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:236:ASN:O	3:C:238:GLY:N	2.44	0.50
1:D:22:LEU:CD1	3:F:619:LEU:HD23	2.31	0.50
1:A:53:VAL:HB	1:A:57:ILE:HD12	1.92	0.50
1:D:149:ARG:O	1:D:151:LYS:HG2	2.12	0.50
3:F:625:LEU:HD13	3:F:713:LEU:HD21	1.93	0.50
2:H:29:GLY:HA2	2:H:61:SER:HB2	1.93	0.50
3:I:229:THR:HG22	3:I:374:LYS:HG3	1.92	0.50
3:C:401:HIS:ND1	3:C:679:MET:HE1	2.27	0.50
3:C:428:LYS:HE2	3:C:428:LYS:CA	2.39	0.50
3:C:747:ASN:HB3	3:C:756:ILE:HD13	1.93	0.50
1:D:107:ASP:O	1:D:108:ASN:HB2	2.10	0.50
3:I:428:LYS:HE2	3:I:428:LYS:CA	2.39	0.50
3:C:297:PHE:N	3:C:297:PHE:HD2	2.09	0.50
1:D:92:GLU:HB2	1:D:94:HIS:NE2	2.27	0.50
3:F:354:PRO:HD3	3:F:365:MET:SD	2.51	0.50
1:G:263:GLU:HG2	1:G:270:PRO:HB3	1.94	0.50
3:I:203:VAL:HG13	3:I:204:ASP:N	2.27	0.50
1:D:215:MET:HE1	1:D:245:TRP:N	2.25	0.50
3:F:199:SER:OG	3:F:376:THR:HG23	2.11	0.50
3:I:236:ASN:O	3:I:238:GLY:N	2.43	0.50
3:C:184:ASP:HB2	3:C:390:PHE:HE1	1.76	0.50
3:C:229:THR:HG22	3:C:374:LYS:HG3	1.94	0.50
3:C:467:LEU:HD22	3:C:548:SER:OG	2.12	0.50
1:D:46:VAL:HG21	1:D:66:SER:HA	1.93	0.50
1:D:198:VAL:HA	1:D:252:PRO:CG	2.38	0.50
3:I:236:ASN:C	3:I:238:GLY:N	2.65	0.50
1:A:232:LYS:HD2	1:A:232:LYS:O	2.12	0.50
1:D:207:ASN:HD21	2:E:13:HIS:HD2	1.57	0.50
3:F:498:ALA:HB2	3:F:553:VAL:HA	1.93	0.50
1:G:146:GLU:CD	3:I:629:ARG:HH22	2.19	0.50
3:C:305:THR:HG21	3:C:543:PRO:HG3	1.94	0.50
3:F:664:GLU:C	3:F:666:THR:H	2.18	0.50
1:G:107:ASP:O	1:G:108:ASN:HB2	2.10	0.50
3:I:690:VAL:HG11	3:I:707:HIS:HB3	1.94	0.50
3:F:622:VAL:HG13	3:F:643:TYR:CE2	2.47	0.50
3:I:279:VAL:HB	3:I:334:VAL:HG13	1.94	0.50
1:A:92:GLU:HB2	1:A:94:HIS:NE2	2.27	0.49
1:A:215:MET:HE1	1:A:245:TRP:N	2.26	0.49
2:B:21:ASN:CG	2:B:22:PHE:H	2.18	0.49
1:D:263:GLU:HG2	1:D:270:PRO:HB3	1.94	0.49
3:F:150:ASN:HA	3:F:153:VAL:HG22	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:345:LEU:HB3	3:I:349:MET:CE	2.41	0.49
3:C:467:LEU:HD21	3:C:544:PHE:CE2	2.47	0.49
1:D:176:GLY:O	1:D:177:ARG:C	2.54	0.49
3:F:234:HIS:ND1	3:F:235:ALA:O	2.45	0.49
3:F:236:ASN:O	3:F:238:GLY:N	2.44	0.49
1:G:18:GLN:O	1:G:19:ASP:CB	2.59	0.49
3:I:135:LEU:HD23	3:I:432:MET:SD	2.52	0.49
2:E:33:SER:HB3	2:E:62:PHE:CE2	2.47	0.49
3:F:502:LEU:O	3:F:506:ILE:HG13	2.12	0.49
3:F:635:MET:HE1	3:F:726:PHE:CZ	2.46	0.49
3:C:724:GLY:O	3:C:725:ALA:C	2.55	0.49
1:D:131:LEU:HD21	1:D:158:ARG:CZ	2.43	0.49
3:F:724:GLY:O	3:F:725:ALA:C	2.55	0.49
1:D:188:VAL:HB	1:D:273:VAL:HG21	1.93	0.49
1:D:238:GLY:HA3	2:E:67:TYR:CZ	2.48	0.49
3:I:192:VAL:HG12	3:I:193:LYS:H	1.76	0.49
3:I:209:LEU:HD12	3:I:210:VAL:N	2.22	0.49
3:I:234:HIS:ND1	3:I:235:ALA:O	2.46	0.49
1:A:198:VAL:HA	1:A:252:PRO:CG	2.42	0.49
3:F:166:ALA:HB1	3:F:389:ILE:CD1	2.43	0.49
1:G:150:HIS:O	1:G:151:LYS:HB2	2.12	0.49
3:I:237:PHE:O	3:I:267:LYS:HG2	2.13	0.49
1:A:228:GLU:OE2	1:G:134:ARG:NH2	2.46	0.49
3:C:655:ARG:HH11	3:C:655:ARG:CG	2.24	0.49
1:D:104:MET:HE3	1:D:169:LEU:HD23	1.95	0.49
3:C:712:LEU:C	3:C:712:LEU:HD23	2.38	0.49
3:C:753:VAL:HG13	3:F:473:SER:CB	2.41	0.49
1:D:8:LEU:HB2	1:D:169:LEU:HD13	1.94	0.49
3:F:209:LEU:HD12	3:F:210:VAL:N	2.27	0.49
1:G:18:GLN:H	1:G:18:GLN:NE2	2.10	0.49
3:I:184:ASP:HB2	3:I:390:PHE:HE1	1.77	0.49
1:A:135:ALA:HB1	1:A:140:ALA:HB3	1.95	0.48
1:A:176:GLY:O	1:A:177:ARG:C	2.55	0.48
3:C:494:PHE:HA	3:C:556:CYS:O	2.13	0.48
1:D:23:SER:OG	1:D:73:ASP:OD2	2.30	0.48
3:F:203:VAL:HG11	3:F:207:GLY:HA2	1.94	0.48
3:F:345:LEU:HB3	3:F:349:MET:CE	2.43	0.48
1:G:31:VAL:O	1:G:34:GLN:HB2	2.12	0.48
1:A:18:GLN:O	1:A:19:ASP:CB	2.59	0.48
1:A:35:LEU:CD2	1:A:49:ARG:HG3	2.42	0.48
3:F:305:THR:HG21	3:F:543:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:LEU:HD12	3:I:619:LEU:HD23	1.95	0.48
1:G:92:GLU:HB2	1:G:94:HIS:NE2	2.28	0.48
1:A:31:VAL:O	1:A:34:GLN:HB2	2.13	0.48
1:A:57:ILE:HG12	1:A:175:LEU:CD2	2.43	0.48
1:A:150:HIS:NE2	1:A:152:ILE:HB	2.27	0.48
1:A:198:VAL:CG2	1:A:199:THR:N	2.75	0.48
3:C:310:THR:HG22	3:C:313:PHE:CE1	2.48	0.48
3:C:595:GLY:O	3:C:599:ILE:HG12	2.13	0.48
1:D:90:SER:C	1:D:92:GLU:H	2.20	0.48
3:F:279:VAL:HB	3:F:334:VAL:HG13	1.96	0.48
3:F:401:HIS:ND1	3:F:679:MET:HE1	2.28	0.48
1:G:57:ILE:HG12	1:G:175:LEU:CD2	2.43	0.48
2:H:1:ILE:HG23	2:H:1:ILE:O	2.13	0.48
2:E:21:ASN:CG	2:E:22:PHE:H	2.19	0.48
3:F:192:VAL:HG12	3:F:193:LYS:H	1.77	0.48
3:F:247:TYR:CD1	3:F:247:TYR:N	2.81	0.48
1:G:46:VAL:HG21	1:G:66:SER:HA	1.96	0.48
1:G:135:ALA:HB1	1:G:140:ALA:HB3	1.96	0.48
3:I:595:GLY:O	3:I:599:ILE:HG12	2.12	0.48
3:I:635:MET:HE1	3:I:726:PHE:CZ	2.47	0.48
1:A:22:LEU:O	1:A:23:SER:O	2.32	0.48
1:A:263:GLU:HG2	1:A:270:PRO:HB3	1.96	0.48
1:D:31:VAL:O	1:D:34:GLN:HB2	2.12	0.48
3:F:690:VAL:HG11	3:F:707:HIS:HB3	1.94	0.48
1:G:131:LEU:HD21	1:G:158:ARG:CZ	2.44	0.48
3:C:414:PRO:HG2	3:C:572:THR:HG22	1.96	0.48
1:G:198:VAL:CG2	1:G:199:THR:N	2.77	0.48
1:A:236:PRO:HG2	2:B:65:LEU:HD22	1.96	0.48
3:C:191:GLN:NE2	3:C:222:TYR:H	2.12	0.48
3:C:625:LEU:HD13	3:C:713:LEU:CD2	2.43	0.48
1:D:191:THR:O	1:D:192:HIS:HB3	2.14	0.48
1:G:90:SER:C	1:G:92:GLU:H	2.21	0.48
3:I:214:GLU:O	3:I:216:PRO:HD3	2.14	0.48
1:A:53:VAL:C	1:A:55:SER:H	2.21	0.48
1:D:191:THR:CG2	1:D:202:ARG:HB3	2.44	0.48
1:G:53:VAL:HB	1:G:57:ILE:HD12	1.95	0.48
3:I:467:LEU:HD22	3:I:548:SER:OG	2.13	0.48
1:A:18:GLN:H	1:A:18:GLN:NE2	2.11	0.48
1:D:18:GLN:H	1:D:18:GLN:NE2	2.12	0.48
1:D:198:VAL:CG2	1:D:199:THR:N	2.76	0.48
3:F:155:ARG:NH1	3:F:419:SER:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:VAL:C	1:G:55:SER:H	2.21	0.48
3:I:166:ALA:HB1	3:I:389:ILE:CD1	2.44	0.48
1:A:90:SER:C	1:A:92:GLU:H	2.20	0.48
3:C:178:LEU:O	3:C:179:SER:C	2.55	0.48
3:C:622:VAL:HG13	3:C:643:TYR:CE2	2.49	0.48
1:D:57:ILE:HG12	1:D:175:LEU:CD2	2.44	0.48
1:D:256:GLN:HE22	1:D:257:ARG:HG3	1.79	0.48
2:E:56:PHE:HB3	2:E:62:PHE:CD1	2.49	0.48
3:F:122:LEU:O	3:F:123:TYR:CB	2.61	0.48
3:C:155:ARG:NH1	3:C:419:SER:HB3	2.28	0.47
3:C:247:TYR:CD1	3:C:247:TYR:N	2.81	0.47
1:A:49:ARG:O	1:A:50:THR:CB	2.61	0.47
3:C:664:GLU:C	3:C:666:THR:N	2.72	0.47
3:F:178:LEU:O	3:F:179:SER:C	2.55	0.47
3:I:247:TYR:CD1	3:I:247:TYR:N	2.81	0.47
3:C:194:ASP:CG	3:C:195:SER:N	2.73	0.47
1:G:23:SER:OG	1:G:73:ASP:OD2	2.32	0.47
1:G:35:LEU:CD2	1:G:49:ARG:HG3	2.44	0.47
3:I:603:HIS:CD2	3:I:603:HIS:C	2.92	0.47
3:C:502:LEU:O	3:C:506:ILE:HG13	2.14	0.47
3:C:724:GLY:O	3:C:726:PHE:N	2.48	0.47
1:G:176:GLY:O	1:G:177:ARG:C	2.57	0.47
1:G:264:HIS:ND1	1:G:266:GLY:N	2.47	0.47
1:A:25:PHE:CD1	1:A:25:PHE:N	2.82	0.47
1:A:264:HIS:ND1	1:A:266:GLY:N	2.49	0.47
3:C:122:LEU:O	3:C:126:ASP:OD2	2.33	0.47
1:D:49:ARG:O	1:D:50:THR:CB	2.62	0.47
3:F:203:VAL:HG13	3:F:204:ASP:N	2.29	0.47
3:F:494:PHE:HA	3:F:556:CYS:O	2.14	0.47
1:G:191:THR:CG2	1:G:202:ARG:HB3	2.45	0.47
1:A:8:LEU:HB2	1:A:169:LEU:HD13	1.95	0.47
1:A:40:ASP:OD2	1:A:40:ASP:C	2.57	0.47
1:A:46:VAL:HG21	1:A:66:SER:HA	1.97	0.47
1:A:191:THR:O	1:A:192:HIS:HB3	2.14	0.47
3:C:205:LYS:HB2	3:C:370:SER:O	2.14	0.47
3:C:690:VAL:HG11	3:C:707:HIS:HB3	1.96	0.47
1:D:22:LEU:O	1:D:23:SER:O	2.33	0.47
3:F:531:LYS:HD3	3:F:531:LYS:C	2.39	0.47
6:G:309:GOL:C3	3:I:646:ARG:HH21	2.24	0.47
3:I:178:LEU:O	3:I:179:SER:C	2.57	0.47
3:I:708:THR:HG22	3:I:711:ALA:N	2.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:192:VAL:HG12	3:C:193:LYS:H	1.77	0.47
1:D:28:LEU:CD2	1:D:38:PHE:CD1	2.95	0.47
3:F:479:PHE:O	3:F:551:PRO:HG2	2.15	0.47
1:G:120:GLY:CA	2:H:31:HIS:CE1	2.98	0.47
3:C:345:LEU:HB3	3:C:349:MET:CE	2.45	0.47
3:C:635:MET:HE1	3:C:726:PHE:CZ	2.48	0.47
1:D:35:LEU:CD2	1:D:49:ARG:HG3	2.45	0.47
1:D:150:HIS:CD2	1:D:153:ARG:H	2.27	0.47
1:A:92:GLU:CB	1:A:94:HIS:NE2	2.78	0.47
3:C:236:ASN:O	3:C:237:PHE:HB2	2.15	0.47
1:G:104:MET:HE3	1:G:169:LEU:HD23	1.96	0.47
1:G:236:PRO:HG2	2:H:65:LEU:HD22	1.97	0.47
3:I:163:GLU:O	3:I:167:LEU:HD13	2.14	0.47
3:I:622:VAL:HG13	3:I:643:TYR:CE2	2.50	0.47
3:C:747:ASN:N	3:C:747:ASN:HD22	2.13	0.46
3:F:149:GLU:O	3:F:151:SER:N	2.48	0.46
1:A:191:THR:CG2	1:A:202:ARG:HB3	2.46	0.46
3:C:628:TYR:O	3:C:632:ILE:HG12	2.15	0.46
3:C:699:HIS:CD2	3:C:701:PHE:HB2	2.50	0.46
1:D:179:VAL:HG12	1:D:179:VAL:O	2.16	0.46
2:H:16:GLU:O	2:H:17:ASN:C	2.58	0.46
3:I:664:GLU:CD	3:I:664:GLU:N	2.60	0.46
3:I:747:ASN:HB3	3:I:756:ILE:HD13	1.97	0.46
3:C:483:ASN:ND2	3:C:540:ALA:HB3	2.31	0.46
1:D:209:TYR:HA	1:D:210:PRO:O	2.15	0.46
3:F:153:VAL:CG2	3:F:154:PRO:CD	2.94	0.46
3:F:747:ASN:HB3	3:F:756:ILE:HD13	1.97	0.46
1:G:256:GLN:HE22	1:G:257:ARG:HG3	1.79	0.46
1:A:104:MET:HE3	1:A:169:LEU:HD23	1.97	0.46
3:C:166:ALA:HB1	3:C:389:ILE:CD1	2.46	0.46
1:D:92:GLU:CB	1:D:94:HIS:NE2	2.79	0.46
3:F:149:GLU:C	3:F:151:SER:N	2.72	0.46
3:F:664:GLU:C	3:F:666:THR:N	2.73	0.46
3:C:231:LYS:CG	3:C:253:SER:HB3	2.46	0.46
1:D:194:VAL:HG22	1:D:199:THR:CG2	2.44	0.46
3:F:712:LEU:HD23	3:F:712:LEU:C	2.40	0.46
1:A:207:ASN:HD21	2:B:13:HIS:CD2	2.33	0.46
3:C:153:VAL:CG2	3:C:154:PRO:CD	2.94	0.46
2:E:29:GLY:HA2	2:E:61:SER:HB2	1.97	0.46
1:G:40:ASP:C	1:G:40:ASP:OD2	2.59	0.46
1:G:218:LEU:HB2	1:G:259:THR:HG1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:GLU:HG2	2:H:83:ASN:HB3	1.98	0.46
3:I:155:ARG:NH1	3:I:419:SER:HB3	2.29	0.46
2:B:56:PHE:HB3	2:B:62:PHE:CD1	2.51	0.46
3:C:150:ASN:C	3:C:153:VAL:HG22	2.41	0.46
3:C:603:HIS:CD2	3:C:603:HIS:C	2.93	0.46
2:E:17:ASN:HA	2:E:72:PRO:O	2.16	0.46
2:H:45:ARG:HG3	2:H:45:ARG:O	2.16	0.46
3:I:149:GLU:C	3:I:151:SER:N	2.73	0.46
3:I:724:GLY:O	3:I:726:PHE:N	2.47	0.46
2:B:16:GLU:O	2:B:17:ASN:C	2.58	0.46
3:C:639:LEU:HD12	3:C:639:LEU:HA	1.73	0.46
1:D:135:ALA:HB1	1:D:140:ALA:HB3	1.97	0.46
1:G:22:LEU:O	1:G:23:SER:O	2.33	0.46
2:H:56:PHE:HB3	2:H:62:PHE:CD1	2.51	0.46
1:A:150:HIS:O	1:A:151:LYS:HB2	2.15	0.46
1:D:146:GLU:CD	3:F:629:ARG:HH22	2.24	0.46
3:F:603:HIS:CD2	3:F:603:HIS:C	2.94	0.46
3:F:625:LEU:HD13	3:F:713:LEU:CD2	2.45	0.46
1:G:50:THR:CG2	1:G:52:TRP:CD1	2.99	0.46
3:I:625:LEU:HD13	3:I:713:LEU:CD2	2.45	0.46
3:I:712:LEU:C	3:I:712:LEU:HD23	2.40	0.46
1:A:144:LYS:O	1:A:148:GLU:HG3	2.16	0.46
3:I:153:VAL:CG2	3:I:154:PRO:CD	2.94	0.46
1:A:4:ARG:N	1:A:4:ARG:CD	2.79	0.45
3:C:260:GLY:C	3:C:262:ILE:H	2.22	0.45
1:D:4:ARG:O	1:D:4:ARG:HG2	2.16	0.45
3:F:194:ASP:CG	3:F:195:SER:N	2.74	0.45
3:F:231:LYS:CG	3:F:253:SER:HB3	2.46	0.45
1:G:4:ARG:HG2	1:G:4:ARG:O	2.16	0.45
1:G:35:LEU:CD2	1:G:35:LEU:C	2.89	0.45
1:G:49:ARG:O	1:G:50:THR:CB	2.63	0.45
3:I:414:PRO:HG2	3:I:572:THR:HG22	1.97	0.45
1:A:66:SER:O	1:A:70:LYS:HG3	2.17	0.45
1:A:178:GLY:O	1:A:182:GLN:HB2	2.16	0.45
1:D:25:PHE:N	1:D:25:PHE:CD1	2.83	0.45
2:E:54:LEU:HD11	2:E:62:PHE:HB3	1.99	0.45
3:F:747:ASN:N	3:F:747:ASN:HD22	2.14	0.45
1:G:25:PHE:CD1	1:G:25:PHE:N	2.84	0.45
1:G:198:VAL:HA	1:G:252:PRO:CG	2.44	0.45
3:C:149:GLU:O	3:C:151:SER:N	2.50	0.45
3:C:279:VAL:HB	3:C:334:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:316:PHE:CD1	3:F:740:TRP:CH2	3.04	0.45
3:C:531:LYS:HD3	3:C:531:LYS:C	2.41	0.45
1:D:53:VAL:C	1:D:55:SER:H	2.24	0.45
1:D:150:HIS:O	1:D:151:LYS:HB2	2.17	0.45
3:F:699:HIS:CD2	3:F:701:PHE:H	2.34	0.45
1:G:230:GLU:CD	1:G:230:GLU:H	2.25	0.45
2:H:35:ILE:HD11	2:H:82:VAL:CG1	2.46	0.45
3:I:150:ASN:C	3:I:153:VAL:HG22	2.41	0.45
3:I:236:ASN:O	3:I:237:PHE:HB2	2.17	0.45
3:I:316:PHE:O	3:I:319:THR:HB	2.16	0.45
3:I:544:PHE:O	3:I:548:SER:HB2	2.16	0.45
3:C:149:GLU:C	3:C:151:SER:N	2.74	0.45
1:D:4:ARG:N	1:D:4:ARG:CD	2.79	0.45
1:D:110:THR:HG21	1:D:166:PRO:HG3	1.98	0.45
1:G:18:GLN:H	1:G:18:GLN:CD	2.24	0.45
1:G:22:LEU:O	1:G:23:SER:HB3	2.16	0.45
3:I:600:LYS:HB3	3:I:608:ASN:ND2	2.32	0.45
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.97	0.45
1:D:40:ASP:OD2	1:D:40:ASP:C	2.59	0.45
2:E:35:ILE:HD11	2:E:82:VAL:CG1	2.46	0.45
3:F:507:GLU:O	3:F:511:GLN:HG3	2.17	0.45
1:G:178:GLY:O	1:G:182:GLN:HB2	2.16	0.45
1:G:209:TYR:HA	1:G:210:PRO:O	2.16	0.45
1:A:23:SER:OG	1:A:73:ASP:OD2	2.34	0.45
1:A:74:HIS:HB3	3:C:646:ARG:NH1	2.32	0.45
1:A:209:TYR:HA	1:A:210:PRO:O	2.16	0.45
3:F:316:PHE:O	3:F:319:THR:HB	2.16	0.45
1:G:92:GLU:CB	1:G:94:HIS:NE2	2.80	0.45
3:I:494:PHE:HA	3:I:556:CYS:O	2.16	0.45
3:I:496:VAL:HG22	3:I:555:PHE:HB3	1.99	0.45
3:C:435:ASP:O	3:C:436:MET:C	2.60	0.45
3:C:448:ILE:HD13	3:C:598:VAL:HG11	1.99	0.45
3:F:232:LEU:HD11	3:F:256:ILE:HB	1.99	0.45
3:F:493:ASN:ND2	3:F:495:LYS:HZ2	2.05	0.45
3:I:194:ASP:CG	3:I:195:SER:N	2.75	0.45
1:A:35:LEU:CD2	1:A:35:LEU:C	2.90	0.45
1:A:49:ARG:HD2	2:B:53:ASP:OD2	2.16	0.45
3:F:414:PRO:HG2	3:F:572:THR:HG22	1.98	0.45
3:F:435:ASP:O	3:F:436:MET:C	2.59	0.45
2:H:17:ASN:HA	2:H:72:PRO:O	2.17	0.45
3:I:439:LYS:C	3:I:441:GLY:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:618:LEU:HD12	3:I:618:LEU:HA	1.81	0.45
3:C:232:LEU:HB3	3:C:367:THR:HG23	1.98	0.45
3:C:310:THR:N	3:C:311:PRO:CD	2.79	0.45
3:C:316:PHE:O	3:C:319:THR:HB	2.16	0.45
1:D:144:LYS:O	1:D:148:GLU:HG3	2.16	0.45
1:D:230:GLU:H	1:D:230:GLU:CD	2.25	0.45
2:E:36:GLU:HG2	2:E:83:ASN:HB3	1.99	0.45
1:G:144:LYS:O	1:G:148:GLU:HG3	2.17	0.45
2:H:54:LEU:HD11	2:H:62:PHE:HB3	1.98	0.45
3:I:531:LYS:HD3	3:I:531:LYS:C	2.42	0.45
3:C:186:HIS:CE1	3:C:316:PHE:CE2	3.05	0.45
1:D:53:VAL:HA	1:D:57:ILE:HG13	1.99	0.45
3:F:518:THR:HG22	3:F:520:GLN:HB2	1.99	0.45
1:G:179:VAL:HG12	1:G:179:VAL:O	2.17	0.45
1:A:50:THR:CG2	1:A:52:TRP:CD1	3.00	0.44
2:B:17:ASN:HA	2:B:72:PRO:O	2.17	0.44
2:B:35:ILE:HD11	2:B:82:VAL:CG1	2.47	0.44
2:B:68:THR:HG22	2:B:69:GLU:O	2.17	0.44
1:D:35:LEU:CD2	1:D:35:LEU:C	2.91	0.44
1:D:114:TRP:HB3	1:D:126:PHE:HB3	1.99	0.44
1:D:178:GLY:O	1:D:182:GLN:HB2	2.17	0.44
2:E:35:ILE:HD11	2:E:82:VAL:HG13	2.00	0.44
3:F:122:LEU:O	3:F:126:ASP:OD2	2.35	0.44
1:G:215:MET:HE3	1:G:246:ILE:HG23	1.99	0.44
3:I:507:GLU:O	3:I:511:GLN:HG3	2.17	0.44
1:A:114:TRP:HB3	1:A:126:PHE:HB3	1.99	0.44
3:C:240:LYS:HE3	3:C:240:LYS:HB2	1.87	0.44
3:F:724:GLY:O	3:F:726:PHE:N	2.50	0.44
2:H:35:ILE:HD11	2:H:82:VAL:HG13	1.99	0.44
3:I:186:HIS:CE1	3:I:316:PHE:CE2	3.05	0.44
3:I:231:LYS:CG	3:I:253:SER:HB3	2.46	0.44
1:A:85:GLU:HG3	3:C:629:ARG:HD3	2.00	0.44
3:F:163:GLU:O	3:F:167:LEU:HD13	2.17	0.44
3:F:595:GLY:O	3:F:599:ILE:HG12	2.16	0.44
1:D:18:GLN:O	1:D:19:ASP:CB	2.60	0.44
2:E:16:GLU:O	2:E:17:ASN:C	2.59	0.44
2:E:45:ARG:O	2:E:45:ARG:HG3	2.18	0.44
1:A:254:GLU:O	1:A:255:GLU:C	2.61	0.44
1:D:9:HIS:HB3	1:D:113:TYR:OH	2.18	0.44
3:F:515:HIS:CD2	3:F:518:THR:H	2.35	0.44
3:F:640:GLN:OE1	3:F:643:TYR:HD1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:TRP:HB3	1:G:126:PHE:HB3	1.99	0.44
3:I:149:GLU:O	3:I:151:SER:N	2.50	0.44
3:I:345:LEU:C	3:I:349:MET:HE3	2.43	0.44
3:I:479:PHE:O	3:I:551:PRO:HG2	2.18	0.44
3:I:588:ARG:HH11	3:I:588:ARG:HG3	1.83	0.44
1:A:18:GLN:H	1:A:18:GLN:CD	2.24	0.44
1:A:256:GLN:HE22	1:A:257:ARG:HG3	1.82	0.44
2:B:31:HIS:CB	2:B:32:PRO:CD	2.96	0.44
2:B:39:LEU:CD2	2:B:80:CYS:HB3	2.47	0.44
3:C:147:LEU:CD2	3:C:165:LEU:HD11	2.48	0.44
3:F:483:ASN:ND2	3:F:540:ALA:HB3	2.32	0.44
3:I:122:LEU:O	3:I:126:ASP:OD2	2.35	0.44
3:I:528:TRP:CG	3:I:529:ALA:N	2.85	0.44
1:A:110:THR:HG21	1:A:166:PRO:HG3	1.99	0.44
2:B:54:LEU:HD11	2:B:62:PHE:HB3	2.00	0.44
3:C:476:LEU:HB2	3:F:680:ARG:HH22	1.83	0.44
1:D:22:LEU:O	1:D:23:SER:HB3	2.18	0.44
1:D:50:THR:CG2	1:D:52:TRP:CD1	3.01	0.44
2:E:1:ILE:HG23	2:E:1:ILE:O	2.18	0.44
3:F:191:GLN:NE2	3:F:222:TYR:H	2.16	0.44
1:G:4:ARG:N	1:G:4:ARG:CD	2.79	0.44
1:G:28:LEU:CD2	1:G:38:PHE:CD1	2.97	0.44
3:I:240:LYS:HE3	3:I:240:LYS:HB2	1.90	0.44
2:B:1:ILE:HG23	2:B:1:ILE:O	2.16	0.44
2:B:45:ARG:O	2:B:45:ARG:HG3	2.17	0.44
3:C:163:GLU:O	3:C:167:LEU:HD13	2.17	0.44
3:C:221:ALA:O	3:C:222:TYR:HB2	2.17	0.44
1:D:18:GLN:H	1:D:18:GLN:CD	2.25	0.44
1:D:115:LYS:HE3	1:D:125:GLU:OE2	2.18	0.44
1:D:204:ARG:NH2	2:E:11:SER:O	2.51	0.44
3:F:211:TYR:O	3:F:212:LEU:HB3	2.18	0.44
3:I:448:ILE:HD13	3:I:598:VAL:HG11	2.00	0.44
3:I:747:ASN:N	3:I:747:ASN:HD22	2.15	0.44
1:A:28:LEU:CD2	1:A:38:PHE:CD1	2.96	0.44
3:C:272:GLU:OE1	3:C:331:ASN:HB2	2.17	0.44
3:C:498:ALA:HB2	3:C:553:VAL:HA	1.98	0.44
3:F:150:ASN:C	3:F:153:VAL:HG22	2.43	0.44
3:F:348:ASN:HD22	3:F:348:ASN:N	2.15	0.44
2:H:31:HIS:O	2:H:62:PHE:CD2	2.71	0.44
3:I:628:TYR:O	3:I:632:ILE:HG12	2.18	0.44
1:A:230:GLU:CD	1:A:230:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:SER:HA	2:H:22:PHE:O	2.18	0.43
3:I:664:GLU:C	3:I:666:THR:N	2.73	0.43
2:B:36:GLU:HG2	2:B:83:ASN:HB3	1.98	0.43
3:C:588:ARG:HG3	3:C:588:ARG:HH11	1.84	0.43
2:E:39:LEU:CD2	2:E:80:CYS:HB3	2.47	0.43
2:B:4:THR:OG1	2:B:5:PRO:HD2	2.18	0.43
3:C:232:LEU:HD11	3:C:256:ILE:HB	1.99	0.43
1:G:121:GLN:NE2	2:H:1:ILE:CG2	2.81	0.43
1:G:191:THR:O	1:G:192:HIS:HB3	2.16	0.43
3:I:348:ASN:N	3:I:348:ASN:HD22	2.16	0.43
3:I:699:HIS:CD2	3:I:701:PHE:HB2	2.53	0.43
1:A:49:ARG:HH11	2:B:53:ASP:CG	2.25	0.43
2:B:35:ILE:HD11	2:B:82:VAL:HG13	2.01	0.43
3:C:528:TRP:CG	3:C:529:ALA:N	2.87	0.43
2:E:31:HIS:CB	2:E:32:PRO:CD	2.96	0.43
3:F:236:ASN:O	3:F:237:PHE:HB2	2.18	0.43
3:F:293:ALA:HB2	3:F:339:ARG:NH1	2.33	0.43
3:F:439:LYS:C	3:F:441:GLY:H	2.26	0.43
1:A:98:VAL:HA	1:A:115:LYS:O	2.19	0.43
1:A:115:LYS:HE3	1:A:125:GLU:OE2	2.18	0.43
1:A:126:PHE:CE2	1:A:128:PRO:HG3	2.54	0.43
3:F:190:ILE:HB	3:F:458:PHE:CE2	2.54	0.43
3:F:628:TYR:O	3:F:632:ILE:HG12	2.18	0.43
2:H:9:VAL:HG21	2:H:95:TRP:HA	1.99	0.43
3:I:125:ASP:O	3:I:129:ARG:HG3	2.19	0.43
3:I:260:GLY:C	3:I:262:ILE:H	2.24	0.43
3:I:310:THR:N	3:I:311:PRO:CD	2.81	0.43
3:I:515:HIS:CD2	3:I:518:THR:H	2.36	0.43
1:A:57:ILE:CA	1:A:175:LEU:HD21	2.43	0.43
3:C:122:LEU:N	3:C:122:LEU:HD12	2.34	0.43
2:E:68:THR:HG22	2:E:69:GLU:O	2.18	0.43
3:F:699:HIS:CD2	3:F:701:PHE:HB2	2.53	0.43
3:F:717:LYS:O	3:F:720:LYS:HG2	2.19	0.43
1:G:78:VAL:HG22	3:I:622:VAL:HG11	2.01	0.43
3:I:448:ILE:HD13	3:I:598:VAL:CG1	2.48	0.43
1:A:194:VAL:HG22	1:A:199:THR:CG2	2.45	0.43
3:C:179:SER:HB3	3:C:394:LYS:HG3	2.01	0.43
3:C:243:PHE:HB3	3:C:274:LEU:HD11	2.00	0.43
3:C:268:VAL:HG21	3:C:334:VAL:HG21	2.01	0.43
3:C:290:ILE:O	3:C:339:ARG:NH2	2.51	0.43
3:F:260:GLY:C	3:F:262:ILE:H	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:31:HIS:CB	2:H:32:PRO:CD	2.97	0.43
3:I:483:ASN:ND2	3:I:540:ALA:HB3	2.33	0.43
1:A:131:LEU:HD21	1:A:158:ARG:CZ	2.48	0.43
3:C:135:LEU:HD13	3:C:592:GLU:HB2	2.01	0.43
3:C:515:HIS:CD2	3:C:518:THR:H	2.37	0.43
2:E:21:ASN:N	2:E:70:PHE:O	2.46	0.43
3:F:122:LEU:N	3:F:122:LEU:HD12	2.34	0.43
3:F:125:ASP:O	3:F:129:ARG:HG3	2.19	0.43
3:F:496:VAL:HG22	3:F:555:PHE:HB3	1.99	0.43
3:F:504:THR:HG22	3:F:508:LYS:HE2	2.01	0.43
3:F:528:TRP:CG	3:F:529:ALA:N	2.86	0.43
3:C:699:HIS:CD2	3:C:701:PHE:H	2.36	0.43
2:E:37:VAL:HG22	2:E:82:VAL:HG22	2.00	0.43
3:F:467:LEU:HD22	3:F:548:SER:OG	2.19	0.43
1:G:115:LYS:HE3	1:G:125:GLU:OE2	2.18	0.43
3:I:435:ASP:O	3:I:436:MET:C	2.60	0.43
1:A:22:LEU:HD12	3:C:619:LEU:CD2	2.46	0.43
2:B:21:ASN:N	2:B:70:PHE:O	2.46	0.43
3:C:129:ARG:HH11	3:C:129:ARG:HB3	1.84	0.43
3:C:348:ASN:N	3:C:348:ASN:HD22	2.17	0.43
3:C:544:PHE:O	3:C:548:SER:HB2	2.19	0.43
1:D:198:VAL:CG2	1:D:199:THR:H	2.32	0.43
1:G:53:VAL:HG23	1:G:54:SER:N	2.34	0.43
3:I:229:THR:CG2	3:I:374:LYS:HG3	2.49	0.43
3:I:243:PHE:HB3	3:I:274:LEU:HD11	2.01	0.43
3:I:600:LYS:O	3:I:608:ASN:ND2	2.52	0.43
1:A:4:ARG:O	1:A:4:ARG:HG2	2.18	0.42
2:B:9:VAL:HG21	2:B:95:TRP:HA	2.01	0.42
3:C:250:VAL:O	3:C:251:ASN:C	2.61	0.42
3:C:600:LYS:HB3	3:C:608:ASN:ND2	2.32	0.42
3:C:618:LEU:HD12	3:C:618:LEU:HA	1.81	0.42
1:D:49:ARG:NH1	2:E:53:ASP:OD2	2.38	0.42
1:D:209:TYR:CD1	1:D:209:TYR:C	2.97	0.42
3:F:588:ARG:HG3	3:F:588:ARG:HH11	1.84	0.42
1:G:28:LEU:HD21	1:G:38:PHE:CD1	2.54	0.42
3:I:502:LEU:O	3:I:506:ILE:HG13	2.19	0.42
1:A:254:GLU:OE2	1:A:257:ARG:NH1	2.53	0.42
3:F:147:LEU:CD2	3:F:165:LEU:HD11	2.48	0.42
2:H:40:LEU:HA	2:H:44:GLU:O	2.19	0.42
3:I:129:ARG:HH11	3:I:129:ARG:HB3	1.84	0.42
3:I:518:THR:HG22	3:I:520:GLN:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:LYS:O	3:C:208:ARG:NH1	2.52	0.42
1:D:126:PHE:CE2	1:D:128:PRO:HG3	2.54	0.42
1:D:254:GLU:O	1:D:255:GLU:C	2.62	0.42
2:E:40:LEU:HA	2:E:44:GLU:O	2.18	0.42
3:F:193:LYS:NZ	3:F:217:GLY:O	2.42	0.42
3:F:229:THR:HA	3:F:373:VAL:O	2.19	0.42
3:F:290:ILE:O	3:F:339:ARG:NH2	2.52	0.42
1:G:202:ARG:CZ	2:H:99:MET:HG2	2.48	0.42
3:I:122:LEU:HD12	3:I:122:LEU:N	2.34	0.42
3:I:268:VAL:HG21	3:I:334:VAL:HG21	2.01	0.42
3:I:349:MET:HG2	3:I:367:THR:HA	2.01	0.42
1:A:209:TYR:CD1	1:A:209:TYR:C	2.97	0.42
3:C:439:LYS:C	3:C:441:GLY:H	2.27	0.42
3:C:580:ILE:HA	3:C:581:PRO:HD2	1.88	0.42
3:F:335:GLN:NE2	3:F:336:THR:H	2.17	0.42
1:G:235:LEU:HD13	2:H:10:TYR:CZ	2.54	0.42
3:I:135:LEU:HD13	3:I:592:GLU:HB2	2.01	0.42
3:I:232:LEU:HB3	3:I:367:THR:HG23	2.00	0.42
3:C:229:THR:CG2	3:C:374:LYS:HG3	2.49	0.42
1:G:49:ARG:HH11	2:H:53:ASP:CG	2.27	0.42
1:G:66:SER:O	1:G:70:LYS:HG3	2.18	0.42
1:G:192:HIS:CB	1:G:201:LEU:HD23	2.49	0.42
2:H:68:THR:HG22	2:H:69:GLU:O	2.19	0.42
1:A:110:THR:HG22	1:A:111:GLU:N	2.35	0.42
3:C:222:TYR:CE2	3:C:308:PRO:HG3	2.54	0.42
3:C:479:PHE:O	3:C:551:PRO:HG2	2.19	0.42
2:E:31:HIS:O	2:E:62:PHE:CD2	2.69	0.42
3:F:243:PHE:HB3	3:F:274:LEU:HD11	2.01	0.42
3:I:293:ALA:HB2	3:I:339:ARG:NH1	2.35	0.42
1:A:206:LEU:CD1	2:B:14:PRO:HD3	2.50	0.42
3:F:129:ARG:HH11	3:F:129:ARG:HB3	1.84	0.42
3:F:211:TYR:CE2	3:F:344:LYS:HD2	2.55	0.42
3:F:349:MET:HG2	3:F:367:THR:HA	2.00	0.42
3:F:509:THR:O	3:F:513:VAL:HG23	2.18	0.42
1:G:63:LEU:HD21	3:I:657:THR:HG22	2.02	0.42
3:I:509:THR:O	3:I:513:VAL:HG23	2.20	0.42
3:C:263:THR:HG22	3:C:264:PHE:N	2.35	0.42
3:C:349:MET:HG2	3:C:367:THR:HA	2.02	0.42
1:D:66:SER:O	1:D:70:LYS:HG3	2.19	0.42
3:F:455:ALA:CB	3:F:461:VAL:HB	2.50	0.42
2:B:37:VAL:HG22	2:B:82:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:640:GLN:OE1	3:C:643:TYR:HD1	2.02	0.42
3:F:250:VAL:O	3:F:251:ASN:C	2.62	0.42
3:F:310:THR:N	3:F:311:PRO:CD	2.82	0.42
3:F:580:ILE:HA	3:F:581:PRO:HD2	1.88	0.42
3:F:639:LEU:HA	3:F:639:LEU:HD12	1.73	0.42
1:G:198:VAL:HG23	1:G:250:VAL:O	2.20	0.42
2:H:37:VAL:HG22	2:H:82:VAL:HG22	2.01	0.42
3:I:186:HIS:CE1	3:I:316:PHE:CZ	3.08	0.42
1:A:192:HIS:CB	1:A:201:LEU:HD23	2.50	0.42
1:A:237:ASN:O	1:A:239:ASP:N	2.50	0.42
2:B:40:LEU:HA	2:B:44:GLU:O	2.19	0.42
3:C:124:TRP:HH2	3:C:596:GLN:HG2	1.83	0.42
1:D:22:LEU:HD12	3:F:619:LEU:CG	2.49	0.42
1:D:37:VAL:HG22	1:D:38:PHE:N	2.35	0.42
3:F:518:THR:C	3:F:520:GLN:N	2.78	0.42
3:F:723:ASN:O	3:F:725:ALA:N	2.53	0.42
1:G:82:THR:HG23	3:I:629:ARG:NH2	2.35	0.42
1:G:255:GLU:OE1	1:G:255:GLU:N	2.52	0.42
2:H:4:THR:OG1	2:H:5:PRO:HD2	2.20	0.42
3:I:699:HIS:CD2	3:I:701:PHE:H	2.37	0.42
3:C:168:TYR:O	3:C:172:GLN:HG2	2.20	0.41
3:C:507:GLU:O	3:C:511:GLN:HG3	2.20	0.41
3:C:518:THR:C	3:C:520:GLN:N	2.78	0.41
3:C:518:THR:HG22	3:C:520:GLN:HB2	2.01	0.41
3:C:539:ASN:ND2	3:C:541:ALA:HB3	2.35	0.41
3:C:664:GLU:O	3:C:666:THR:N	2.53	0.41
1:D:150:HIS:ND1	3:F:640:GLN:HB3	2.35	0.41
1:D:254:GLU:OE2	1:D:257:ARG:NH1	2.53	0.41
2:E:15:ALA:HB2	2:E:95:TRP:CZ2	2.55	0.41
3:F:149:GLU:C	3:F:151:SER:H	2.28	0.41
3:F:536:THR:OG1	3:F:538:ASP:OD1	2.35	0.41
3:F:539:ASN:ND2	3:F:541:ALA:HB3	2.35	0.41
1:G:110:THR:HG22	1:G:111:GLU:N	2.34	0.41
3:I:154:PRO:HA	3:I:413:GLY:O	2.19	0.41
3:I:192:VAL:CG1	3:I:193:LYS:N	2.83	0.41
3:I:290:ILE:O	3:I:339:ARG:NH2	2.53	0.41
1:A:99:ILE:HG23	1:A:99:ILE:O	2.20	0.41
3:C:345:LEU:C	3:C:349:MET:HE3	2.45	0.41
3:C:715:ASN:ND2	3:C:731:PHE:HB2	2.34	0.41
3:F:229:THR:CG2	3:F:374:LYS:HG3	2.50	0.41
3:F:655:ARG:CG	3:F:655:ARG:NH1	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:TYR:CD1	1:G:209:TYR:C	2.98	0.41
3:I:498:ALA:HB2	3:I:553:VAL:HA	2.01	0.41
1:A:22:LEU:O	1:A:23:SER:HB3	2.20	0.41
1:D:235:LEU:HB3	2:E:10:TYR:OH	2.20	0.41
2:E:12:ARG:NH2	2:E:22:PHE:CD2	2.78	0.41
3:F:298:PHE:CG	3:F:299:GLY:N	2.88	0.41
3:F:446:ARG:HH11	3:F:602:THR:HA	1.85	0.41
3:F:709:LEU:HD12	3:F:709:LEU:HA	1.84	0.41
1:G:98:VAL:HA	1:G:115:LYS:O	2.21	0.41
1:G:254:GLU:OE2	1:G:257:ARG:NH1	2.53	0.41
3:I:551:PRO:HD3	3:I:682:GLU:CB	2.50	0.41
3:I:593:VAL:HG23	3:I:594:ALA:N	2.35	0.41
1:A:9:HIS:HB3	1:A:113:TYR:OH	2.20	0.41
1:A:49:ARG:NH1	2:B:53:ASP:OD2	2.37	0.41
1:A:53:VAL:HG23	1:A:54:SER:N	2.34	0.41
1:A:179:VAL:HG12	1:A:179:VAL:O	2.18	0.41
2:B:12:ARG:NH2	2:B:22:PHE:CD2	2.77	0.41
3:C:293:ALA:HB2	3:C:339:ARG:NH1	2.36	0.41
3:C:555:PHE:CD1	3:C:555:PHE:C	2.98	0.41
3:F:154:PRO:HA	3:F:413:GLY:O	2.20	0.41
3:F:192:VAL:CG1	3:F:193:LYS:N	2.82	0.41
3:F:518:THR:HG22	3:F:520:GLN:CG	2.50	0.41
1:G:235:LEU:HD13	2:H:10:TYR:CE1	2.55	0.41
2:H:12:ARG:HG2	2:H:13:HIS:CE1	2.54	0.41
3:I:168:TYR:O	3:I:172:GLN:HG2	2.20	0.41
3:I:210:VAL:HG12	3:I:211:TYR:CD1	2.44	0.41
3:I:705:GLY:HA3	3:I:707:HIS:CE1	2.55	0.41
1:A:35:LEU:HD23	1:A:36:PHE:N	2.36	0.41
1:A:229:PHE:HD1	1:A:230:GLU:O	2.03	0.41
3:C:518:THR:HG22	3:C:520:GLN:CG	2.50	0.41
1:D:192:HIS:CB	1:D:201:LEU:HD23	2.50	0.41
1:G:121:GLN:CG	2:H:1:ILE:HG22	2.50	0.41
1:G:150:HIS:CD2	1:G:153:ARG:H	2.29	0.41
3:I:191:GLN:NE2	3:I:222:TYR:H	2.18	0.41
3:I:493:ASN:ND2	3:I:495:LYS:HZ2	2.14	0.41
1:A:198:VAL:HG23	1:A:250:VAL:O	2.21	0.41
1:A:206:LEU:HD11	2:B:14:PRO:HD3	2.02	0.41
2:B:79:ALA:HB1	2:B:93:VAL:O	2.20	0.41
3:C:205:LYS:NZ	3:C:205:LYS:HB3	2.35	0.41
3:C:263:THR:CG2	3:C:264:PHE:N	2.84	0.41
3:C:353:CYS:HB2	3:C:363:CYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:232:LEU:HB3	3:F:367:THR:HG23	2.01	0.41
3:F:345:LEU:C	3:F:349:MET:HE3	2.45	0.41
1:G:49:ARG:HD2	2:H:53:ASP:OD2	2.21	0.41
1:G:110:THR:CG2	1:G:111:GLU:N	2.83	0.41
1:G:254:GLU:O	1:G:255:GLU:C	2.62	0.41
2:H:21:ASN:N	2:H:70:PHE:O	2.45	0.41
3:I:124:TRP:HH2	3:I:596:GLN:HG2	1.85	0.41
3:I:250:VAL:O	3:I:251:ASN:C	2.64	0.41
3:I:704:SER:O	3:I:707:HIS:CE1	2.74	0.41
3:I:723:ASN:O	3:I:725:ALA:N	2.53	0.41
1:A:110:THR:CG2	1:A:111:GLU:N	2.83	0.41
2:E:4:THR:OG1	2:E:5:PRO:HD2	2.21	0.41
1:G:9:HIS:HB3	1:G:113:TYR:OH	2.20	0.41
1:G:35:LEU:HD23	1:G:36:PHE:N	2.35	0.41
3:I:147:LEU:CD2	3:I:165:LEU:HD11	2.50	0.41
3:I:298:PHE:CG	3:I:299:GLY:N	2.88	0.41
1:A:120:GLY:CA	2:B:31:HIS:CE1	3.04	0.41
3:C:149:GLU:C	3:C:151:SER:H	2.29	0.41
3:C:565:TYR:CE2	3:C:570:MET:HE3	2.56	0.41
3:F:166:ALA:HB1	3:F:389:ILE:HD13	2.02	0.41
3:F:236:ASN:HD21	3:F:258:ARG:HE	1.68	0.41
3:F:241:LYS:O	3:F:244:GLU:HB3	2.21	0.41
1:G:194:VAL:HG22	1:G:199:THR:CG2	2.44	0.41
3:I:655:ARG:CG	3:I:655:ARG:NH1	2.81	0.41
3:I:667:ASP:HB3	3:I:670:VAL:CG1	2.48	0.41
1:A:11:LEU:O	1:A:27:ALA:HA	2.21	0.41
1:A:37:VAL:HG22	1:A:38:PHE:N	2.35	0.41
1:A:198:VAL:CG2	1:A:199:THR:H	2.32	0.41
2:B:12:ARG:HG2	2:B:13:HIS:CE1	2.56	0.41
3:C:125:ASP:O	3:C:129:ARG:HG3	2.20	0.41
3:C:150:ASN:O	3:C:161:LYS:NZ	2.52	0.41
3:C:241:LYS:O	3:C:244:GLU:HB3	2.21	0.41
3:C:298:PHE:CG	3:C:299:GLY:N	2.88	0.41
3:C:550:ILE:O	3:C:551:PRO:C	2.63	0.41
1:D:57:ILE:HG12	1:D:175:LEU:HD21	2.03	0.41
1:D:213:ILE:HG12	1:D:214:THR:N	2.36	0.41
3:F:268:VAL:HG21	3:F:334:VAL:HG21	2.02	0.41
3:I:149:GLU:C	3:I:151:SER:H	2.29	0.41
1:A:215:MET:HE3	1:A:246:ILE:HG23	2.02	0.41
3:C:229:THR:HA	3:C:373:VAL:O	2.21	0.41
3:C:723:ASN:O	3:C:725:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:LEU:HD21	1:D:38:PHE:CD1	2.55	0.41
2:E:76:ASP:O	2:E:97:ARG:NH2	2.54	0.41
3:F:429:LEU:O	3:F:433:PHE:HD1	2.04	0.41
3:F:551:PRO:HD3	3:F:682:GLU:CB	2.51	0.41
2:H:15:ALA:HB2	2:H:95:TRP:CZ2	2.56	0.41
2:H:76:ASP:O	2:H:97:ARG:NH2	2.54	0.41
3:I:555:PHE:CD1	3:I:555:PHE:C	2.98	0.41
1:A:235:LEU:HD13	2:B:10:TYR:CE1	2.56	0.40
2:B:11:SER:HA	2:B:22:PHE:O	2.20	0.40
2:B:13:HIS:O	2:B:21:ASN:OD1	2.39	0.40
3:C:392:VAL:HG22	3:C:393:ILE:N	2.36	0.40
3:C:455:ALA:CB	3:C:461:VAL:HB	2.51	0.40
3:C:705:GLY:HA3	3:C:707:HIS:CE1	2.56	0.40
1:D:6:HIS:HA	1:D:32:ASP:OD1	2.21	0.40
3:F:448:ILE:HD13	3:F:598:VAL:CG1	2.51	0.40
3:F:704:SER:O	3:F:707:HIS:CE1	2.75	0.40
1:G:6:HIS:HA	1:G:32:ASP:OD1	2.21	0.40
1:G:67:GLN:HE22	3:I:657:THR:HB	1.85	0.40
1:G:74:HIS:HB3	3:I:646:ARG:NH1	2.36	0.40
3:I:350:GLU:O	3:I:365:MET:O	2.39	0.40
3:I:505:LEU:HD12	3:I:505:LEU:O	2.21	0.40
3:I:518:THR:HG22	3:I:520:GLN:CG	2.50	0.40
1:A:28:LEU:HD21	1:A:38:PHE:CD1	2.56	0.40
1:A:53:VAL:HA	1:A:57:ILE:HG13	2.02	0.40
3:C:186:HIS:CE1	3:C:316:PHE:CZ	3.10	0.40
3:C:319:THR:CG2	3:C:321:PHE:H	2.32	0.40
3:C:691:SER:HA	3:C:692:PRO:HD3	1.94	0.40
1:D:145:LEU:HB3	1:D:149:ARG:NH2	2.36	0.40
3:F:593:VAL:HG23	3:F:594:ALA:N	2.36	0.40
3:I:190:ILE:HB	3:I:458:PHE:CE2	2.55	0.40
3:I:263:THR:HB	3:I:266:GLU:CG	2.50	0.40
3:I:353:CYS:HB2	3:I:363:CYS:O	2.22	0.40
3:C:154:PRO:HA	3:C:413:GLY:O	2.21	0.40
3:C:335:GLN:NE2	3:C:336:THR:H	2.19	0.40
1:D:9:HIS:CE1	1:D:30:TYR:HB2	2.57	0.40
3:F:168:TYR:O	3:F:172:GLN:HG2	2.21	0.40
3:F:272:GLU:OE1	3:F:331:ASN:HB2	2.22	0.40
3:F:518:THR:HG22	3:F:520:GLN:CB	2.51	0.40
3:F:550:ILE:O	3:F:551:PRO:C	2.63	0.40
3:F:664:GLU:O	3:F:666:THR:N	2.54	0.40
1:G:247:THR:CG2	1:G:248:LEU:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:455:ALA:HB3	3:I:461:VAL:HB	2.04	0.40
1:A:50:THR:HG22	1:A:52:TRP:CD1	2.56	0.40
3:C:132:SER:O	3:C:136:ASP:OD1	2.39	0.40
3:C:448:ILE:HD13	3:C:598:VAL:CG1	2.51	0.40
2:E:68:THR:HG22	2:E:69:GLU:N	2.36	0.40
3:F:618:LEU:HA	3:F:618:LEU:HD12	1.84	0.40
1:G:110:THR:HG21	1:G:166:PRO:HG3	2.02	0.40
3:I:573:TYR:O	3:I:574:LYS:C	2.64	0.40
1:A:21:GLY:C	1:A:22:LEU:O	2.65	0.40
3:C:153:VAL:HG23	3:C:161:LYS:CE	2.47	0.40
3:C:163:GLU:HG3	3:C:387:LEU:HD12	2.03	0.40
3:C:203:VAL:HG22	3:C:210:VAL:HG12	2.04	0.40
3:C:326:SER:C	3:C:328:GLY:H	2.29	0.40
3:C:350:GLU:O	3:C:365:MET:O	2.39	0.40
3:C:496:VAL:HG22	3:C:555:PHE:HB3	2.03	0.40
3:C:551:PRO:HD3	3:C:682:GLU:CB	2.52	0.40
3:C:708:THR:HG22	3:C:711:ALA:N	2.03	0.40
1:D:21:GLY:C	1:D:22:LEU:O	2.64	0.40
1:D:250:VAL:HG11	1:D:258:TYR:CE1	2.57	0.40
3:F:150:ASN:HA	3:F:153:VAL:HG13	2.03	0.40
3:F:386:ILE:HG22	3:F:387:LEU:N	2.37	0.40
3:F:506:ILE:O	3:F:510:MET:HG3	2.22	0.40
3:F:600:LYS:HB3	3:F:608:ASN:ND2	2.33	0.40
3:I:122:LEU:O	3:I:123:TYR:CB	2.59	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	270/275 (98%)	233 (86%)	24 (9%)	13 (5%)	2 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	270/275 (98%)	230 (85%)	26 (10%)	14 (5%)	1	5
1	G	270/275 (98%)	230 (85%)	27 (10%)	13 (5%)	2	6
2	B	97/99 (98%)	83 (86%)	9 (9%)	5 (5%)	1	5
2	E	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	1	5
2	H	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	1	5
3	C	633/640 (99%)	575 (91%)	45 (7%)	13 (2%)	5	20
3	F	633/640 (99%)	572 (90%)	47 (7%)	14 (2%)	5	19
3	I	633/640 (99%)	573 (90%)	47 (7%)	13 (2%)	5	20
All	All	3000/3042 (99%)	2664 (89%)	241 (8%)	95 (3%)	3	11

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	22	LEU
1	A	44	ARG
2	B	31	HIS
3	C	153	VAL
3	C	722	ASN
3	C	724	GLY
3	C	725	ALA
3	C	752	ASP
1	D	19	ASP
1	D	22	LEU
1	D	44	ARG
2	E	31	HIS
3	F	153	VAL
3	F	205	LYS
3	F	722	ASN
3	F	724	GLY
3	F	725	ALA
3	F	752	ASP
1	G	19	ASP
1	G	22	LEU
1	G	44	ARG
2	H	31	HIS
3	I	153	VAL
3	I	205	LYS
3	I	722	ASN

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Mol	Chain	Res	Type
3	I	724	GLY
3	I	725	ALA
3	I	752	ASP
1	A	177	ARG
2	B	17	ASN
3	C	212	LEU
3	C	366	VAL
3	C	440	ASP
1	D	177	ARG
1	D	255	GLU
1	D	256	GLN
2	E	17	ASN
3	F	366	VAL
3	F	440	ASP
1	G	177	ARG
2	H	17	ASN
3	I	210	VAL
3	I	366	VAL
3	I	440	ASP
1	A	23	SER
1	A	90	SER
1	A	255	GLU
1	A	256	GLN
2	B	32	PRO
3	C	150	ASN
3	C	208	ARG
1	D	23	SER
1	D	90	SER
2	E	32	PRO
3	F	150	ASN
1	G	23	SER
1	G	90	SER
1	G	255	GLU
1	G	256	GLN
2	H	32	PRO
3	I	150	ASN
1	A	50	THR
1	A	239	ASP
2	B	97	ARG
3	C	123	TYR
3	C	360	ASP
3	C	665	LYS

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Mol	Chain	Res	Type
1	D	50	THR
1	D	207	ASN
2	E	97	ARG
3	F	360	ASP
1	G	50	THR
1	G	207	ASN
2	H	97	ARG
1	A	207	ASN
1	D	239	ASP
3	F	123	TYR
3	F	665	LYS
1	G	239	ASP
3	I	123	TYR
3	I	360	ASP
1	A	236	PRO
1	D	16	SER
1	D	236	PRO
2	E	90	PRO
3	F	237	PHE
1	G	236	PRO
2	H	90	PRO
3	I	237	PHE
2	B	90	PRO
1	D	252	PRO
1	G	252	PRO
1	A	252	PRO
3	F	210	VAL

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	244/249 (98%)	231 (95%)	13 (5%)	20	52
1	D	244/249 (98%)	230 (94%)	14 (6%)	18	49
1	G	244/249 (98%)	231 (95%)	13 (5%)	20	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	92/94 (98%)	91 (99%)	1 (1%)	65	87
2	E	92/94 (98%)	91 (99%)	1 (1%)	65	87
2	H	92/94 (98%)	91 (99%)	1 (1%)	65	87
3	C	544/549 (99%)	501 (92%)	43 (8%)	11	35
3	F	544/549 (99%)	504 (93%)	40 (7%)	13	37
3	I	544/549 (99%)	502 (92%)	42 (8%)	12	36
All	All	2640/2676 (99%)	2472 (94%)	168 (6%)	16	44

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	18	GLN
1	A	19	ASP
1	A	34	GLN
1	A	35	LEU
1	A	41	HIS
1	A	49	ARG
1	A	153	ARG
1	A	197	SER
1	A	232	LYS
1	A	255	GLU
1	A	256	GLN
1	A	269	GLN
2	B	70	PHE
3	C	146	LEU
3	C	153	VAL
3	C	160	GLN
3	C	181	VAL
3	C	183	ARG
3	C	184	ASP
3	C	203	VAL
3	C	205	LYS
3	C	206	ASN
3	C	223	SER
3	C	227	THR
3	C	229	THR
3	C	247	TYR
3	C	297	PHE
3	C	319	THR

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Mol	Chain	Res	Type
3	C	324	SER
3	C	336	THR
3	C	345	LEU
3	C	348	ASN
3	C	353	CYS
3	C	365	MET
3	C	376	THR
3	C	453	TRP
3	C	496	VAL
3	C	524	GLN
3	C	531	LYS
3	C	533	GLU
3	C	535	LEU
3	C	558	CYS
3	C	559	GLU
3	C	583	LEU
3	C	612	GLU
3	C	618	LEU
3	C	633	LYS
3	C	639	LEU
3	C	640	GLN
3	C	646	ARG
3	C	655	ARG
3	C	664	GLU
3	C	708	THR
3	C	709	LEU
3	C	716	LEU
3	C	753	VAL
1	D	13	MET
1	D	18	GLN
1	D	19	ASP
1	D	34	GLN
1	D	35	LEU
1	D	41	HIS
1	D	49	ARG
1	D	153	ARG
1	D	197	SER
1	D	232	LYS
1	D	236	PRO
1	D	255	GLU
1	D	256	GLN
1	D	269	GLN

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Mol	Chain	Res	Type
2	E	70	PHE
3	F	146	LEU
3	F	153	VAL
3	F	160	GLN
3	F	181	VAL
3	F	183	ARG
3	F	184	ASP
3	F	203	VAL
3	F	223	SER
3	F	227	THR
3	F	229	THR
3	F	247	TYR
3	F	297	PHE
3	F	319	THR
3	F	324	SER
3	F	336	THR
3	F	348	ASN
3	F	353	CYS
3	F	365	MET
3	F	376	THR
3	F	453	TRP
3	F	496	VAL
3	F	524	GLN
3	F	531	LYS
3	F	533	GLU
3	F	535	LEU
3	F	558	CYS
3	F	559	GLU
3	F	583	LEU
3	F	612	GLU
3	F	618	LEU
3	F	633	LYS
3	F	639	LEU
3	F	640	GLN
3	F	646	ARG
3	F	655	ARG
3	F	664	GLU
3	F	708	THR
3	F	709	LEU
3	F	716	LEU
3	F	753	VAL
1	G	13	MET

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Mol	Chain	Res	Type
1	G	18	GLN
1	G	19	ASP
1	G	34	GLN
1	G	35	LEU
1	G	41	HIS
1	G	49	ARG
1	G	153	ARG
1	G	197	SER
1	G	232	LYS
1	G	255	GLU
1	G	256	GLN
1	G	269	GLN
2	H	70	PHE
3	I	146	LEU
3	I	153	VAL
3	I	160	GLN
3	I	181	VAL
3	I	183	ARG
3	I	184	ASP
3	I	203	VAL
3	I	204	ASP
3	I	223	SER
3	I	227	THR
3	I	229	THR
3	I	247	TYR
3	I	297	PHE
3	I	319	THR
3	I	324	SER
3	I	336	THR
3	I	345	LEU
3	I	348	ASN
3	I	353	CYS
3	I	365	MET
3	I	376	THR
3	I	453	TRP
3	I	496	VAL
3	I	524	GLN
3	I	531	LYS
3	I	533	GLU
3	I	535	LEU
3	I	558	CYS
3	I	559	GLU

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Mol	Chain	Res	Type
3	I	583	LEU
3	I	612	GLU
3	I	618	LEU
3	I	633	LYS
3	I	639	LEU
3	I	640	GLN
3	I	646	ARG
3	I	655	ARG
3	I	664	GLU
3	I	708	THR
3	I	709	LEU
3	I	716	LEU
3	I	753	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	18	GLN
1	A	67	GLN
1	A	87	HIS
1	A	121	GLN
1	A	150	HIS
1	A	156	GLN
1	A	157	ASN
1	A	168	GLN
1	A	171	GLN
1	A	193	HIS
1	A	222	GLN
1	A	256	GLN
1	A	269	GLN
2	B	13	HIS
2	B	21	ASN
2	B	24	ASN
2	B	31	HIS
2	B	51	HIS
2	B	83	ASN
3	C	150	ASN
3	C	186	HIS
3	C	191	GLN
3	C	198	ASN
3	C	206	ASN

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Mol	Chain	Res	Type
3	C	215	ASN
3	C	236	ASN
3	C	285	GLN
3	C	302	HIS
3	C	379	ASN
3	C	483	ASN
3	C	493	ASN
3	C	515	HIS
3	C	539	ASN
3	C	603	HIS
3	C	608	ASN
3	C	640	GLN
3	C	684	HIS
3	C	699	HIS
3	C	747	ASN
1	D	9	HIS
1	D	18	GLN
1	D	64	GLN
1	D	67	GLN
1	D	74	HIS
1	D	87	HIS
1	D	97	GLN
1	D	121	GLN
1	D	150	HIS
1	D	157	ASN
1	D	168	GLN
1	D	171	GLN
1	D	207	ASN
1	D	222	GLN
1	D	256	GLN
1	D	269	GLN
2	E	21	ASN
2	E	24	ASN
2	E	51	HIS
2	E	83	ASN
3	F	150	ASN
3	F	186	HIS
3	F	191	GLN
3	F	198	ASN
3	F	215	ASN
3	F	236	ASN
3	F	285	GLN

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Mol	Chain	Res	Type
3	F	302	HIS
3	F	318	HIS
3	F	379	ASN
3	F	483	ASN
3	F	493	ASN
3	F	515	HIS
3	F	539	ASN
3	F	603	HIS
3	F	608	ASN
3	F	684	HIS
3	F	699	HIS
3	F	743	GLN
3	F	747	ASN
1	G	9	HIS
1	G	18	GLN
1	G	87	HIS
1	G	121	GLN
1	G	123	HIS
1	G	150	HIS
1	G	157	ASN
1	G	168	GLN
1	G	171	GLN
1	G	193	HIS
1	G	222	GLN
1	G	256	GLN
1	G	269	GLN
2	H	21	ASN
2	H	24	ASN
2	H	31	HIS
2	H	51	HIS
2	H	83	ASN
3	I	150	ASN
3	I	186	HIS
3	I	191	GLN
3	I	197	GLN
3	I	198	ASN
3	I	215	ASN
3	I	236	ASN
3	I	285	GLN
3	I	302	HIS
3	I	318	HIS
3	I	379	ASN

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Mol	Chain	Res	Type
3	I	483	ASN
3	I	493	ASN
3	I	515	HIS
3	I	539	ASN
3	I	603	HIS
3	I	608	ASN
3	I	699	HIS
3	I	743	GLN
3	I	747	ASN

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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	G	309	-	5,5,5	1.82	2 (40%)	5,5,5	0.99	0
4	NAG	I	902	3	14,14,15	0.46	0	17,19,21	1.04	2 (11%)
4	NAG	F	901	3	14,14,15	0.59	0	17,19,21	0.87	1 (5%)
4	NAG	C	900	3	14,14,15	0.66	0	17,19,21	0.82	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	G	309	-	-	2/4/4/4	-
4	NAG	I	902	3	-	2/6/23/26	0/1/1/1
4	NAG	F	901	3	-	2/6/23/26	0/1/1/1
4	NAG	C	900	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	309	GOL	O2-C2	2.98	1.52	1.43
6	G	309	GOL	C3-C2	2.20	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	901	NAG	C2-N2-C7	-2.79	119.16	122.90
4	I	902	NAG	C2-N2-C7	-2.64	119.36	122.90
4	C	900	NAG	C2-N2-C7	-2.49	119.56	122.90
4	I	902	NAG	C4-C3-C2	-2.04	108.03	111.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	309	GOL	C1-C2-C3-O3
6	G	309	GOL	O2-C2-C3-O3
4	F	901	NAG	O5-C5-C6-O6
4	F	901	NAG	C4-C5-C6-O6
4	I	902	NAG	C4-C5-C6-O6
4	C	900	NAG	O5-C5-C6-O6
4	C	900	NAG	C4-C5-C6-O6
4	I	902	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	309	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.